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Abstract

Non-collinear magnetic structures provide a promising platform for energy-efficient carriers of information. Periodic non-collinear spin arrangements generated as the interference pattern of spin waves are an extensive subclass known as multi- q magnets. The study of their electronic properties is of central importance for the implementation in future technology. As the length scale of a multi- q spin texture approaches the lattice constant of its host material, gapped topological states may form in the associated electronic system, similar to the formation of Landau levels in the presence of magnetic fields. Given that the textures at these length scales are discrete and lattice incommensurate, we challenge the prevailing notion that their description relies on emergent magnetic fields. Instead, we adopt a C^* -algebraic viewpoint that harmonises with these properties and facilitates the computation of invariants associated with the topology of the electronic states. We implement a computational programme of non-commutative K -theory to compute all Chern numbers associated with real, momentum and mixed space. As a central application, we tune texture parameters to create discontinuous jumps in the real space winding number of skyrmionic textures and observe the relation to the Chern numbers. We find a peculiar discrepancy between the behaviour of the momentum space Chern number and the winding number, and identify a single energy level that contributes to the real space Chern number. The non-commutative framework also provides access to the computation of the orbital magnetisation in accordance with modern theory even in the presence of finite magnetic flux. This allows us to compare the orbital magnetisation with the texture and electronic state topology and investigate the scaling behaviour with respect to the texture length scale and magnetic flux.

Nichtkollineare magnetische Strukturen bieten eine vielversprechende Plattform für energieeffiziente Informationsträger. Periodische nichtkollineare Spinanordnungen, die als Interferenzmuster von Spinwellen erzeugt werden, sind eine weitreichende Unterklasse bekannt als Multi- q -Magneten. Die Untersuchung ihrer elektronischen Eigenschaften ist von zentraler Bedeutung für ihren Einsatz in zukünftiger Technologie. Wenn sich die Größenordnung der Multi- q Spintextur der Gitterkonstante des sie beherbergenden Materials nähert, können sich topologische Zustände mit Energielücke im zugehörigen elektronischen System bilden. Dies ist ähnlich zur Ausbildung von Landau-Niveaus in Anwesenheit magnetischer Felder. Da die Texturen in diesen Größenordnungen diskret und gitterinkommensurat sind, stellen wir die vorherrschende Anschauung in Frage, dass ihre Beschreibung auf emergenten Magnetfeldern beruht. Stattdessen nehmen wir einen C^* -algebraischen Blickwinkel ein, der sich gut mit diesen Eigenschaften verträgt und die Berechnung von Invarianten erleichtert, die mit der Topologie der elektronischen Zustände zusammenhängen. Wir implementieren ein Programm für Berechnungen nichtkommutativer K -Theorie, um alle Chernnummern zu berechnen, die mit dem Realraum, Impulsraum und Mischraum assoziiert sind. Als eine zentrale Anwendung modifizieren wir Texturparameter, um unstetige Sprünge in der Realraumwindungszahl von Skyrmiomtexturen zu erzeugen und beobachten die Beziehung zu den Chernnummern. Wir entdecken eine auffällige Diskrepanz zwischen dem Verhalten der Impulsraum-Chernnummer und der Windungszahl und identifizieren ein einzelnes Energieniveau, das zur Realraum-Chernnummer beiträgt. Der nichtkommutative Rahmen ermöglicht uns außerdem die Berechnung der Orbitalmagnetisierung in Übereinstimmung mit der modernen Theorie, sogar in der Anwesenheit eines endlichen magnetischen Flusses. Das erlaubt uns die Orbitalmagnetisierung mit der Textur und der Topologie der elektrischen Zustände zu vergleichen und ihr Skalierungsverhalten bezüglich der Größenordnung der Textur und des magnetischen Flusses zu untersuchen.

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Introduction

The study of magnetic materials that exhibit non-collinear spin arrangements is a prolific research area for prospective information technologies. It contains, most famously, the seminal field of spin transport electronics, aka spintronics, the concept of availing the intrinsic spin of the electron in addition to its electronic charge as an information carrier in solid-state devices. Periodic non-collinear spin structures that are dominated by their lowest Fourier modes can be characterised by phase-coherent superpositions of multiple spin spirals with wave vector $\mathbf{q}$. Materials featuring these emerging interference patterns are known as multi- q magnets. The diverse class of multi- q spin textures comprises the one-dimensional helicoids found in chiral materials [Ada+12; Jan+13], two-dimensional skyrmion crystals in MnSi [Neu+09; Müh+09], two-dimensional vortex crystals in frustrated magnets [Wan+15], and three-dimensional hedgehog lattices in MnGe [Tan+15]. The characteristic wave vectors of multi- q order can be detected experimentally, for instance by small angle neutron scattering [Müh+09; Ada+12]. They are a hallmark in the identification of these materials.

Multi- q textures

A particular scientific focus is directed towards the study of skyrmion materials. Skyrmions are stable spin swirls arising from competing interactions in their host materials. They are characterised by the non-zero winding number of the underlying spin vector field, which renders them topologically stable. This stability refers to the coupling energy between neighbouring spins, which emulates the continuity of the mapping and must be overcome for the skyrmion to dissolve into the background magnetisation. Skyrmions exhibit sensitivity to applied forces, including magnetic and electric fields, mechanical stress, and local and global temperature changes. By applying electric fields, they can be purposefully manipulated, which can be capitalised for a variety of auspicious applications such as memory storage [Tom+14], quantum computing [Not+22], and neuromorphic reservoir computing [Gro+20].

Skyrmions

The study of skyrmion lattices and their electronic states is of paramount importance for comprehending these structures and devising adroit methods of their detection. For instance, the presence of skyrmions has been demonstrated to contribute to the conductance perpendicular to an applied current [Neu+09]. This contribution can be measured with minimal equipment, which makes this mode of detection suitable for spintronic devices. The phenomenon is referred to as the topological Hall effect (THE), drawing parallels with the classical Hall effect caused that arises from the presence of a permeating magnetic field. It can also be explained by this analogy, in the language of emergent magnetic fields [Sch+12]. When the spin of the electron aligns with the spin texture, one can rotate the electron Hamilton operator into the collinear co-moving frame of reference at the price of a modified kinetic energy term that resembles the presence

Topological Hall effect

Introduction

of an electromagnetic vector potential. The emergent local field strength coincides with the solid angle of the spin vector field, which integrates over one texture period to the winding number. Accordingly, the THE is attributed to the real space topology of the spin texture.

For the system to be considered suitable for this description, each skyrmion should encompass a sufficient number of atomic lattice sites to emulate continuity and even smoothness of the texture. Skyrmion materials that satisfy this requirement are MnSi [Neu+09; Müh+09], FeGe [Yu+11; Ler+18], and Cu₂OSeO₃ [Ada+12; Sek+12; Lan+14; Hua+20]. They host skyrmion lattices with periodicities in the order of tens of nanometres, which corresponds to wave vectors of length $q \sim 0.01 \frac{2\pi}{a}$ in relation to their respective lattice constants a . Beyond that exist materials that feature nano-scale skyrmions with sizes in the single nanometre range, such as the centrosymmetric materials Gd₂PdSi₃ [Kur+19], Gd₃Ru₄Al₁₂ [Hir+19], and GdRu₂Si₂ [Kha+20], with wave number $q \sim 0.1 \frac{2\pi}{a}$.

Electronic state topology

As the length scale of a multi- q texture approaches the lattice constant of its host material, the resulting interference effects can lead to the formation of gapped topological states in the electronic state spectrum similar to the formation of Landau levels. These states are topological in the sense that they can be interpreted as sections of a non-trivial vector bundle over a parameter manifold. A suitable manifold is, for instance, given by the continuous spectrum of an operator that commutes with the Hamilton operator, resulting in simultaneous eigenstates. If such an operator exists, then the space of energy eigenstates can be decomposed into eigenspaces that can be interpreted as fibres at each parameter point. In most use cases, it is the momentum eigenstates that belong to vector space fibres over the crystal momentum space, namely the Brillouin zone manifold. If the energy gaps stay open over the whole parameter range, the positioning of the gaped states over the manifold relative to all other states is a topological property in the realm of topological K -Theory [Hat03].

Quantum Hall effect

This has physical consequences for the electronic transport properties, as the local curvature of the energy eigenstates measures how much they transition into all other energy states as governed by the time evolution of the Schrödinger equation along a path in parameter space. This is known as the Berry curvature [Ber84], and it has been employed to understand the quantum Hall effect (QHE) of the Landau levels in constant magnetic fields and periodic potentials [Tho+82]. The integral of the Berry curvature of occupied states over the Brillouin zone is an integer known as the Chern number of the vector bundle, and it is proportional to the Hall conductance. In the presence of disorder this is reflected experimentally in a resistivity curve with sharp steps [KDP80; Lau81].

Quantum anomalous Hall effect

Similar effects attributed to the momentum space topology of the electronic states have been reported for topological insulators (TI), that exhibit gaps with non-zero Chern number [Nag+10]. It is invoked by the presence of spin-orbit coupling breaking time-reversal symmetry that otherwise would cause the Berry curvature over the Brillouin zone to compensate itself. This transverse conductance has been coined the quantum anomalous Hall effect (QAHE) due to its occurrence in the absence of an external magnetic field.

Since the presence of non-collinear magnetism also breaks time-reversal symmetry, it has been conjectured that non-collinear textures such as skyrmion crystals also elicit a quantised Hall effect [HEN15]. This has been quantified for skyrmion crystals by mapping this quantised topological Hall effect (QTHE) to the QHE through making the emergent magnetic field homogeneous [Göb+17b; Göb+17a]. By doing this one assigns the electronic bands to Landau levels carrying integer Chern numbers and observes an unconventional behaviour arising from the topology of the structural lattice. However, we conjecture that the relationship is more intricate than this.

*Quantised
topological Hall
effect*

The nanometric skyrmion lattices that induce the formation of gapped states realise each skyrmion on a small number of lattice sites, and are moreover reportedly lattice incommensurate [Kha+20]. The first caveat poses an issue for the validity of the approximation of the spin texture as a smooth vector field, and the second obstructs the construction of a well-defined parameter manifold. A lattice incommensurate texture has a periodicity with an irrational ratio to the periodicity of the structural lattice and is therefore lattice-aperiodic. Consequently, there exists no super-cell on which the translation operators commutes with the Hamilton operator, such that the crystal momentum is no longer a quantum number and the Brillouin zone is no longer a well-defined topological space. Systems like this can be addressed by the algebraic generalisation of the geometric methods discussed above in the mathematical domain of non-commutative geometry [Con94].

*The continuous
issue of topology*

A fascinating duality between topology and algebra states that the properties of topological spaces can be encoded into the commutative algebra of continuous functions over them. With this identification, classes of vector bundles over the topological spaces from topological K -theory become classes of projective modules over the function algebras [Ser55; Swa62]. This description, however, no longer requires the commutativity of the algebra. The algebraic methods can equally be applied to non-commutative algebras, such as the observable algebra of a tight-binding Hamilton operator coupled to an incommensurate spin texture. The term observable algebra in this context refers to the smallest C^* -algebra containing all physical observables that are obtained as functions of the Hamilton operator in the sense of spectral calculus.

*Non-
commutative
 K -Theory*

Algebras of bounded operators that are complete in the metric induced by the operator norm are C^* -algebras and can be abstracted on account of their characterising commutation relations. Operator K -theory is the non-commutative generalisation of topological K -theory to Banach algebras, and can, thus, be employed to classify projection operators from the observable algebra. This includes in particular the Fermi projections onto the occupied states below the Fermi energy positioned in an energy gap at zero temperature. Accordingly, operator K -theory can be used to classify the spectral gaps that arise in the electronic spectrum from the coupling of the electron's spin to the multi- q spin texture.

Non-commutative geometry was first applied to the solid state physics of the quantum Hall effect by Jean Bellissard [Bel86]. For quantum Hall systems with an irrational number of magnetic flux quanta per unit cell, the observable algebra exhibits the defining relations of the so-called non-commutative torus, which is the epitome of a non-commutative space. With each translation the electronic states receive a complex phase proportional to the

*Non-
commutative
torus*

Introduction

flux, such that an infinite number of translations never return to the same phase but densely sample the space of phases, the unit circle S^1 . For incommensurate multi- q textures we witness the same exact behaviour with respect to the phases specifying the orientation of the spin along each individual spin wave.

Ergodicity This incidentally also solves our first caveat with nanoscale spin structures, which is the loss of smoothness. On an infinite lattice all possible spin orientations are densely sampled, such that the sum per unit volume converges to the integral of the corresponding continuous vector field. This property of the time average (where each translation corresponds to one time step) coinciding with the space average is known as ergodicity.

Strong disorder In his seminal work, Jean Bellissard demonstrated how the Chern number assigned to a spectral gap is preserved in the presence of strong disorder that populates the gaps with localised states. He managed to achieve this by associating the Chern number to the index of a suitable Fredholm module. This technique could presumably also be applied to disordered multi- q systems, nevertheless, this work rather focusses on the evaluation and juxtaposition of different Chern numbers associated with real and momentum space.

Hofstadter's butterfly In case of the QHE, the electronic spectrum in dependence of the magnetic flux forms a fractal, self-similar pattern known as Hofstadter's butterfly [Hof76] due to its axis symmetric wing shaped gaps. In a prior work of the author, spearheaded by Fabian Lux [Lux+24], we constructed the observable algebra for a tight-binding Hamiltonian coupled to multi- q spin textures and analysed the dependence of the density of states (DOS) on the wave number, or pitch, of the texture. Following the work of [LP20], we extracted some mixed-space Chern numbers from the fingerprints of the gaps in the integrated density of states (IDS). The spectral gaps appear as line features in the IDS that are polynomials in the pitch with integer coefficients related to various Chern numbers. This relation is a generalisation of the classical Středa formula [Str82], that relates the IDS to the Hall conductance in terms of the momentum space Chern number. The proof for the generalised Středa formulas for higher dimensional magnetic fields using Itô-derivatives is due to Emil Prodan [PS16]. A modified version of the proof encompassing also the pitch of multi- q textures is conceived by the author for Thm. 3.8 within this dissertation.

Topological phase transition The central research question of the author's doctoral project was sparked by the communication that the continuous tuning of texture properties, such as the relative phase between the individual spin waves of a multi- q texture, can induce singularities by destructive interference that drive transitions of the real space topology in terms of the winding number [HOM21; Shi+22]. The hypothesis was formed that these changes would be reflected in the behaviour of the electronic state topology as well.

Computational program In order to pursue this endeavour, the author adapted the computational non-commutative geometry programme devised by Emil Prodan for the application to disordered topological insulators [Pro17] to the use case of multi- q systems. This comprises in particular the adaption of the differential calculus and the finite volume approximation for computation. The latter makes it viable to evaluate Chern numbers and general correlation functions for large supercells with approximately incommensurate textures by which we refer to systems with rational ratio between texture and lattice periodicity, such that the periods only align after several iterations. From a physics

standpoint this yields no restriction to the model as the electrons possess a finite mean free path [MNA21]. We find the finite volume approximation converging faster than any inverse power of the finite supercells' volume as derived for Thm. 4.1 following the proof of the corresponding statement in [Pro17].

One pivotal instance for another correlation function that can be evaluated in the C^* -algebra framework is the orbital magnetisation of the system. The corresponding formula was derived in [ST13] using Itô-derivates, and it coincides with the Bloch function expression from the modern theory of orbital magnetisation in the limit of smooth periodic textures. The modern theory of orbital magnetisation was first devised for the application to periodic insulators [Tho+05; XSN05] in terms of semi-classical considerations. Shortly thereafter, it was generalised to multi-band insulators, Chern insulators, and metals [Cer+06], and alternative derivations such as by quantum perturbation theory [Shi+07], which made it valid at weak and strong magnetic fields, were discovered.

*Orbital
magnetisation*

The non-commutative formula is derived from the same thermodynamic definition as in the perturbation theory approach, i.e. as the response of the free energy to changes in the external magnetic field. Here, the C^* -algebra approach has the definite advantages, that derivations with respect to the magnetic field can be calculated in a straightforward way using Itô derivatives and that aperiodic systems can be considered. The semi-classical picture identifies two contributions to the orbital magnetisation from the itinerant and local circulation of the electrons. We identify these contributions in our framework and consider their behaviour separately.

The modern formalism has been applied to skyrmion lattices in several publications [Lux+18; Göb+19; GSM25]. In this dissertation, we consider additionally the dependence on the texture parameters and real space topology, and we consider the simultaneous presence of a skyrmion texture and an external magnetic field as it is common in experimental setups.

Main results The most significant findings from the numerical results for the physical systems can be summarised in a few central statements:

Physical results

1. We corroborate the results from our IDS analysis in [Lux+24] by numerical evaluating the gap labels for all considered textures.
2. We reproduce the unconventional behaviour in skyrmion crystals of the momentum space Chern number at the van-Hove singularity (VHS) of the structural lattice reported in [Göb+17b] and find a similar behaviour of the real space and mixed space Chern numbers. In particular, in the absence of an external magnetic field we identify the states at the VHS as sole contributors to the real space Chern number.
3. We observe a disparity between the behaviour of the momentum space Chern numbers and the winding number of the spin texture that contradicts the approach of mapping the energy levels to the Landau levels of the averaged emergent magnetic field from [Göb+17b] for some areas of our the parameter range.

Introduction

4. We identify a topological phase transition of the momentum space Chern number along the line in parameter space for which the average magnetisation in the z -direction vanishes.
5. We reproduce the qualitative shape of the orbital magnetisation for the skyrmion crystals on the triangular lattice reported in [Göb+19].
6. We observe a shift in the DOS over the magnetic flux (Hofstadter’s butterfly) for the electronic states with spin aligned and anti-aligned to the spin texture that corresponds to the textures pitch.
7. We find the magnetic flux and texture pitch competing in the orbital magnetisation which leads to non-linear responses.

The findings 2, 3, and 4 were reported in [Pra+24] for the case of the helical skyrmion lattice and expanded to a sinusoidal skyrmion lattice for this dissertation.

Mathematical results

In [Lux+24; Pra+24], the C^* -algebraic framework, gap labelling theorem, and non-commutative geometry computational programme of [PS16; Pro17] were adopted for the application to systems coupled to multi- q spin textures while omitting the inclusion of an external magnetic field and disorder. This dissertation re-includes the magnetic field and elucidates several technical details of the adaptation.

1. We clarify the construction of the family of covariant representations used to construct the C^* -completion of the twisted crossed product algebra.
2. We expand on the derivation of the differential calculus in terms of the Fourier calculus and the characterisation of the smooth subalgebra.
3. We construct the Itô derivatives with respect to the pitch of the spin texture and determine the corresponding Itô-like product rule in Eq. (3.41), which is different from that in Eq. (3.40) of the established Itô derivatives with respect to the magnetic flux.
4. We prove the generalised Středa formula for the cases involving the texture’s pitch for Thm. 3.8 and remedy a sign inconsistency in the higher gap labelling formula of Thm. 3.9.
5. We decompose the formula for the orbital magnetisation into terms that can be associated with the contributions identified in the semi-classical derivation of the modern theory formula.
6. We clarify the mapping onto the finite volume approximation algebras and their convergence to the projective limit on infinite volume.
7. We produce a proof for the hyper-polynomially fast decaying upper bound of the error estimation for the finite volume approximation in Thm. 4.1 and corroborate it with numerical results.

Publications The publications by the author that accrued during the doctoral project are

*Non-commutative
K-theory of
multi-q systems*

- [Lux+24]: F. R. Lux, S. Ghosh, P. Prass, E. Prodan, and Y. Mokrousov, „Unified topological characterization of electronic states in spin textures from noncommutative K -theory“, *Phys. Rev. Res.* **6**, 013102 (2024)

F.R.L. discovered the affiliation of multi- q systems to the non-commutative torus algebra, implemented the DOS and IDS computation, calculated the Chern number decompositions, and created the figures. S.G. provided the spin helix superposition. F.R.L. and P.P. devised the differential calculus. F.R.L. derived the relation to the Berry curvature and the emergent magnetic fields. F.R.L., S.G., P.P., E.P., and Y.M. discussed the results and reviewed the manuscript.

- [Pra+24]: P. Prass, F. R. Lux, E. Prodan, D. van Straten, and Y. Mokrousov, „A C^* -algebraic view on the interaction of real- and reciprocal space topology in skyrmion crystals“, *SciPost Phys. Core* **7**, 080 (2024)

P.P. investigated the relationship between texture winding number and electronic Chern numbers. P.P. and F.R.L. adapted the differential calculus and its finite volume presentation to the case of multi- q textures. P.P. implemented the computational programme with guidance from F.R.L., E.P., and Y.M., and created the figures. P.P. and F.R.L. wrote the manuscript. P.P., F.R.L., E.P., D.v.S, and Y.M. discussed the results and reviewed the manuscript.

Another approach to study the electronic properties of non-collinear magnets, that the author engaged in, was pursued in the joined work with Fabian Lux:

*Semi-classical
gradient
expansion*

- [Lux+20b]: F. R. Lux, P. Prass, S. Blügel, and Y. Mokrousov, *Effective Seiberg-Witten gauge theory of noncollinear magnetism*, 2020

F.R.L. found the relation to the Seiberg-Witten map, performed the numerical calculation and wrote the manuscript. P.P. contributed on the relation to the work of Jean Bellissard about the quantum Hall effect. F.R.L., P.P., S.B., and Y.M. discussed the results and reviewed the manuscript.

This approach is based on the semi-classical gradient expansion of quantum observables in terms of real space derivations of the magnetisation and expresses the operators in the phase space formalism of Wigner and Weyl. Fabian Lux found a relation between the expansion of the Berry curvature and the Seiberg-Witten map, which is a construction commonly used in string theory to map the gauge theories emerging from different regularisation schemes onto each other. In this work, it is used to map the ordinary gauge theory arising from Bloch theory to the non-commutative gauge theory in the phase space formalism. Applying these results to the Rashba model, the Seiberg-Witten map provides an explanation to a mixed space Berry curvature contribution and a first order correction to the anomalous Hall coefficient, coined the chiral Hall effect in [Lux+20a]. This formalism applies to smooth noncollinear spin textures, which is complementary to the nanometric textures considered in the dissertation.

Chapter 1 **Structure and structural remarks** In chapter 1, we introduce the magnetic textures that are the prime subject of study in this dissertation. To motivate their existence, section 1.1 describes the emergence of magnetism in materials through the interplay of orbital magnetic momenta and intrinsic spin of the electrons. Then, in section 1.2, we discuss the stabilisation mechanisms which create non-collinear spin structures, introduce skyrmions, and present the multi- q textures that we apply our formalism to. To understand the real space topology of non-collinear spin textures, in section 1.3 we fastidiously introduce the mathematical concept of the winding number and use it as an introductory example for the application of methods from geometry and non-commutative geometry as well as topological phase transitions.

Chapter 2 Chapter 2 is devoted to the introduction of the electronic properties under investigation. For this, section 2.1 discusses the behaviour of electrons in solid state systems and justifies the study of non-interacting tight-binding models. Section 2.2 introduces the concepts of geometric phases in terms of the Berry connection in Bloch theory, which provides the framework in which electronic transport properties and orbital magnetisation are commonly described. Accordingly, section 2.3 gives a brief overview of different kinds of Hall effects and their relation to the momentum space topology of electronic states. Equally, section 2.4 introduces the modern theory formulation of orbital magnetisation in terms of Bloch functions.

Chapter 3 With chapter 3, the exposition of the mathematical framework which is the centrepiece of this dissertation starts. After a brief introduction into the basic concepts of C^* -algebras, we start to construct the observable algebra describing the physical system in section 3.1. For this, we decode the translation behaviour in presence of a multi- q spin texture and external magnetic field into a twisted crossed product algebra, construct its representation, and complete it to a C^* known as the non-commutative torus in order to include all physical observables. In section 3.2, we construct the differential calculus on this algebra which comprises a canonical trace and derivations stemming from a Fourier calculus, and Itô derivatives for the differentiation with respect to the magnetic fluxes and pitches of the texture. Next, in section 3.3 we give a concise introduction to operator K -theory and cyclic cocycles to motivate the definition of Chern numbers, and we derive generalised Středa formulas for their decomposition. Eventually, everything is set up and in section 3.4, we can demonstrate that the tight-binding Hamiltonian of multi- q systems belongs to the constructed algebra, perform the Chern number decomposition for the multi- q textures of section 1.2, and derive the non-commutative formula for the orbital magnetisation.

Chapter 4 In order to compute numerical results in the established framework, chapter 4 presents an approximate programme. For this, section 4.1 introduces the finite volume approximations for the algebra and the differential calculus, and discusses their infinite volume limit. Using this, section 4.2 presents the algorithm for the numerical evaluation and the expressions for implantation. The error bounds for the approximated program are derived in section 4.3.

Chapter 5 presents the Chern number and gap label results for several multi- q textures in the absence of a magnetic field. Section 5.1, starts with an analysis of the scaling behaviour of the DOS and IDS, which is then substantiated and extended on by the numerical results of section 5.2. In section 5.3, we focus exclusively on the two skyrmion textures and probe the topological phase transitions in dependence on the texture's parameters and winding number. The absence of the necessary spectral flow during these transitions is addressed and solved in section 5.4.

Chapter 5

In chapter 6 we consider solely the helical skyrmion lattice and its orbital magnetisation in zero and finite magnetic fields. Section 6.1 presents the zero field results including phase transitions. Then, section 6.2 considers the general influence of finite magnetic flux, and section 6.3 applies it to the orbital magnetisation. At last, in section 6.4, we also apply it to the meron-antimeron lattice, which is the special case of the helical skyrmion lattice at the winding number transition parameter. For this spin texture, the mathematical description fails, and we assess its implications.

Chapter 6

The appendix contains two parts, appendix A contains a collection of all calculations and proofs which were too extensive to be featured in the main body of the text, and appendix B presents the relevant excerpts of the implementation which contains all functions laid out in section 4.2.

Appendix

To conclude the introduction, we would like to offer some remarks on the choices made regarding the structure of the dissertation and how it is intended to be read. We endeavour to render every section as self-consistent as possible to facilitate access at any point. For this, we commence each section with a brief synopsis of the concept presented within, accompanied by an overview of the content. To enhance the clarity of the text arrangement, we employ margin notes with short captions to each group of paragraphs on a given topic.

*Structural
remarks*

In general, we strive for a language accessible to all individuals with the necessary knowledge in the field, irrespective of their level of familiarity with the concepts presented herein. Nevertheless, in order to maintain conciseness, the mathematical terminology for the concepts is also included to not confuse the initiated reader, even if it is not established prior or used further. These text passages may be bypassed by the lay reader without compromising the intended comprehension. All extended calculations and proofs are relocated to the appendix to not detract from the corresponding statements in the main text. They are meticulously referenced at their respective occurrences and reference back for easy accessibility back and forth.

1 | Magnetic Textures

Magnetic textures are arrangements of local magnetic moments in a solid state system. They comprise ferromagnetic and antiferromagnetic textures with parallel or antiparallel collinear spins as well as non-collinear spin textures such as skyrmion crystals.

Magnetism in materials emerges from an intricate interplay of electromagnetism and quantum properties of matter. The magnetic moment of a free atom receives contributions from the spins and orbital angular momenta of its electrons. These combine and compensate in accordance with complex rules imposed by the quantum mechanical exclusion principle for fermions, the rotation symmetry of the atom, and the energy hierarchy of competing interactions. For atoms in a solid held together by chemical bonds, the electrons are affected by the neighbouring atoms such that the emerging magnetic properties change significantly. They can be described with two contrasting models, one that considers the electrons localised to the atomic sites and one that considers the electrons itinerant in the material. For the localised model, the rules for the emergence of magnetic momenta are heavily modified. For many materials the orbital contribution is completely quenched by the electric field of the atoms and the primary contribution to the magnetic moment is due to the spin. In the itinerant model the magnetism is interwoven with the electronic properties of the materials. Magnetic textures arise then as a consequence of magnetic order, which is enforced by interactions between the magnetic momenta due to the Coulomb interaction and the exclusion principle. The magnetic order can be studied by the micromagnetic approach in which the magnetisation is approximated by a continuous function and the magnetic ground state is determined by minimising an energy functional containing the relevant interactions.

Magnetic origin

The focus of this dissertation lies with non-collinear textures for which the local magnetic momenta are arranged into complex patterns. They occur in different kinds of materials and can be stabilised by an antisymmetric exchange interaction such as the Dzyaloshinskii-Moriya interaction (DMI) that favours canting of neighbouring spins or Fermi surface mechanisms that favour long range helical spin waves. Such spin waves and their phase-coherent superposition patterns are referred to as multi- q textures if they can be characterised by the wave vectors $\mathbf{q}$. The coupling of electrons to a non-collinear texture can result in peculiar electronic structures that manifests for instance in unconventional transport properties.

Non-collinear textures

Of particular interest for the spintronic community are skyrmion lattices which can be classified by their topological properties in real space. The continuous vector field which describes the texture can be associated with a winding number, which is a topological invariant counting how often the magnetic moments wrap around a sphere. This property

Topological textures

1. Magnetic Textures

can only change, if the local momenta overcome the interactions emulating the continuity of the texture.

Chapter content

In this chapter, we introduce the origin of non-collinear magnetism, present the specific textures studied in this dissertation, and discuss their topological properties.

In Sec. 1.1, we present a comprehensive overview of the magnetism of free atoms and solids. We discuss the plethora of phenomena that determine the magnetic properties of the most common magnetic materials, with particular reference to intermetallic and rare earth elements. Then, we discuss the prevailing mechanisms for magnetic order and the transition to the micromagnetic approximation of continuous magnetisation.

Subsequently, in Sec. 1.2, we discuss the stabilisation of non-collinear textures. We follow this up with a brief description of single skyrmions and a comprehensive introduction to multi- q magnetic textures. We finish this part by introducing the four multi- q textures studied in this dissertation. These comprise a one-dimensional spin wave superposition, two two-dimensional skyrmion lattices generated by different spin waves and with different winding numbers, and one two-dimensional vortex lattice.

For the end of this chapter, in Sec. 1.3, we introduce the winding number in terms of the mathematical concept of the degree of a continuous mapping. Then, we present some examples for the diverse applications of this concept ranging from the total curvature of a surface to Chern numbers of vector bundles. Finally, we discuss discontinuous transitions of the winding number. For that, we visualise a transition of the single skyrmion to a ferromagnet, and subsequently administer a regularisation to render the transition continuous.

1.1. Magnetism

Magnetism is an emergent phenomenon. It arises from the most fundamental interactions and requires various different effective descriptions for different length scales. The theory of solid state magnetism combines properties from electromagnetism, special relativity, and quantum physics.

Electromagnetism

All electric and magnetic phenomena originate from the fundamental electromagnetic force between electrically charged particles. According to the theory of quantum electrodynamics (QED), this force is mediated by virtual photons acting as exchange particles. In order to adhere to the principles of special relativity, elementary particles possess an additional intrinsic property, spin, that couples to the electromagnetic force. In the limit of non-relativistic quantum mechanics, the electromagnetic force is governed by Coulomb's law while the spin remains a significant property, resulting in the generation of a magnetic dipole moment analogous to that generated by a charged particle's angular momentum.

On the other side of the length scale, macroscopically, magnetism can be described as a classical force field with a vector potential. According to the Maxwell equations it is connected to the electric field, electric charges, and electric currents. This description is manifestly invariant under the change of initial system according to special relativity.

The fundamental building blocks of solid state magnetism are the magnetic moments of the electrons of each atom, even though the transition from the free to the bound atom is not straight forward. While most elements in the atomic state exhibit a non-zero magnetic moment, only a few of them retain a magnetic moment when they bond to an arrangement of atoms such as a molecule, liquid, or solid. These elements possess unfilled $3d$, $4f$, or $5f$ shells, and thus belong to the iron, lanthanide (or rare earth), or actinide series of the elemental table [TGS02, Table 3.1-3.2]. A unique case is Sm which has no magnetic moment in the atomic state, but is antiferromagnetic when forming a solid.

*Solid state
magnetism*

In this section, we give an introductory overview of magnetism in solid state systems. We start with the free atom for which the magnetic moment is determined by the combination of the spin and orbital magnetic momenta of its electrons. Then, we discuss the magnetisation of solids consisting of bound atoms where electrons occupy hybridised orbits and are affected by the surrounding electric charges. For them, we introduce the leading interactions that cause magnetic order and introduce the convenient viewpoint of micromagnetics, where the magnetisation of a material is approximated as a continuous vector field. This is especially relevant for the subsequent section where we introduce non-collinear magnetism.

Section Content

1.1.1. Atomic State Magnetism

A free atom may exhibit a magnetic moment with contributions from two principal sources: The electron spin and the orbital angular momentum of the electrons around the nucleus. Whether an element is magnetic in the atomic state depends on its total angular momentum, determined by the filling of its orbits. This is a direct consequence of the quantum mechanical Pauli exclusion principle and spin-orbit coupling. In the following, we introduce the sources of the magnetic moment and discuss how the total magnetic moment of an element in the atomic state emerges. For this, we follow [TGS02, Chap. 7] and [Tim19, Chap. 1-2], and refer to the latter for more details on the calculations.

We start by considering a single electron within an atom. The orbital contribution to the magnetic moment can be motivated by classical electrodynamics according to which the movement of an electronic charge generates a magnetic field. If we assume the single electron orbits the nucleus on a circle of constant radius and with constant angular momentum, we can approximate it by the averaged magnetic field induced by the averaged current density $\mathbf{j}$ using the *Biot-Savart law*.

Orbital moment

For the far-field, we can perform a multipole expansion to identify a dipole as leading contribution since the magnetic field is divergence-free and thus there exist no magnetic monopoles [Jac14]. The corresponding magnetic dipole moment is of the form:

$$\mathbf{m}_0 = \frac{1}{2} \int_V dV \mathbf{r} \times \mathbf{j}(\mathbf{r}) = -\frac{e}{2m_e} \mathbf{L}_0, \quad (1.1)$$

with the classical orbital momentum $\mathbf{L}_0 = m_e \mathbf{r} \times \mathbf{v}$.

Since the electron does not orbit the nucleus as a classical particle would, we need to apply quantum mechanics for the description of its orbital momentum. The Hamiltonian for the electron in the central coulomb potential is $SO(3)$ rotation invariant and has

1. Magnetic Textures

thus simultaneous eigenstates with the representations of the rotation generators, the components of the *orbital angular momentum operator* $\mathbf{l}$. Many properties of the basis of eigenstates are dictated by the commutation relations of the *angular momentum algebra* $\mathfrak{so}(3)$. Since the individual components of $\mathbf{l}$ do not commute with each other, one commonly chooses the mutually commuting operators $\mathbf{l}^2$ and l_i ($i = 3$ by convention), with integer eigenvalues $l(l+1)$ and $m_l = -l, \dots, 0, \dots, l$, to differentiate and label the energy eigenstates. Moreover, the corresponding energy eigenvalues do not depend on m and the energy states are $(2l+1)$ -times degenerate. This means, that the representation of the rotation group on the Hilbert space can be decomposed into the direct sum of $(2l+1)$ dimensional irreducible representations.

For hydrogen-like atoms consisting of a single electron and a nucleus the energy depends only on the principal quantum number $n \in \mathbb{N}$ and energy eigenstates exist for $0 \leq l \leq n-1$. If one chooses the Hilbert space of square-integrable functions $\mathcal{H} = L^2(\mathbb{R}^3)$ in spherical coordinates and separates the variables, n and l are the quantum numbers which specify the radial part of the solution.

With the above considerations one finds the permitted values for the angular momentum quantized in integer multiples of the reduced Planck constant $\hbar$. The orbital angular magnetic moment for a single quantum electron is therefore

$$\mathbf{m}_l = -\frac{e}{2m_e}\hbar\mathbf{l} = -\mu_B\mathbf{l},$$

with the Bohr magneton $\mu_B = \frac{e\hbar}{2m_e}$.

Spin moment

Apart from the orbital contribution there is another intrinsic contribution to the magnetic moment generated by an electron. The experimental observation of this contribution in the *Stern-Gerlach experiment* 1922 [GS22] was the first indication of this intrinsic property of the electron, which was coined *spin* in analogy with the angular momentum of a spinning classical particle. In this experiment, only two distinct magnetic moments were observed, which is incompatible with an angular magnetic moment with quantised integer values but instead requires the existence of half-integer eigenvalues, in particular $s = \frac{1}{2}$, such that $m_s = -\frac{1}{2}, \frac{1}{2}$.

The spin in quantum mechanics is described by the *spin operator* $\mathbf{s}$ whose components are a representation of the Lie algebra $\mathfrak{su}(2)$, which is isomorphic to $\mathfrak{so}(3)$, such that they obey identical commutation relations. For that reason, the spin behaves like a quantum mechanical angular momentum and the spin magnetic moment for a single quantum electron can be expressed as

$$\mathbf{m}_s = -g\frac{e}{2m_e}\hbar\mathbf{s} = -g\mu_B\mathbf{s},$$

where the *g-factor* $g \approx 2$ describes the strength of the magnetic moment generated by the spin. For a classical spinning charged sphere with uniform mass and charge distribution, one would find $g = 1$ instead. The energy of the eigenstates for electrons with spin is independent of s and m_s such that the energy states are $(2n+1)(2l+1)(2s+1)$ -times degenerate with $(2s+1) = 2$.

The quantum mechanical spin arises from the relativistic *Dirac quantum theory* in the non-relativistic limit and has no classical correspondence. The form of the spin operators as a representation of $\mathfrak{su}(2)$ is determined by the behaviour of the electron under *Lorentz-transformation* and derives from representations of the Lorentz group. From the non-relativistic limit $v \ll c$ of the Dirac equation one finds $g = 2$. A more detailed discussion of the representation of spin and the coupling to the magnetic field is also essential for the description of the electronic structure and can be found in Rem 2.1.

Dirac theory

The g-factor 2 is not the precise value observed in experiments, which is due to higher order interactions of the electronic charge with the electromagnetic field. Those corrections are described in *Quantum Electro Dynamics* (QED) as *anomalous magnetic moment* and can be evaluated to high accuracy. One finds $g = 2 + \frac{\alpha}{\pi} + \mathcal{O}(\alpha^2)$, where $\alpha = \mu_0 \frac{e^2 c}{2\hbar}$ is the *fine-structure constant*. Fine-structure refers to the splitting of the energy levels due to further relativistic effects, that we will discuss later on, and the energy gaps are of magnitude $(Z\alpha)^2$ with the atomic number Z .

Remark 1.1 (Fine-structure constant). The fine structure constant can be measured very precisely from quantised magnetic effects such as the *Quantum Hall Effect* (QHE) [KDP80].

The *total magnetic dipole moment* generated by a single electron in an atom is the sum $\mathbf{m}_t$ of orbital contribution $\mathbf{m}_l$ and the spin contribution $\mathbf{m}_s$. With $g = 2$ it is collinear with $\mathbf{l} + 2\mathbf{s}$ rather than with the total angular momentum $\mathbf{j} = \mathbf{l} + \mathbf{s}$. However, it still commutes with the Hamiltonian and is therefore a constant of motion, i.e. constant under time evolution of the system.

Total magnetic moment

Remark 1.2 (Nuclear magnetic moment). All charged elementary particles with spin produce a magnetic moment. Therefore, the protons and neutrons in the nucleus, which are formed by charged quarks with spin, also possess magnetic moments each. However, those are suppressed by the larger proton and neutron masses $m_e \ll m_p \approx m_n$ such that they can be neglected.

In the case of an atom with many electrons, the situation becomes immensely more complicated due to the interactions between the individual electrons. As this many-particle problem cannot be solved exactly, one commonly solves instead the one-particle problem for each electron with an effective potential. Such an effective potential for one electron is, for instance, obtained by the *Hartree approximation*, for which the interaction with the other electrons is modelled as their averaged charge density. The new potential is still spherically symmetric, so the angular momentum operators $\mathbf{l}_i$ and $\mathbf{s}_i$ still commute with the Hamiltonian. The solution is therefore of the same form as for the hydrogen-like atom, except for the energies of the eigenstates depending on l such that the $(2n+1)$ -degeneracy is lifted. We define the total orbital angular momentum $\mathbf{L}$ and the total spin $\mathbf{S}$ by

Many electrons

$$\mathbf{L} := \sum_{i=1}^N \mathbf{l}_i \quad \text{and} \quad \mathbf{S} := \sum_{i=1}^N \mathbf{s}_i.$$

With the Pauli exclusion principle inhibiting N electrons at the same energy from occupying the same state more than once, the remaining degeneracy of $2(2l+1)$ for each

1. Magnetic Textures

electron leads to $\binom{2(2l+1)}{N}$ different *configurations* for each energy level. For filled shells, i.e. $N = 2(2l + 1)$ electrons at the same energy, there is only one allowed configuration and the expectation values of the individual $\mathbf{l}_i$ and $\mathbf{s}_i$ compensate each other respectively, such that the expectation values of $\mathbf{L}$ and $\mathbf{S}$ vanish. As a consequence the total magnetic moment of the atom vanishes as well. Clearly, incompletely occupied shells are required for magnetism.

Filling the shells

The way that the electrons fill the shells follows the set of empirical *Hund rules*, that can be explained by the Coulomb interaction beyond the Hartree approximation and the so-called spin-orbit interaction which is a higher order (in $\frac{v}{c}$) effect occurring in the non-relativistic limit of the Dirac theory. The Coulomb interaction operator commutes no longer with the individual angular momentum operators $\mathbf{l}_i$ and $\mathbf{s}_i$ but instead with $\mathbf{L}$, $\mathbf{L}^2$, $\mathbf{S}$ and $\mathbf{S}^2$ such that the configurations can be classified in terms of the quantum numbers L, m_L, S, m_S and the $\binom{2(2l+1)}{N}$ configurations split into energy levels, so-called *terms*, with degeneracy $(2L+1)(2S+1)$. The terms are shifted in energy with differences of order 10eV as the Pauli principle indirectly affects the strength of the Coulomb interaction: Electrons with the same spin or aligned orbital angular momenta, i.e. large L , are further apart and thus experience lower Coulomb repulsion, leading to lower energy. The ground-state term is the one with the lowest energy.

Spin-orbit coupling

The spin-orbit coupling (SOC) is a higher order contribution to the non-relativistic Hamiltonian that couples $\mathbf{l}$ and $\mathbf{s}$ of each electron. Its origin can be explained from the reference system of the electron in which the orbiting nucleus generates a magnetic dipole moment interacting with the electrons' spin moment. One can compress several cases for it into a compact form

$$H_{\text{SO}} = \lambda \mathbf{L} \cdot \mathbf{S} = \frac{\lambda}{2} [\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2] \quad (1.2)$$

with a prefactor λ that depends on the filling [Tim19, Chap. 2.3]. For less than half full shells one has $\lambda < 0$ and one has $\lambda > 0$ for shells at more than half-filling. The spins and orbital moments are therefore preferably parallel or antiparallel, which also leads to the alignment of the individual spins. For the second equality one defines the total angular momentum operator $\mathbf{J} := \mathbf{L} + \mathbf{S}$ and assumes $g = 2$. Including this term the Hamiltonian commutes with $\mathbf{J}$, $\mathbf{J}^2$, $\mathbf{L}^2$, and $\mathbf{S}^2$, but no longer with $\mathbf{L}$ and $\mathbf{S}$. From Eq. (1.2) follows, that the energy depends on L , S , and J . This splits the $(2L+1)(2S+1)$ -degeneracy in the terms into *multiplets* with remaining degeneracy $2J+1$ in which $\mathbf{L}$ and $\mathbf{S}$ are collinear. The energy difference depends on the atomic number and is of order $10^{-2}\text{eV} - 10^{-1}\text{eV}$ in the iron group and of order 1eV for rare earths. The ground state multiplet is determined by the sign of λ , which is known as the third Hund rule. It has minimal $J = |L - S|$ for $\lambda < 0$ and maximal $J = L + S$ for $\lambda > 0$. For half-filled shells, one has $J = S$.

Observable magnetic moment

The magnetic moment of an atom in the ground state with S , L , and J is given by $\mathbf{m}_J = \mathbf{m}_L + \mathbf{m}_S$, which is not collinear to $\mathbf{J}$ and does not commute with the Hamiltonian. It is therefore not a constant of motion and thus also not a suitable observable. Since most experiments are slow in comparison to the time evolution of $\mathbf{m}_J$, we consider instead the observable time-averaged magnetic moment $\mathbf{m}_{\text{obs}}$ obtained by projecting onto $\mathbf{J}$:

$$\mathbf{m}_{\text{obs}} = -\left(1 - \frac{1}{2} \frac{J(J+1) + S(S+1) - L(L+1)}{J(J+1)}\right) \mu_B \mathbf{J} := -g_J \mu_B \mathbf{J}.$$

The new factor g_J , the so-called *Landé g-factor*, arises from the projection and takes values between 0 and 2. Its value contains information about the respective contributions of spin and orbital moment. The observable magnetic moment is therefore proportional to $\mathbf{J}$ and vanishes for $J = 0$, in particular, it requires unfilled shells in which spin and orbital contributions to the total magnetic moment do not fully compensate.

1.1.2. Solid State Magnetism

For solids, magnetism is described by the magnetisation, i.e. the magnetic moment per volume. As in the atomic state, magnetisation in solids has two main contributions: Spin magnetisation and orbital magnetisation. However, the magnetic moments in the solid state are generally not the same as in the atomic state. In fact, most solid materials are non-magnetic, while their constituent elements have a non-zero magnetic moment as a free atom.

There are two models for describing the magnetism of solids, the *localised electron model* and the *itinerant electron model*. In the former, the electrons are localised at the atomic sites, similar to the atomic state, whereas in the latter, the electrons contributing to magnetisation are fully delocalised in the conduction band. In both cases, the electrons are influenced by the electric field of the neighbouring atoms breaking the isotropy of space, which can have a variety of consequences depending on its strength compared to other interactions. For example, in the case of most transition metal salts, the observable orbital angular momentum gets strongly suppressed, such that the main contribution to the magnetisation is mostly due to the electron spin.

In the following, we introduce how magnetic moments arise in solids according to the different models and how the orbital contribution is quenched. For further details we refer to [TGS02, Chap. 7-8] and [Tim19, Chap. 4, 10].

Solid substances consist of atoms held together by chemical bonds formed by sharing or exchanging electrons from different elements. For covalent or ionic bonds the electrons are localised around the atomic sites and the sharing or exchange of electrons leads to orbits with full occupation and thus compensating contributions to the magnetic moment. Only if there are remaining partially filled shells, a permanent magnetic moment can emerge, but even then, the orbits are perturbed by the electric field of the neighbouring atoms such that the magnetic moment arises differently from the individual electron dipole moments than in the free case.

Bound atoms

With metallic bonds the electrons from the outermost occupied shells become the delocalised conduction electrons that behave like an electron gas in the periodic electric potential from the ionised atoms, which leads to band formation. If the conduction band is equally occupied by electrons with spin up and down, the total magnetic moments vanish as well. In general, such as the atomic magnetic moment required non-saturated shells, a permanent magnetic moment in a solid requires unpaired electrons.

1. Magnetic Textures

Localised model

The localised electron model applies to insulators and most materials with rare earth elements [TGS02, Chap. 7] and allows for a quantitative treatment of the magnetic moments. As motivated above, partially filled electronic shells are required for permanent magnetism. For them to remain partially filled while bonded to other atoms, the shells need to be internal, i.e. there are occupied shells further from the nucleus that participate in bonding instead. There are two main groups for which such shells exist, the *iron group* with partially filled inner $3d$ shell that is surrounded by the $4s$ electrons, and the *rare earths* with partially filled inner $4f$ shell surrounded by the $5s$, $5d$, and $6s$ shells. For transition metals from the other series the non-saturated $4d$ or $5d$ shells are more delocalised and take part in bonding, while the elements with partially filled $5f$ shells are radioactive.

The observed magnetic moments in magnetic materials with localised electrons often differ from the magnetic moment of the free atom. Especially for the salts of the $3d$ iron group, the magnetic moments are often closer to the spin moment contribution than to the total angular moments, as can be seen in [Kit18, Chap. 11, Tab. 2], whereas in the case of rare earth ions the moments are in much better agreement [Kit18, Chap. 11, Tab. 1]. This is due to the strength hierarchy of the various interactions, including the spin-orbit coupling and correlation between electrons, in comparison to the crystal field, which breaks isotropy in space and influences the spatial motion of electrons, consequently affecting their orbital angular momentum. We refer to [TGS02, Chap. 7.3] for the discussion of some individual elements and compounds for better illustration. In general, it is very difficult to give exact predications of the magnetic moment of any compound due to the perturbation of the ground state.

Orbital quenching

For transition metal salts the $3d$ shell is only weakly shielded from the electric field of the surrounding atoms. Therefore, for the energy splitting the crystal field needs to be considered first and spin-orbit coupling acts as a small perturbation to it [Tim19, Chap. 3.3]. The anisotropic crystal field leads to a decrease in symmetry and thus lifting of the degeneracy in the terms. For sufficiently low symmetry, all degeneracies except for the spin degrees are lifted. As a matter of fact, if the symmetry of the crystal is not low enough to lift the degeneracy completely, the crystal might even distort to compensate for this. The quadratic energy increase for the elastic deformation is more than recouped by the linear decrease from the splitting of the degenerate state [Blü17, Chap. 3.4]. This is known as the Jahn-Teller effect [JT37], and it leads to a non-degenerate ground state.

Then, for non-degenerate states, the expectation value for the total orbital angular momentum is zero, as can be seen by a brief line of arguments [Tim19, Chap. 3.3.2]: The Hamiltonian including the crystal field is a real operator in the Schrödinger representation and thus one can choose a real many-electron ground state wave function. Further, $\mathbf{L}$ is hermitian and purely imaginary in the Schrödinger representation. Consequently, the expectation value $\langle 0 | \mathbf{L} | 0 \rangle$ must be real as well as imaginary and thus,

$$\langle 0 | \mathbf{L} | 0 \rangle = 0.$$

This is known as *quenching* of the orbital angular momentum. A small orbital contribution is restored by the spin-orbit coupling perturbation. Then, the magnetic moment contains

an induced orbital magnetic moment from the second order contribution and an anisotropy energy term of the spin arises.

For rare earth ions, which are better shielded from the nuclear electric field, spin-orbit coupling is still relevant, and the crystal field can be assumed as a small perturbation breaking isotropy. This leads to splitting in the J multiplets, which manifests in the emergence of an easy axis and a hard axis (easy-plane) anisotropy. A detailed description in terms of irreducible tensor operators is given in [Ste52].

There is also the possibility of the crystal field being even stronger than the interactions responsible for Hund's rules [Tim19, Chap. 3.2]. In that case, the effect of the crystal field has to be considered for each single electron, before the interaction is applied. Then, the population of the $3d$ orbits maximises the orbital momentum first, before maximising the spin. This is known as a *low spin state*, as the spin contribution is either compensated or arises from a single electron at most. At the same time, the orbital moment is significantly larger than expected from Hund's rules, but still completely quenched by the strong crystal field.

For the description of $3d$, $4d$, and $5d$ transition metal atoms in the metallic state, the localised electron model does not apply, and instead the itinerant model gives a reasonable qualitative description [TGS02, Chap. 8]. As mentioned above, metallic bonds delocalise the electrons from the outermost occupied shells creating a gas of electrons propagating in the periodic electric potential of the ionised atoms. The influence of this potential leads to the formation of energy bands over the Brillouin zone. Since the valence electrons that contributed to the magnetic moment of the atoms in the atomic state are now delocalised, the magnetic moment in the solid state differs drastically. Indeed, the magnetism is intimately interwoven with the electronic structure of the system that in turn depends on the system's atomic arrangement, composition, and dimensionality.

Itinerant model

Macroscopic magnetisation arises with magnetic order through the interplay of Coulomb repulsion and the Pauli principle. For band electrons this is taken into account by the Stoner model as we briefly discuss in Sec. 1.1.3. It describes a repulsion between electrons of opposite spin such that an energetic dissymmetry arises in the spin occupation of the conduction band, leading to uncompensated magnetic moments. This explains in particular, why the size of the magnetic moment on the atomic sites is not an integer multiple of the Bohr magneton μ_B at zero temperature.

For the transition metals the s electrons are fully delocalised, while the d electrons are more localised to the atomic sites. Since the d orbitals of neighbouring sites overlap with each other, this can be described in a so-called tight-binding model. It constructs the wave function as a linear combination of atomic orbitals with the itinerant electrons hopping between the sites [TGS02, Chap. 8.6]. As the density of states for the s electrons is much weaker than for the d electrons, the magnetic properties of transition metals is dominated by the latter. One finds the atomic sites exhibiting stable, quasi-static local magnetic moments when averaged over times longer than the hopping times of the itinerant electrons (in the order of femtoseconds) since the hopping electrons leaving and entering the sites are correlated in a way that preserves the orientation of their magnetic spin moment [Blü17, Chap. 2.3]. This is not the general case for other elements.

1. Magnetic Textures

For rare earth materials the $4f$ electrons responsible for the magnetic moment are localised, but the $5d$ and $6s$ itinerant electrons mediate the interactions between them, making the effective interaction long ranged in comparison to the short ranged interactions in the local model. We will discuss the effects of this phenomenon in Sec. 1.2.1 for its part in the stabilisation of non-collinear magnetic order.

*Orbital
magnetisation*

Although, the orbital magnetic moment is quenched in many common materials, it is not negligible in all materials. The orbital magnetisation arising from electronic properties in an infinitely extended system was challenging to calculate for a long while [Tho11]. This has been amended by the modern theory of orbital magnetisation approach that we present in Chap. 2.4 in the context of the properties of electronic systems.

1.1.3. Magnetic Order

Interactions between neighbouring magnetic moments energetically favour specific arrangements, which may result in spatially extended magnetic order. The most prevalent ordered arrangements are ferromagnetic and antiferromagnetic magnetism, with fully parallel or antiparallel neighbouring moments.

The obvious interaction between magnetic momenta is the dipole-dipole interaction, which is however too weak to enforce order at finite temperatures above 0.3K [Tim19, Chap. 1.3]. Instead, the predominant interaction in many materials with localised electrons is the Heisenberg exchange interaction, which emerges from the Coulomb interaction mediated to spin states by the fundamental quantum-mechanical Pauli exclusion principle. For itinerant electrons the same principles affect the band electrons, such that magnetic order occurs also in metals. The strength of the exchange interaction determines the critical temperature (Curie temperature T_C for ferromagnets, Néel temperature T_N for antiferromagnets) above which the magnetic order vanishes again [Tim19, Chap. 6.1]. It heavily depends on the material properties and can reach high temperatures.

In the following, we present a quantum mechanical derivation of the exchange interaction between two electrons. Then, we discuss further exchange interactions in insulators and metals that generate magnetic order.

*Heisenberg
exchange*

The Heisenberg exchange interaction is a spin-spin interaction generated by the interplay of the spin-independent Coulomb interaction and the Pauli exclusion principle in materials with covalent or ionic bonds. This interplay causes the potential energy to minimise when the wave function overlap of two electrons is reduced. This can be achieved by producing antisymmetric spacial wave functions when the electrons occupy overlapping orbits, favouring parallel aligned spins, or by producing symmetric spacial wave functions when the orbits are localised around different ions, favouring antiparallel aligned spins [Blü17, Chap. 2.3].

The exchange interaction can be efficiently expressed by an effective spin model, which reduces the model to the spin degrees of freedom and summarises the electronic degrees of freedom by exchange parameters. For an extensive account in second-quantisation formalism applied to an ionic crystal, we refer to [Tim19, Chap. 4.1-4.2]. Here, we sketch a derivation of the exchange interaction between two electrons, following [KZP17, Chap. 1]: The two-electron Hamiltonian with spin degrees of freedom takes the form

$$H = H_A + H_B + H_{\text{coul}} \quad \text{with} \quad H_{\text{coul}} = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|},$$

where $H_{A/B}$ denotes the single-electron Hamiltonian of the electron A/B at positions $\mathbf{r}_1, \mathbf{r}_2$ and H_{coul} describes the Coulomb interaction between the electron charges e .

Since all contributions to the Hamiltonian H are explicitly spin independent, its solutions have the product form $\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \phi(\mathbf{r}_1\mathbf{r}_2)\chi(\sigma_1\sigma_2)$. For two spin- $\frac{1}{2}$ particles like the electron, there are four possible spin wave functions: Three of them are symmetric under exchange of the particles and have total spin $S = 1$, referred to as the triplet state $\chi_T(\sigma_1, \sigma_2) = +\chi_T(\sigma_2, \sigma_1)$, whereas the last one is antisymmetric under exchange and exhibits total spin $S = 0$, referred to as the singlet $\chi_S(\sigma_1, \sigma_2) = -\chi_S(\sigma_2, \sigma_1)$.

The Pauli exclusion principle states, that the total wave function describing two Fermions need to be antisymmetric with respect to exchange of the particles, i.e. $\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = -\Psi(\mathbf{r}_2\sigma_2, \mathbf{r}_1\sigma_1)$. Consequently, the symmetric triplet state χ_T is paired with an antisymmetric orbital state ϕ_- , and the antisymmetric singlet state χ_S is paired with a symmetric orbital state ϕ_+ . Those orbital states are constructed from the single-particle orbital wave functions as follows:

$$\phi_{\pm}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}[\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) \pm \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)].$$

Since the spacial charge distributions of the total states associated with singlet and triplet states consequently differ, they exhibit different coulomb energies. Their difference can be evaluated as exchange integral

$$J_{\text{ex}} = E_S - E_T = 2 \int \phi_a^*(\mathbf{r}_1)\phi_b^*(\mathbf{r}_2)H\phi_b(\mathbf{r}_1)\phi_a(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2.$$

One can understand this exchange energy difference as being caused by the coulomb repulsion between electrons in orthogonal orbitals. If it is positive, the symmetric triplet state has lower energy leading to parallel spin orientations, and if it is negative, the antisymmetric singlet state is energetically favoured leading to an antiparallel arrangement.

After successfully integrating out the orbital degrees of freedom, we can express the Hamiltonian H as effective spin Hamiltonian. For that, we use the spin operator $\mathbf{s}_i$ of the electron i with expectation value $\langle \mathbf{s}_i^2 \rangle = \frac{1}{2}(\frac{1}{2} + 1) = \frac{3}{4}$. The total spin $\mathbf{S}^2 = \mathbf{s}_1 + \mathbf{s}_2$ has the expectation value $\langle \mathbf{S}^2 \rangle = \langle \mathbf{s}_1^2 \rangle + \langle \mathbf{s}_2^2 \rangle + 2\langle \mathbf{s}_1 \cdot \mathbf{s}_2 \rangle$ which needs to be 0 for the singlet and $2 = 1(1 + 1)$ for the triplet. Consequently, the expectation value of the product $\langle \mathbf{s}_1 \cdot \mathbf{s}_2 \rangle$ is $\frac{1}{4}$ for the triplet and $-\frac{3}{4}$ for the singlet. The Hamiltonian can thus be effectively expressed in terms of these energies as

$$H = \frac{1}{4}(E_S + 3E_T) + (E_T - E_S) \langle \mathbf{s}_1 \cdot \mathbf{s}_2 \rangle.$$

Since the first term is constant, we can drop it to obtain the effective spin Hamiltonian $H_{\text{eff}} = -J_{\text{ex}} \mathbf{s}_1 \cdot \mathbf{s}_2$, that can be generalised to the lattice to obtain

$$H_{\text{ex}} = - \sum_{i < j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j, \quad (1.3)$$

1. Magnetic Textures

where the sum considers all pairs of lattice sites. In its classical limit, the spin operators are replaced by classical vectors of length 1. Since the coulomb interaction is short ranged, the coupling constant J_{ij} can in many models assumed to be constant for nearest neighbours and zero otherwise. With positive value it favours ferromagnetic and with negative value antiferromagnetic order.

Further interactions

The exchange interaction might be the dominant one in most system with localised electrons, but it is by far not the only spin-spin interaction. For instance one can obtain higher-order spin terms, such as the biquadratic exchange $\propto (\mathbf{s}_i \cdot \mathbf{s}_j)^2$ or ring-exchange $\propto (\mathbf{s}_i \cdot \mathbf{s}_j)(\mathbf{s}_k \cdot \mathbf{s}_l) + (\mathbf{s}_i \cdot \mathbf{s}_l)(\mathbf{s}_k \cdot \mathbf{s}_j) - (\mathbf{s}_i \cdot \mathbf{s}_k)(\mathbf{s}_j \cdot \mathbf{s}_l)$ for square or cubic lattices, where the indices run over the corners of a square [Tim19, Chap. 4.2].

In ionic crystals with magnetic ions separated by non-magnetic anions, the direct exchange interaction is comparably small. Instead, the dominant interaction is given by the so-called superexchange or semicovalent exchange interaction, which arises from electrons hopping between the ions and anions rather than sharing an overlapping orbit [Tim19, Chap. 4.3]. It was first described by Kramers and Anderson [Kra34; And50]. This type of exchange can be estimated by the Goodenough-Kanamori rules [Goo55; Goo58; Kan59], which attribute strong antiferromagnetic coupling to the cases where half-filled orbits of the cations overlap with the same empty or filled orbit of the mediating anion, and weak ferromagnetic coupling to the cases where they overlap with orthogonal orbits of the same anion.

An important antisymmetric exchange interaction is the Dzyaloshinskii-Moriya interaction (DMI) [Dzy58; Dzy64; Mor60], that may also arise from superexchange as a correction due to spin-orbit coupling and favours canting of neighbouring spins. In Sec. 1.2.1, we will discuss the implications of the DMI for non-collinear magnetisation.

Itinerant order

Also, for materials with metallic bonds, magnetic order arises from the interplay of the Coulomb interaction and the exclusion principle, however, acting on the itinerant electrons occupying the bands over the Brillouin zone [Tim19, Chap. 10.1]. This reduces the energy for electron pairs with parallel spin, leading to ferromagnetic order in metals. Since the electrons form a Fermi surface, this type of exchange interaction is typically long ranged.

The mobile electrons screen the Coulomb interaction from affecting electrons further apart. This effect is captured in the Stoner model [Sto39], describing electrons in an effective magnetic field proportional to the polarisation $\frac{N_\uparrow - N_\downarrow}{N_e}$, generated by N_e electrons of which $N_\uparrow$ are spin-up and $N_\downarrow$ spin-down [Tim19, Chap. 10.2]. This leads to an energy shift in the density of states for differently polarised electrons, such that the conduction band is mostly occupied by electrons of the same orientation, leading to ferromagnetism.

If both itinerant and localised electrons contribute to the creation of magnetic order, as is the case in intermetallic rare-earth compounds, the best description is the Ruderman-Kittel-Kasuya-Yosida (RKKY) model [RK54; Kas56; Yos57] from which non-collinear order might arise as discussed in Sec. 1.2.1.

1.1.4. The Micromagnetic Model

The micromagnetic model describes mesoscopic magnetism as continuous properties of the material. At the considered length scale of several micrometers the discrete atomic substructure can be ignored, while magnetic structures are resolved. The magnetic ground state of a system can for instance be determined by minimising an energy density functional with continuous contributions raised by interactions.

In the following, we introduce the key concepts of the micromagnetic approximation and its application on the example of the Heisenberg exchange interaction. This section follows closely the introduction in [KZP17, Chap. 3].

The concept of micromagnetics has been developed by Landau and Lifshitz [LL35; LL13] and Brown [Bro40; Bro63]. It was devised for the study of domain walls which are of small size in relation to the magnetic domains at a time when the quantum theory and atomistic model was not yet established. Instead of considering individual magnetic moments the micromagnetic model approximates the distribution of magnetisation over the sample volume as a continuous function $\mathbf{M}$. The density of the magnetic moments per unit volume, the so-called saturation magnetisation

Micromagnetic approximation

$$M_s = \sum_i \frac{\mu_i}{V},$$

determines the absolute value of the magnetisation, i.e. $\mathbf{M} = M_s \mathbf{n}$ with $|\mathbf{n}| = 1$.

There are different approaches to achieve the explicit transition between the atomistic and micromagnetic model. Here, we want to present the approach laid out in [KZP17, Chap. 3] for the exemplary case of the Heisenberg exchange interaction in a two-dimensional lattice. The exchange interaction term from Eq. (1.3) can be rewritten to

Exchange interaction

$$H_{\text{ex}} = - \sum_{i < j} J_{ij} \left(1 - \frac{1}{2} |\mathbf{n}_i - \mathbf{n}_j|^2 \right)$$

for magnetic momenta $\mathbf{n}_i$ of unit length, such that $\mathbf{n}_i^2 = 1$ for all atomic sites i . This can be brought into the form of a sum over local energy density terms at the individual lattice sites

$$H_{\text{ex}} = \sum_i \epsilon_i \quad \text{with} \quad \epsilon_i = -\frac{1}{2} \sum_s J_s \sum_j^{N(s)} \left(1 - \frac{1}{2} \sum_{\alpha=1}^2 (n_{\alpha}(\mathbf{r}_i) - n_{\alpha}(\mathbf{r}_i + \mathbf{r}_{ij}))^2 \right),$$

where S denotes the number of shells (sets of equidistant neighbouring lattice sites), J_s the coupling constant for the shell s , $N(s)$ the number of neighbours in the shell s , $\mathbf{r}_i$ the position of the atom i , and $\mathbf{r}_{ij}$ the relative position of the neighbour atom j . This can be expressed in terms of the lattice constant a .

In the micromagnetic approximation, where the distribution of the vectors $\mathbf{n}(\mathbf{r}_i)$ can be described by continuous functions differentiable at $\mathbf{r}_i$, the energy density terms ϵ_i can be approximated by their Taylor expansion

$$\epsilon(\mathbf{r}) \approx \frac{1}{v} \left[\epsilon_i(0) + \frac{a^2}{2} \frac{d^2}{da^2} \epsilon_i(a) \right],$$

1. Magnetic Textures

with volume per lattice site v . We obtain an energy functional in the form of an integral over the whole sample

$$E_{\text{ex}}[\mathbf{n}] = \int_V \epsilon_{\text{ex}}(\mathbf{r}) \, d\mathbf{r} \quad \text{with} \quad \epsilon_{\text{ex}}(\mathbf{r}) = \epsilon_0 + \sum_{\alpha, \beta, \gamma=1}^2 \left(\frac{\partial n_\alpha}{\partial r_\beta} \right) A_{\beta\gamma} \left(\frac{\partial n_\alpha}{\partial r_\gamma} \right).$$

Here, α, β, γ indicate the real space indices and $A_{\beta\gamma} = \frac{1}{4v} \sum_s J_s \sum_j^{N(s)} r_j^\beta r_j^\gamma$ is the micro-magnetic exchange coupling tensor in its most general form. For the common case of a high-symmetry crystal, such as square lattice, it reduces to a scalar A .

$$\epsilon_{\text{ex}}(\mathbf{r}) = \epsilon_0 + \sum_{\alpha, \beta=1}^2 A \left(\frac{\partial n_\alpha}{\partial r_\beta} \right)^2$$

Minimising the energy functional lets us determine the stable magnetic ground state. Together with further competing interactions this ground state might be non-collinear as discussed in the next section.

1.2. Non-collinear Magnetism

Non-collinear magnetism describes arrangements of local magnetic moments which are neither parallel nor antiparallel but follow a more complicated pattern.

Isolated structures

A common occurrence of non-collinear magnetism is in the form of isolated structures in a ferro- or antiferromagnetic background. Their prototypical example are domain walls that separate areas of different orientation from each other. In a homogeneous background in two dimensions, they are often of circular shape and encompass an oppositionally oriented centre. These magnetic bubbles are also known as skyrmions if their underlying continuous vector field can be classified by a non-zero winding number. Because of their stability and soliton property, they can be described as quasi-particles for the purpose of their dynamics. A presentation of a variety of further magnetic quasi-particles can be found in [GMT21].

Multi- q textures

A rich class of noncollinear magnets comprises periodic spin textures dominated by their lowest-order Fourier modes [Hei+11]. They can be characterised by phase-coherent superpositions of multiple spin waves with wave vector $\mathbf{q}$, and are referred to as multi- q textures. The most basic instance is the single- q state that describes periodicity in one direction and manifests in two dimensions as a striped pattern of domain walls. Multi- q textures are fully determined by the phases of the superimposed spin waves and this homogeneity makes them ideal candidates for the study of the electronic structure of non-collinear magnetic materials. They feature a variety of unconventional electronic structure and transport properties that arise from an interplay of topological attributes in real- and reciprocal space [HEN15; Göb+17b; Lux+24; Hay23].

The multi- q texture that holds the highest significance for the context of this dissertation is the skyrmion lattice. Skyrmionic multi- q states appear in the family of chiral B20 materials such as MnSi [Müh+09; Neu+09], FeGe [Yu+11; Ler+18], and $\text{Fe}_{1-x}\text{Co}_x\text{Si}$ thin films [Mün+10; Yu+10], chiral multiferroic insulators such as Cu_2OSeO_3 [Ada+12; Sek+12; Lan+14; Hua+20], and centrosymmetric rare-earth intermetallic compounds such as Gd_2PdSi_3 [Kur+19], GdRu_2Si_2 [Kha+20], and $\text{Gd}_3\text{Ru}_4\text{Al}_{12}$ [Hir+19].

The length scale of the period in the multi- q materials is typically in the order of tens of nanometres, with each skyrmion comprising many atomic sites. This is expressed by their wave number $q \sim 0.01 \frac{2\pi}{a}$ in relation to their respective lattice constants a . These textures can be assumed to be lattice commensurate which entails that the spins on the lattice sites are the same for each cell of the spin lattice. Conversely, the more recently discovered skyrmion textures in the centrosymmetric systems have periodicities in the order of single nanometres with lattice incommensurate wave number $q \sim 0.1 \frac{2\pi}{a}$. The spins in each texture cell differ slightly from the ones in all other cells such that all spin orientations are realised in an infinite system.

In general, non-collinear structures are stabilised to be the magnetic ground state by an interplay of competing interactions. Large skyrmions with extended ferromagnetic centre and narrow domain wall are for instance stabilised by the dipole-dipole interaction [GMT21]. They can reach diameters of several micrometers. The skyrmions smaller than a few hundred nanometres that occur in non-centrosymmetric chiral magnets are typically stabilised by the Dzyaloshinskii-Moriya interaction (DMI) [Dzy58; Mor60; Dzy64; Dzy65] in competition with ferromagnetic interactions, such as the Heisenberg exchange interaction and magnetocrystalline anisotropy, the Zeeman interaction with an external magnetic field, and a multitude of influences, such as thermal and quantum fluctuations or disorder introduced by impurities. In itinerant magnets nanometric skyrmion lattices can be stabilised by itinerant frustration between long-range interactions mediated by electrons such as the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [RK54; Kas56; Yos57]. The wave number has its origin in the nesting of the Fermi surface, which favours specific wave vectors related by the rotation symmetry of the system. This applies to the centrosymmetric rare-earth intermetallic compounds mentioned above.

Stabilisation

We begin this section with a discussion of the main stabilisation mechanisms in non-centrosymmetric and centrosymmetric systems, the DMI and RKKY interaction. Then, we present a parametrisation of a single skyrmion, which allows an easy analytic notion for its winding number, polarity, and vorticity.

Section Content

The main part of the section focuses on the aforementioned multi- q textures. We specify their general characterisation, their topological classification with the winding number, and their realisation on a structural atomic lattice. Following this, we present the precise examples of multi- q textures that are studied in this dissertation. They contain a $2q$ spin wave superposition in one dimension, two separate $3q$ skyrmion lattices, respectively generated from helical and sinusoidal spin waves, and a $3q$ vortex lattice generated by spin density waves. All the $3q$ textures are hosted on a two-dimensional triangular lattice. For the two skyrmion lattices, we further present the dependence of their real space properties on texture parameters regarding the superposition.

1. Magnetic Textures

1.2.1. Stabilisation Mechanisms

Non-collinear spin textures are stabilised by the competing interplay of various interactions between the spins and charges of local and itinerant electrons.

In non-centrosymmetric systems, where non-collinear magnetism was first observed, the dominating energy terms arise from the Heisenberg exchange interaction and the Dzyaloshinskii-Moriya interaction (DMI). Such materials include B20 compounds, magnetic insulators, and magnetic monolayers. Spin textures also occur in itinerant magnets, where they are stabilised, *inter alia*, by the DMI and Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. The latter are also stable in centrosymmetric systems where the DMI is replaced by biquadratic interactions, examples of which include several Gd compounds.

In the following, we briefly introduce the leading stabilisation mechanisms for the different scenarios. We start with the Dzyaloshinskii-Moriya interaction in non-centrosymmetric systems. Then, we discuss the case of itinerant magnets following [HM21b] and introduce the RKKY interaction that extends to centrosymmetric systems.

DMI The Dzyaloshinskii-Moriya interaction (DMI) was first predicted by Dzyaloshinskii in the context of its absence in centrosymmetric systems [Dzy58]. Its mechanism involving the spin-orbit coupling was explained by Moriya [Mor60], and it was subsequently applied to non-centrosymmetric systems [Dzy64; Dzy65]. In such systems the inversion symmetry is broken, which leads to the DMI as chiral energy correction to the exchange interaction due to spin-orbit coupling [GMT21]

$$H_{DMI} = \frac{1}{2} \sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{s}_i \times \mathbf{s}_j).$$

The DM-vectors $\mathbf{D}_{ij}$ account for the way the inversion symmetry is broken and belong to an antisymmetric tensor $\mathbf{D}$, i.e. $\mathbf{D}_{ij} = -\mathbf{D}_{ji}$. The DMI differs from the exchange interactions caused exclusively by the Coulomb interaction in that it favours a distinct chirality for the spins. Moriya derived a number of symmetry rules for the direction of the DM vectors, that can be found in [Mor60]. The contributions to the free magnetic energy arising from it are known as Lifshitz invariants and can be found in [Bog+02]. They favour the canting of neighbouring magnetic moments which, under the right circumstances, may stabilise long-periodic spatially modulated structures with a fixed sense of rotation of the spin vectors $\mathbf{s}_i$.

The micromagnetic theory for the stabilisation of non-collinear spin structures by DMI had been developed by Bogdanov and Hubert [BY89; BH94; RBP06]. In it, effective energy functional in two dimensions takes the form

$$E[\mathbf{n}] = \int_{\mathbb{R}^2} [A|\nabla\mathbf{n}|^2 + \mathbf{D} : (\nabla\mathbf{n} \times \mathbf{n}) + \mathbf{n} \cdot \mathbf{K} \cdot \mathbf{n} - \mathbf{n} \cdot \mathbf{B}] d^2\mathbf{r}.$$

The first term describes the exchange energy with scalar stiffness A which, for $A > 0$, favours parallel alignment of the spins. The second term describes the DMI contribution with 3-tensor $\mathbf{D}$ favouring spin canting. Here, the colon denotes the tensor contraction. The third term describes the anisotropy with 2-tensor $\mathbf{K}$, which typically favours

alignment along a specific preferred axis. The fourth term describes the influence of an external magnetic field with vector $\mathbf{B}$ favouring alignment along the field's direction. The parameters are material constants and the effects of the competition of the different terms materialise on different length scales. In the right parameter range, periodic textures with non-trivial winding number can emerge. For a modern account we refer to [Mel14; Leo+16].

In itinerant magnets, topological spin textures with significant shorter periods can occur. Their stabilisation involves the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [RK54; Kas56; Yos57], that arises in spin-charge coupled systems and is rooted in the kinetic movement of itinerant electrons. It is a long-ranged interaction, which is best described in momentum space by

RKKY

$$H_{RKKY} = -J_K^2 \sum_{\mathbf{q}} \chi_{\mathbf{q}}^0 \mathbf{s}_{\mathbf{q}} \cdot \mathbf{s}_{-\mathbf{q}}$$

with the bare susceptibility $\chi_{\mathbf{q}}^0$ of itinerant electrons, $\mathbf{s}_{\mathbf{q}}$ denoting the Fourier transform of the localised spin vector $\mathbf{s}_i$, and J_K the exchange coupling constant. The periodicity of the RKKY interaction is set by the Fermi wave number of the itinerant electrons for which the corresponding wave vectors maximise $\chi_{\mathbf{q}}^0$. This is particularly clear in the case of perfect nesting, where all points of the Fermi surface are connected with each other by a single nesting vector. Then, the bare susceptibility exhibits a delta-functional peak at this vector, and the system is unstable towards single- q order by gap opening on the entire Fermi surface. In principle this favours single- q states, however, several Fermi wave vectors related by the rotation symmetry of the system may occur simultaneously. This degeneracy between the different single- q states is known as itinerant frustration. It can be lifted by higher-order multiple-spin contributions such as the effective bilinear-biquadratic interaction [HOM17]

$$H_{BBQ} = s \sum_{\nu} \left[-J \mathbf{s}_{\mathbf{q}_{\nu}} \cdot \mathbf{s}_{-\mathbf{q}_{\nu}} + \frac{K}{N} (\mathbf{s}_{\mathbf{q}_{\nu}} \cdot \mathbf{s}_{-\mathbf{q}_{\nu}})^2 \right],$$

with sum over the set of wave vectors $\mathbf{q}_{\nu}$ giving the peaks in the bare susceptibility. The parameter N denotes the number of sites, J is an energy unit, and K is a positive coupling constant (in the case of itinerant magnets). As a consequence of the degeneracy lifting, multi- q states might be stabilised as superposition of the single- q spin waves [OHM17; HM21a]. This is irrespective of the structural lattice and applies in particular also to centrosymmetric systems.

This stabilisation mechanism for itinerant magnets is elucidated in detail in the review article [HM21b] with application to the centrosymmetric Gd compounds GdRu₂Si₂ [Kha+20; Yas+20] and Gd₃Ru₄Al₁₂ [Hir+19; HHT21]. A demonstration of the RKKY paradigm from first principle for the spin textures in GdRu₂Si₂ and Gd₂PdSi₃ [Kur+19] can be found in [Bou+22]. For them the barrel-shaped structures in the Fermi surface facilitate Fermi surface nesting that leads to single- q spiral states, that transform into skyrmion crystals under an applied magnetic field.

1. Magnetic Textures

1.2.2. Single Skyrmion

The single skyrmion represents an isolated nanoscale whirl in a uniform magnetic background texture. It has axial symmetry and a fixed rotational sense determined by its stabilisation mechanism, such as DMI in materials with broken inversion symmetry. Its size and shape depend on external magnetic fields. In this subsection, we introduce a general parameterisation for an isolated skyrmion which decomposes into radial and azimuthal components and has a simple analytical expression for its winding number. This description is applicable for different radial profiles such as for a simple, spacially confinement profile but also a realistic domain wall profile.

Parametrisation

To parametrise a single skyrmion one commonly proceeds the following way: The continuous magnetisation in real space is described in spherical coordinates for each individual spin

$$\hat{\mathbf{n}} : \mathbb{R}^2 \rightarrow S^2, \mathbf{x} \mapsto \hat{\mathbf{n}}(\mathbf{x}) = \begin{pmatrix} \sin(\theta(\mathbf{x})) \cos(\varphi(\mathbf{x})) \\ \sin(\theta(\mathbf{x})) \sin(\varphi(\mathbf{x})) \\ \cos(\theta(\mathbf{x})) \end{pmatrix}.$$

At the centre of the skyrmion, the spin points downwards and rises continuously and monotonically as the radius increases, transitioning to a ferromagnetic background. If the skyrmion is located at the origin, we require of the polar angle $\theta(0) = \pi$ and $\theta(\mathbf{x}) = 0$ for $|\mathbf{x}| \rightarrow \infty$. By continuity, the azimuthal angle φ along any closed loop in real space around the origin needs to change continuously by a multiple of 2π . This factor $m \in \mathbb{Z}$ determines how often the image of $\hat{\mathbf{n}}$ wraps around the unit sphere S^2 .

For spherical skyrmions it is convenient to parameterise the real space in polar coordinates (ρ, ϕ) and to separate the coordinates in such a way that the polar angle θ of the spin depends only on the radius ρ , while the azimuthal angle φ of the spin depends only on the azimuthal angle ϕ of the coordinates. In this case, the winding number takes a very simple form:

Winding number

$$\begin{aligned} \deg \hat{\mathbf{n}} &= \frac{1}{4\pi} \int_0^\infty d\rho \int_0^{2\pi} d\phi \hat{\mathbf{n}} \cdot (\partial_\rho \hat{\mathbf{n}} \times \partial_\phi \hat{\mathbf{n}}) = \frac{1}{4\pi} \int_0^\infty d\rho \sin(\theta(\rho)) \frac{\partial \theta}{\partial \rho} \int_0^{2\pi} d\phi \frac{\partial \varphi}{\partial \phi} \\ &= -\frac{1}{4\pi} \cos(\theta(\rho)) \Big|_0^\infty \varphi(\phi) \Big|_0^{2\pi}. \end{aligned}$$

With the specifications from above it is $\cos(\theta(\rho)) \Big|_0^\infty = 2$ and $\varphi(\phi) \Big|_0^{2\pi} = 2\pi m$, thus, $\deg \hat{\mathbf{n}} = -m$. One defines further the following values: First, the polarity $p := -\frac{1}{2} \cos(\theta(\rho)) \Big|_0^\infty$, which is -1 , here, and changes if one chooses different initial conditions for the origin and infinity. Experimentally this depends on the direction of the applied external magnetic field [Rom+15]. Next, one defines the vorticity $v := \frac{1}{2\pi} \varphi(\phi) \Big|_0^{2\pi} = m$, with the meaning as discussed above for m . Lastly, one defines the helicity $\gamma := \varphi(0)$, which is the initial condition for the azimuthal angle. It has no influence on the winding number, but determines the symmetry. One differentiates between the special cases $\gamma = 0$

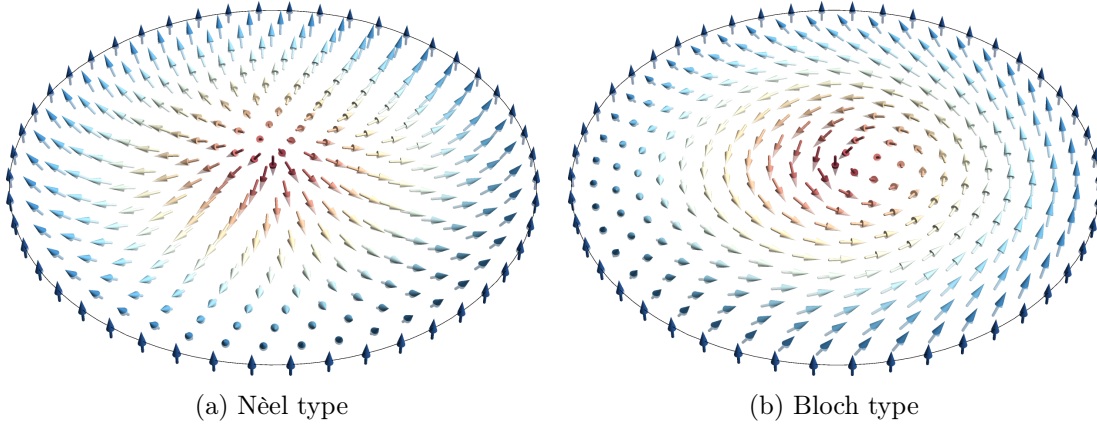


Figure 1.1.: **Single skyrmion** Two skyrmions with winding number $\deg \hat{\mathbf{n}} = -1$ and radial profile from Eq. (1.4). The Nèel type skyrmion (a) is also known as hedgehog skyrmion and has helicity $\gamma = 0$, while the Bloch type skyrmion (b) with helicity $\gamma = \frac{\pi}{2}$ is referred to as spiral skyrmion.

for Nèel type and $\gamma = \frac{\pi}{2}$ for Bloch type skyrmions. For simplicity in models, one often chooses $\varphi(\phi) = m\phi + \gamma$.

The above considerations are true for any precise choice of the radial profile. For a simple mode one can use a profile, which reaches the ferromagnetic background already at radius 1:

$$\theta(\rho) = \arccos((2\rho - 1)\Theta(1 - \rho) + \Theta(\rho - 1)), \quad (1.4)$$

where Θ denotes the Heaviside step function with middle value $\Theta(0) = \frac{1}{2}$. A visualisation of the skyrmion with winding number $\deg \hat{\mathbf{n}} = -1$ as Nèel and Bloch type is depicted in Fig. 1.1. A more realistic radial profile [Rom+15] is given by a 360° domain wall profile

$$\theta(\rho) = \sum_{\pm} \arcsin\left(\tanh\left(-\frac{-\rho \pm c}{\omega/2}\right)\right) + \pi,$$

here c is the radius of the skyrmion centre bounded by the circle with $\theta(c) = \frac{\pi}{2}$ and ω is the width of a 180° domain wall with position c . One can think of a skyrmion with this profile as the overlap of two of those domain walls.

1.2.3. Multi-q Magnetic Textures

Multi- q spin textures are arrangements of local magnetic moments that can be described as phase-coherent superpositions of multiple spin waves. In non-collinear magnetic materials, they are characterised by their dominant lowest Fourier modes, of which the wave vectors can be detected experimentally by small-angle neutron scattering [Müh+09; Ada+12]. The textures studied in this dissertation are constructed as normalised or unnormalised linear superpositions of spin waves. Since the spin orientation at any point in real space is fully determined by the phases of the generating waves, we can conceive the spin vector

Profile

1. Magnetic Textures

fields in real space equivalently as vector fields on the space of these phases, which is isomorphic to a torus. For normalised textures, this allows us to assign a winding number to each texture unit cell as we will discuss in detail in the ensuing Sec. 1.3.

For the study of electronic systems on an atomic lattice hosting multi- q textures, we need to consider interference effects of the lattice and texture periodicities. We do this by expressing the wave vectors in terms of the reciprocal lattice vectors of the structural atomic lattice. Thereby, we obtain an easy description of the spin waves' phases in terms of the site labels and pitch parameters which encode how much the phases change between a site and its neighbours. For lattice incommensurate textures in an infinite system, the realised phases lie dense in the space of phases of the continuous model. The examples for multi- q textures which are the subjects in this dissertation, are a $2q$ superposition of spin waves on an atomic chain, two normalised $3q$ textures on a triangular lattice, that are hexagonal skyrmion crystals with different winding numbers, and one unnormalised $3q$ texture on a triangular lattice, which is a vortex lattice.

In the following, we begin with a general characterisation of multi- q textures and establish their construction from a superposition of stationary spin waves. Subsequently, we discuss the realisation on a discrete lattice and the intricacies of this description. Finally, we present the explicit expression of the textures studied in this dissertation and discuss the parameter dependence of their real space properties. This section closely follows and is partially adapted from [Pra+24, Chap. 2].

Periodic textures

First, we want to consider a general periodic texture $\mathbf{n}: \mathbb{R}^d \rightarrow \mathbb{R}^3$ with Bravais lattice constructed from the vectors $\mathbf{L}_1, \dots, \mathbf{L}_d \in \mathbb{R}^d$. Clearly, it is invariant under the action of the discrete translation group $\{m_1\mathbf{L}_1 + \dots + m_d\mathbf{L}_d \in \mathbb{R}^d | \mathbf{m} \in \mathbb{Z}^d\}$. Let now $\mathbf{Q}_1, \dots, \mathbf{Q}_d \in \mathbb{R}^d$ be the basis for the corresponding reciprocal lattice, such that $\mathbf{L}_i \cdot \mathbf{Q}_j = 2\pi\delta_{ij}$. Then, an arbitrary reciprocal lattice vector is given for any $\mathbf{m} \in \mathbb{Z}^d$ by

$$\mathbf{G}_{\mathbf{m}} = m_1\mathbf{Q}_1 + \dots + m_d\mathbf{Q}_d \in \mathbb{R}^d. \quad (1.5)$$

If the vector field $\mathbf{n}$ is integrable within its unit cell, we can thus expand it as a lattice Fourier series of the form

$$\begin{aligned} \mathbf{n}(\mathbf{x}) &= \sum_{\mathbf{m} \in \mathbb{Z}^d} \mathbf{n}_{\mathbf{G}_{\mathbf{m}}} e^{+i\mathbf{G}_{\mathbf{m}} \cdot \mathbf{x}}, \\ \mathbf{n}_{\mathbf{G}_{\mathbf{m}}} &= \frac{1}{V_{uc}} \int_{V_{uc}} d\mathbf{x} \, \mathbf{n}(\mathbf{x}) e^{-i\mathbf{G}_{\mathbf{m}} \cdot \mathbf{x}}. \end{aligned}$$

The complex Fourier coefficients $\mathbf{n}_{\mathbf{G}_{\mathbf{m}}} \in \mathbb{C}^3$ decay as a sequence of increasing $\|\mathbf{m}\|$ with a rate correspondent to the smoothness of the texture. This can be intuitively understood from the example of the discontinuous square wave $n(x) = \text{sgn}(\sin(x))$ in one dimension whose Fourier coefficients n_m decay only as $1/m$. For a sufficiently smooth texture, the Fourier decomposition will be dominated by its lowest order terms and one can take this as a hallmark of multi- q magnetic order.

In this regime, a periodic magnetic texture can be emulated as a linear superposition of a few fundamental modes

Multi-q order

$$\mathbf{n}(\mathbf{x}) \approx \sum_{i=-r}^r \mathbf{n}_{\mathbf{q}_i} e^{i(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i)}. \quad (1.6)$$

In this case, it is fully determined by the set of $r \in \mathbb{N}$ coexisting wave vectors $\mathbf{q}_1, \dots, \mathbf{q}_r \in \mathbb{R}^d$, $\mathbf{q}_{-i} := -\mathbf{q}_i$, together with their initial phase conditions $\varphi_1, \dots, \varphi_r \in S^1$ and complex amplitudes $\mathbf{n}_{\mathbf{q}_1}, \dots, \mathbf{n}_{\mathbf{q}_r} \in \mathbb{C}^3$ at the origin of some arbitrary but fixed coordinate system, and the zero mode with $\mathbf{q}_0 = 0$, $\varphi_0 = 0$, and $\mathbf{n}_{\mathbf{q}_0} \in \mathbb{R}^3$. The initial phase conditions are put in by design to clarify the intended phases at the origin and could be absorbed by the complex amplitudes. The q -vectors in the summation above can be any of the reciprocal lattice vectors $\mathbf{G}_{\mathbf{m}}$ with the coefficients $m_i \in \{-1, 0, 1\}$ (see Eq.(1.5)), i.e., the lowest order Fourier modes. Consequently, r may exceed the dimensionality d of real space.

A general normalised vector field loses its normalisation after the truncation of higher-order modes, however, a reconstruction of the normalisation as $\hat{\mathbf{n}}(\mathbf{x}) = \mathbf{n}(\mathbf{x})/\|\mathbf{n}(\mathbf{x})\|$ still gives an excellent approximation to the original vector field albeit for the price of re-introducing higher order modes.

The other way around, we can construct magnetic textures, even aperiodic ones, by selecting arbitrary q -vectors from possibly different, and even outright incommensurate reciprocal lattices before assembling them in a linear superposition. This encompasses the Fourier truncation of lattice-periodic textures as a special case but contains more general textures, such as aperiodic Moiré patterns [Shi+21]. We parameterise these superpositions as

Multi-q textures

$$\mathbf{n}(\mathbf{x}) = \sum_{i=1}^r (\psi_i^c \hat{\mathbf{e}}_i^c \cos(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i) + \psi_i^s \hat{\mathbf{e}}_i^s \sin(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i)) + m \hat{\mathbf{e}}^0, \quad (1.7)$$

which is the equivalent trigonometric formulation of Eq. (1.6) and is more commonly used in the literature on multi- q states, e.g., [Shi+21; Shi+22; NK19; Fre+13]. Here, $\psi_i^c, \psi_i^s \in \mathbb{R}$ are the real amplitudes of the cosinusoidal and sinusoidal waves with wave vectors $\mathbf{q}_i$, respectively, $\hat{\mathbf{e}}_i^c$ and $\hat{\mathbf{e}}_i^s$ are real unit vectors, and $\hat{\mathbf{e}}^0$ is another independent unit vector for the direction of the constant net magnetisation of magnitude m . In case of a normalised texture $\hat{\mathbf{n}}(\mathbf{x}) = \mathbf{n}(\mathbf{x})/\|\mathbf{n}(\mathbf{x})\|$, m no longer determines the actual net magnetisation but is still a related parameter. For instance, in its limit $\lim_{m \rightarrow \infty} \hat{\mathbf{n}}(\mathbf{x}) = \hat{\mathbf{e}}^0$ we obtain the collinear ferromagnet.

At first glance, a texture which is constructed from r spin waves depends on r corresponding phases $\omega_i : \mathbb{R}^d \rightarrow S^1$. However, these phases are in general not independent of one another, as they are determined by the choice of the q -vectors by

Phase torus

$$\omega_i(\mathbf{x}) = (\mathbf{q}_i \cdot \mathbf{x} + \varphi_i) \mod 2\pi \in S^1. \quad (1.8)$$

The phase values which are assumed at the same position in real space lie in the image of the map $\omega : \mathbb{R}^d \rightarrow T^r$. Only if we have r $\mathbb{R}$ -linear independent q -vectors we reach every point in this phase space, which is only possible for $r \leq d$.

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We can also consider the scenario where a selection of q -vectors is linearly dependent: The dimension of the image $\omega(\mathbb{R}^d)$ is then not immediately apparent. Let $\tilde{r}$ denote the dimension of the linear subspace of $\mathbb{R}^d$ spanned by the r wave vectors. In case that the $\mathbb{R}$ -linear dependent wave vectors are also linear dependent over $\mathbb{Q}$, there exists a rational relation between the phases and the texture is periodic. Then, the image $\omega(\mathbb{R}^d) \subset T^r$ is of dimension $\tilde{r}$ and isomorphic to $T^{\tilde{r}}$. Otherwise, the image is dense in a submanifold of T^r with dimension equivalent to the number of rationally independent wave vectors. In that case, some q -vectors are from incommensurate lattices and the texture is inevitably aperiodic. A simple example in one dimension is given by two phases with an irrational slope ratio, such that the image of the real line wraps densely around T^2 .

Coming back to the case of periodic textures, there can be at most d $\mathbb{Q}$ -linear independent q -vectors and one has fixed rational relations between the initial phases. As the texture consists of a finite sum of smooth functions over S^1 , it is an element of $C^\infty(T^{\tilde{r}}, \mathbb{R}^3)$, the space of smooth maps from the $\tilde{r}$ -torus to $\mathbb{R}^3$. Whenever $\|\mathbf{n}(\mathbf{x})\| > 0$ for all $\mathbf{x} \in \mathbb{R}^d$, the normalisation procedure will lead to a smooth field of unit vectors $\hat{\mathbf{n}}$, and thus $C^\infty(T^{\tilde{r}}, S^2)$. If we set $\mathbf{x} = 0$, we can conveniently parameterise T^r with the corresponding φ_i and we can restrict the image to $T^{\tilde{r}}$ by using the phase relations. In the case of $d = 2$ with 2 independent q -vectors, we can assign a winding number to every texture unit cell by

$$\deg \hat{\mathbf{n}} = \frac{1}{4\pi} \int_{T^2} d\varphi \hat{\mathbf{n}} \cdot (\partial_{\varphi_1} \hat{\mathbf{n}} \times \partial_{\varphi_2} \hat{\mathbf{n}}) \in \mathbb{Z}. \quad (1.9)$$

1.2.3.1. Multi- q Systems coupled to Lattice Electrons

Electronic properties of multi- q magnets are often studied from the perspective of an electronic tight-binding Hamiltonian which is hosted by its own respective Bravais lattice [HEN15; Göb+17b]. This Bravais lattice can generally be different from the Bravais lattice of the multi- q texture, and non-trivial band structure effects can result from the interference of these two patterns. In the following, we express the wave vectors in terms of the atomic lattice vectors and obtain a simple description for the phases at each lattice site in terms of the pitches of the spin waves. This section is adapted from [Pra+24, Chap. 2.4].

Atomic lattice

For the d -dimensional atomic Bravais lattice we denote the lattice vectors $\{\mathbf{a}_i\}$ and the reciprocal lattice vectors $\{\mathbf{b}_j\}$, satisfying $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$. The real space position of the lattice site with integer label $\mathbf{m} \in \mathbb{Z}^d$ and the r wave vectors $\{\mathbf{q}_i\}$ of the multi- q texture can now be decomposed into

$$\mathbf{x}_{\mathbf{m}} = \sum_j^d m_j \mathbf{a}_j \quad \text{and} \quad \mathbf{q}_i = \sum_{j=1}^d \theta_{ij} \mathbf{b}_j,$$

with the $(r \times d)$ -dimensional matrix θ of pitch parameters.

This implies for the phases at position $\mathbf{x}_m$

$$\mathbf{x}_m \cdot \mathbf{q}_i = \sum_{kl} m_k \theta_{il} \mathbf{a}_k \cdot \mathbf{b}_l = 2\pi \sum_k m_k \theta_{ik} \equiv 2\pi \mathbf{m} \cdot \boldsymbol{\theta}_i,$$

where $\boldsymbol{\theta}_i \in \mathbb{R}^d$ with $(\boldsymbol{\theta}_i)_k = \theta_{ik}$.

The pitch θ_{ij} indicates by how much the phase $\omega_i(\mathbf{x}_m)$ of wave i changes if one moves one site along $\mathbf{a}_j$. From here on, we denote the phase values modulo 2π by $[x] = x \bmod 2\pi \in [0, 2\pi)$ for all $x \in \mathbb{R}$. Then, the phases can be written as

Phases

$$\omega_i(\mathbf{x}_m) = [\mathbf{x}_m \cdot \mathbf{q}_i + \varphi_i] = [2\pi \mathbf{m} \cdot \boldsymbol{\theta}_i + \varphi_i],$$

where φ_i is the phase of wave i at the origin $\mathbf{x}_0 = 0$ [Lux+24]. In matrix notation, one can give a more compact description in terms of

$$\boldsymbol{\omega}(\mathbf{x}_m) = [2\pi \boldsymbol{\theta} \mathbf{m} + \boldsymbol{\varphi}].$$

The natural action τ of the lattice translation group $\mathbb{Z}^d$ on the waves' phases is defined by

Lattice translations

$$\boldsymbol{\omega}(\mathbf{x}_{m+\mathbf{l}}) = [2\pi \boldsymbol{\theta}(\mathbf{m} + \mathbf{l}) + \boldsymbol{\varphi}] = [\boldsymbol{\omega}(\mathbf{x}_m) + 2\pi \boldsymbol{\theta} \mathbf{l}] =: \tau_{\mathbf{l}} \boldsymbol{\omega}(\mathbf{x}_m) \quad (1.10)$$

with $\mathbf{l} \in \mathbb{Z}$. With it we can relate phases at any site back to the phases at the origin:

$$\boldsymbol{\omega}(\mathbf{x}_m) = \tau_{\mathbf{m}} \boldsymbol{\omega}(\mathbf{x}_0) = \tau_{\mathbf{m}} \boldsymbol{\varphi}. \quad (1.11)$$

We want to consider the entire orbit under lattice translations

$$\mathbb{Z}^d \boldsymbol{\varphi} = \{\tau_{\mathbf{m}} \boldsymbol{\varphi} \mid \mathbf{m} \in \mathbb{Z}^d\} \subset \boldsymbol{\omega}(\mathbb{R}^d), \quad (1.12)$$

and refer to the closure of $\mathbb{Z}^d \boldsymbol{\varphi}$ in $\boldsymbol{\omega}(\mathbb{R}^d)$ as the hull Ω of the magnetic pattern. If the translation action is ergodic on $\boldsymbol{\omega}(\mathbb{R}^d)$, then $\mathbb{Z}^d \boldsymbol{\varphi}$ will form a dense subset of $\boldsymbol{\omega}(\mathbb{R}^d)$ whose closure is $\Omega = \boldsymbol{\omega}(\mathbb{R}^d)$ for all $\boldsymbol{\varphi} \in \boldsymbol{\omega}(\mathbb{R}^d)$.

1.2.3.2. 2q Spin Waves

The first and simplest texture we want to consider is a $2q$ texture in one dimension constructed by superimposing two helical spin spirals. This could be realised physically via proximity coupling of a one-dimensional electronic system to two independent atomic spin spirals [Lux+24]. Here, we define the texture and visualise the phase space and the interference pattern.

For two q -vectors ($r = 2$) on a one-dimensional lattice ($d = 1$) with lattice vector $\mathbf{a} = \hat{\mathbf{e}}_x$ and reciprocal lattice vector $\mathbf{b} = 2\pi \hat{\mathbf{e}}_x$ the decompositions is given by $\mathbf{q}_i = 2\pi \theta_i \hat{\mathbf{e}}_x$. With them, we parameterise the texture according to Eq. (1.7) for the case of helical waves, i.e. $\hat{\mathbf{e}}_i^c = \hat{\mathbf{e}}_z$ and $\hat{\mathbf{e}}_i^s = -\hat{\mathbf{e}}_y$ orthogonal to the propagation direction $\hat{\mathbf{e}}_x$, building a right-handed basis of $\mathbb{R}^3$. We further set the amplitudes to equal length 1, and the magnetisation parameter $m = 0$.

1. Magnetic Textures

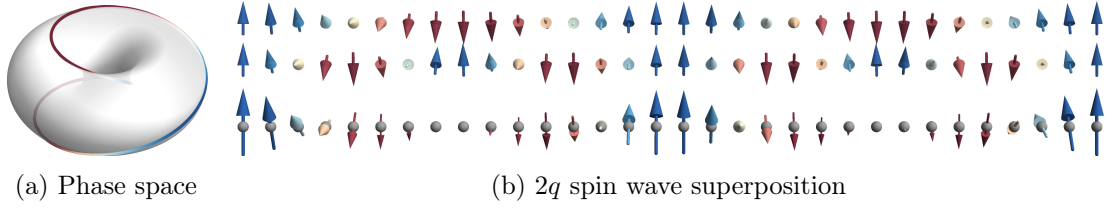


Figure 1.2.: **Spin wave** Superposition of two helical spin waves on 32 sites for $\theta_2 = 2\theta_1$ with $\theta_1 = \frac{2}{31}$ and $\varphi_1 = \varphi_2 = 0$. This figure was adapted from [Lux+24, Fig. 1].

Then, the explicit expression for the texture is given by

$$\mathbf{n}(x) = \sum_{i=1}^2 \hat{\mathbf{e}}_z \cos(2\pi\theta_i x + \varphi_i) - \hat{\mathbf{e}}_y \sin(2\pi\theta_i x + \varphi_i) \quad (1.13)$$

$$= \sum_{i=1}^2 \mathbf{n}_i e^{i(2\pi\theta_i x + \varphi_i)} + \mathbf{n}_i^* e^{-i(2\pi\theta_i x + \varphi_i)}, \quad (1.14)$$

with $\mathbf{n}_i = \frac{1}{2}(\hat{\mathbf{e}}_z + i\hat{\mathbf{e}}_y)$. If we want a periodic texture, we choose a rational ratio $\theta_2 = c\theta_1$, and for ergodicity we choose the q -vectors incommensurate with the underlying lattice $\theta_1 \in \mathbb{R} \setminus \mathbb{Q}$. Fig. 1.2(a) shows the image of $\omega(\mathbb{R})$ in T^2 for $c = 2$ and Fig. 1.2(b) depicts such helical waves and their superposition in the commensurate case.

1.2.3.3. 3q Skyrmion and Vortex Lattices

The focus of this dissertation is on the skyrmionic $3q$ -state, supported by a triangular lattice. Here, we define first the lattices and the q -vectors and discuss the phase space. Then we construct three $3q$ -textures with different properties. Two of them are skyrmion lattices constructed as the normalised superposition of helical and sinusoidal spin waves, respectively. For them, we compute the winding number and display its dependence on the phase relation and net magnetisation parameter. Lastly, we construct a vortex lattice as the unnormalised superposition of the spin density waves, for which a winding number is not defined. This section is partially adapted from [Pra+24, Chap. 2.5].

q-vectors All $3q$ spin textures we consider are constructed as superposition of $r = 3$ spin waves in two-dimensional real space ($d = 2$) with wave vectors of equal length q that sum up to zero (120° apart from each other):

$$\mathbf{q}_1 = \begin{pmatrix} \frac{\sqrt{3}q}{2} \\ -\frac{q}{2} \\ 0 \end{pmatrix}, \quad \mathbf{q}_2 = \begin{pmatrix} 0 \\ q \\ 0 \end{pmatrix}, \quad \text{and} \quad \mathbf{q}_3 = \begin{pmatrix} -\frac{\sqrt{3}q}{2} \\ -\frac{q}{2} \\ 0 \end{pmatrix}. \quad (1.15)$$

Due to their linear dependence, we have a fixed relation between the corresponding phases ω_i . The relation between the phases at the origin offers thus one additional degree of freedom: Their sum $\varphi_1 + \varphi_2 + \varphi_3 = \varphi$, which we refer to as phase shift. All other changes preserving this sum can be compensated by translations in real space.

1.2. Non-collinear Magnetism

For the texture hosting atomic lattice, we consider the two-dimensional triangular lattice with real- and reciprocal space lattice vectors:

*Triangular
lattice*

$$\mathbf{a}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \\ 0 \end{pmatrix}, \quad \mathbf{b}_1 = 2\pi \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{b}_2 = 2\pi \begin{pmatrix} 0 \\ \frac{2}{\sqrt{3}} \\ 0 \end{pmatrix}. \quad (1.16)$$

They satisfy $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$ as required. Expanding the q -vectors in the reciprocal lattice vector basis, we find

$$\mathbf{q}_1 = \frac{q\sqrt{3}}{4\pi}\mathbf{b}_1, \quad \mathbf{q}_2 = \frac{q\sqrt{3}}{4\pi}\mathbf{b}_2, \quad \text{and} \quad \mathbf{q}_3 = \frac{q\sqrt{3}}{4\pi}(-\mathbf{b}_1 - \mathbf{b}_2). \quad (1.17)$$

Let $\vartheta = \frac{q\sqrt{3}}{4\pi}$, then the pitch coefficient matrix θ is given by:

$$\theta = \vartheta \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{pmatrix}. \quad (1.18)$$

The third phase $\omega_3(\mathbf{x}_m) = [\mathbf{x}_m \cdot \mathbf{q}_3 + \varphi_3]$ is artificial in the sense that it can be expressed in terms of the other two phases $\omega_3(\mathbf{x}_m) = [\varphi - \omega_1(\mathbf{x}_m) - \omega_2(\mathbf{x}_m)]$. It can be eliminated from the whole description of the texture from the start. Then it is $r = 2$ and the minimal θ -matrix is given by $\theta = \vartheta \mathbb{1}_2$. However, the construction of the spin textures presented below is much simplified with the superfluous, yet helpful degree of freedom.

Important topological properties of the electronic system coupled to the magnetic texture can be discovered when ϑ takes irrational values. In this case, the map

*Incommensurate
textures*

$$\mathbb{Z}^2 \ni (m_1, m_2) \mapsto ([2\pi\vartheta m_1 + \varphi_1], [2\pi\vartheta m_2 + \varphi_2]) = (\omega_1, \omega_2) \in T^2$$

samples the torus T^2 densely. We find the lattice site labels m_1 and m_2 uniquely associated with either ω_1 or ω_2 . Therefore, we can reduce the claim above to the following proposition: The set $\{[2\pi\vartheta m + \varphi] \mid m \in \mathbb{Z}\}$ is dense in $[0, 2\pi)$ for arbitrary $\varphi \in \mathbb{R}$ and $\vartheta \in \mathbb{R} \setminus \mathbb{Q}$. A proof can be found in [Wey16] and [KH95, Prop. 1.3.3.].

For the two-dimensional lattices just discussed, the hull of the magnetic pattern is then given by

$$\overline{\{([2\pi\vartheta m_1 + \varphi_1, 2\pi\vartheta m_2 + \varphi_2]) \mid (m_1, m_2) \in \mathbb{Z}^2\}} \cong T^2.$$

Consequently, on the infinite discrete lattice all possible local realisations of the magnetic texture are densely approximated when ϑ is irrational.

1. Magnetic Textures

Helical skyrmion lattice The most common type of $3q$ skyrmion lattice is constructed as the normalised superposition of three helical spin waves. This part is partially adapted from [Pra+24, Chap. 2.5].

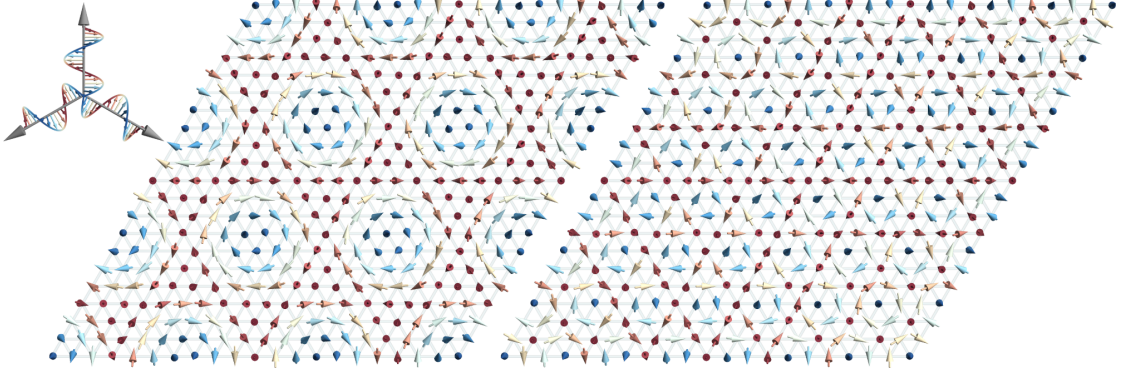


Figure 1.3.: **Helical skyrmion lattice.** Normalised superposition of three helical spin waves with wave vectors summing up to zero, as depicted in the upper left corner, for $\varphi = 0$ and $m = 0$. The winding number in each unit cell is $\deg \hat{\mathbf{n}} = 1$. We present two realisations on a two-dimensional triangular lattice with 21×21 sites for $\vartheta = \frac{3}{20}$ (left) and $\vartheta = \frac{7}{20}$ (right). This figure was adapted from [Pra+24, Fig. 1].

For the parameterisation, we set the amplitudes to $1/\sqrt{3}$ and the unit vectors in such a way that they create helical waves, i.e., $\hat{\mathbf{e}}_i^c$ directs out of the plane in the z -direction and $\hat{\mathbf{e}}_i^s$ is orthogonal to $\mathbf{q}_i$ and $\hat{\mathbf{e}}_i^c$, such that they form a right-handed basis of $\mathbb{R}^3$. The resulting vector field is then given by the normalisation $\hat{\mathbf{n}}$ of their superposition $\mathbf{n}$ [Shi+22]:

$$\mathbf{n}(\mathbf{x}) = \sum_{i=1}^3 \left(\frac{1}{\sqrt{3}} \hat{\mathbf{e}}_z \cos(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i) + \frac{1}{\sqrt{3}} (\hat{\mathbf{q}}_i \times \hat{\mathbf{e}}_z) \sin(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i) \right) + m \hat{\mathbf{e}}_z \quad (1.19)$$

$$= \sum_{i=1}^3 \left(\mathbf{n}_i e^{i(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i)} + \mathbf{n}_i^* e^{-i(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i)} \right) + m \hat{\mathbf{e}}_z, \quad (1.20)$$

with $\mathbf{n}_i = \frac{1}{2\sqrt{3}}(\hat{\mathbf{e}}_z - i\hat{\mathbf{q}}_i \times \hat{\mathbf{e}}_z)$. An example of such a skyrmion lattice for two rational ϑ is displayed in Fig. 1.3.

The winding number of $\hat{\mathbf{n}}$ computed as in Eq. (1.9) is the first important order parameter characterising the texture. In Fig. 1.4(a), we show how $\deg \hat{\mathbf{n}}$ depends on m and φ , reproducing the result of [Shi+22, Fig. 6]. Analytic expressions for the positions of destructive interference, which are the phase boundaries, were already determined in [Shi+22, Eq. (29)-(32)].

Another relevant order parameter for the interpretation of the electronic phase diagrams later on is the net magnetisation

$$\langle \hat{\mathbf{n}} \rangle = \lim_{|V| \rightarrow \infty} \frac{1}{|V|} \int_V d^2\mathbf{x} \, \hat{\mathbf{n}}(\omega(\mathbf{x})) = \frac{1}{|T^2|} \int_{T^2} d^2\varphi \, \hat{\mathbf{n}}(\varphi). \quad (1.21)$$

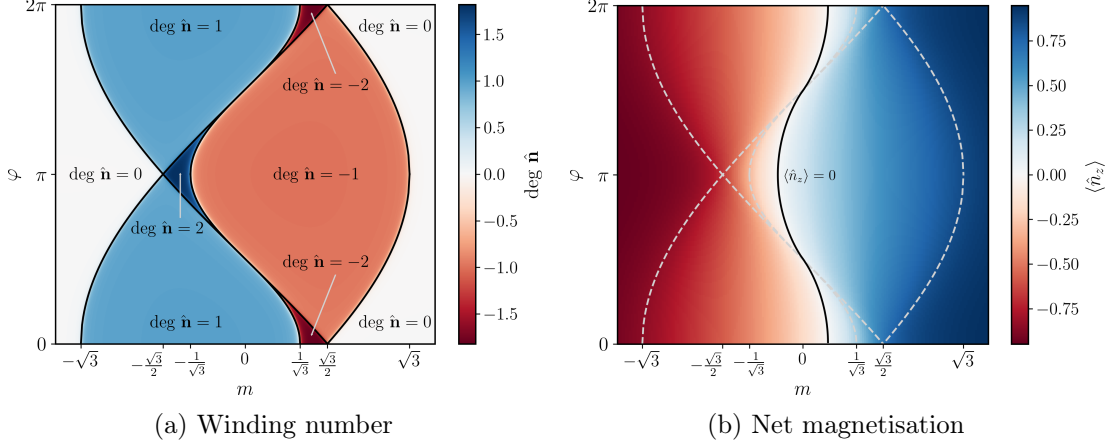


Figure 1.4.: Real space phase diagram. The magnetic texture of the helical $3q$ skyrmion lattice depends on the phase shift φ and net magnetisation parameter m . (a) displays the winding number $\deg \hat{\mathbf{n}}$ with phase boundaries (solid black lines) determined by the condition $\mathbf{n}(\varphi) = 0$ for some $\varphi \in T^2$ (cf. [Shi+22, Fig. 6]). (b) displays the net magnetisation $\langle \hat{n}_z \rangle$ with boundary (solid black line) determined by the condition $\langle \hat{n}_z \rangle = 0$. This figure was adapted from [Pra+24, Fig. 2].

One finds $\langle \hat{n}_x \rangle = \langle \hat{n}_y \rangle = 0$, while $\langle \hat{n}_z \rangle$ shows a non-trivial dependence on m and φ as demonstrated by Fig. 1.4(b). When $\langle \hat{\mathbf{n}} \rangle = 0$, the magnetic texture is time-reversal invariant modulo a proper Euclidean symmetry operation. Since this imposes additional constraints on the associated electronic system, we mark the corresponding parameter points as a solid black line in Fig. 1.4(b).

Sinusoidal skyrmion lattice A second skyrmion lattice can be constructed as normalised superposition of three sinusoidal spin waves and differs from the helical skyrmion lattice in its topological phase diagram [Shi+22; OHM17].

For the construction we only include the cosine part of the waves by setting the amplitudes to $\psi_i^c = 1/\sqrt{3}$ and $\psi_i^s = 0$. The unit vector $\hat{\mathbf{e}}_i^c$ is set orthogonal to $\mathbf{q}_i$ and can otherwise be chosen freely. Since the phase diagram is up to a sign independent of the choice of the angle of the sinusoidal plane, we follow [Shi+22] with their parametrisation to emphasise this freedom:

$$\hat{\mathbf{e}}_1^c = \begin{pmatrix} (-1)^{\Gamma+1} \sin \alpha \\ 0 \\ \cos \alpha \end{pmatrix}, \quad \hat{\mathbf{e}}_2^c = \begin{pmatrix} (-1)^{\Gamma} \frac{1}{2} \sin \alpha \\ \frac{\sqrt{3}}{2} \sin \alpha \\ \cos \alpha \end{pmatrix}, \quad \hat{\mathbf{e}}_3^c = \begin{pmatrix} (-1)^{\Gamma+1} \frac{1}{2} \sin \alpha \\ -\frac{\sqrt{3}}{2} \sin \alpha \\ \cos \alpha \end{pmatrix}, \quad (1.22)$$

where $\Gamma \in \{0, 1\}$ describes the chirality of the texture and affects the sign of the winding number, while $\alpha \in (0, \frac{\pi}{2})$ describes the precise angle. Γ affects also the symmetry: The texture for $\Gamma = 0$ has threefold rotational symmetry, which is not the case for $\Gamma = 1$. $\hat{\mathbf{e}}_2^c$ and $\hat{\mathbf{e}}_3^c$ can be obtained from $\hat{\mathbf{e}}_1^c$ by a $(-1)^{\Gamma} \frac{2\pi}{3}$ and $(-1)^{\Gamma} \frac{4\pi}{3}$ rotation around the z -axis, respectively. The resulting vector field is finally given by the normalisation $\hat{\mathbf{n}}$ of the superposition $\mathbf{n}$ [Shi+22]:

1. Magnetic Textures

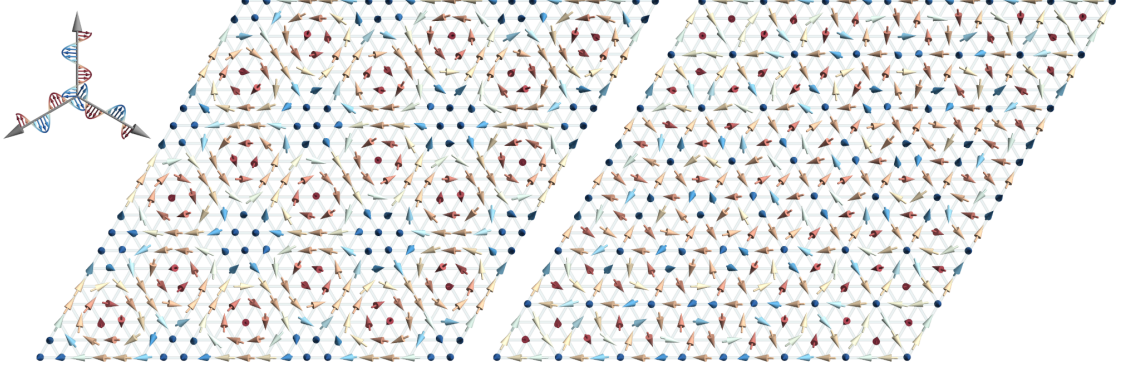


Figure 1.5.: **Sinusoidal skyrmion lattice.** Normalised superposition of three sinusoidal spin waves with wave vectors summing up to zero, as depicted in the upper left corner, and sinusoidal plane given by $\alpha = \arccos\left(\frac{1}{\sqrt{3}}\right)$ and $\Gamma = 0$ for $\varphi = 0$ and $m = 0$. The winding number in each unit cell is $\deg \hat{\mathbf{n}} = -2$. We present two realisations on a two-dimensional triangular lattice with 21×21 sites for $\vartheta = \frac{3}{20}$ (left) and $\vartheta = \frac{7}{20}$ (right).

$$\mathbf{n}(\mathbf{x}) = \sum_{i=1}^3 \frac{1}{\sqrt{3}} \hat{\mathbf{e}}_i^c \cos(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i) + m \hat{\mathbf{e}}_z \quad (1.23)$$

$$= \sum_{i=1}^3 \left(\mathbf{n}_i e^{i(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i)} + \mathbf{n}_i e^{-i(\mathbf{q}_i \cdot \mathbf{x} + \varphi_i)} \right) + m \hat{\mathbf{e}}_z, \quad (1.24)$$

with $\mathbf{n}_i = \frac{1}{2\sqrt{3}} \hat{\mathbf{e}}_i^c$. An example for such a skyrmion lattice is given in Fig. 1.5, commensurate for two different rational ϑ .

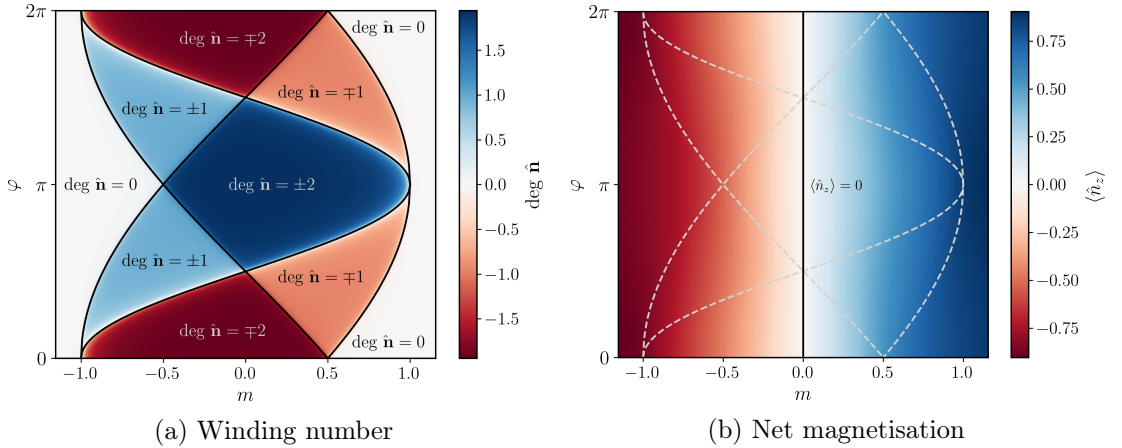


Figure 1.6.: **Real space phase diagram.** The magnetic texture of the sinusoidal $3q$ skyrmion lattice depends on the phase shift φ and net magnetisation parameter m . The diagrams were evaluated for $\Gamma = 0$ and $\alpha = \arccos\left(\frac{1}{\sqrt{3}}\right)$. (a) displays the winding number $\deg \hat{\mathbf{n}}$ with phase boundaries (solid black lines) determined by the condition $\mathbf{n}(\boldsymbol{\varphi}) = 0$ for some $\boldsymbol{\varphi} \in T^2$ (cf. [Shi+22, Fig. 10]). (b) displays the net magnetisation $\langle \hat{n}_z \rangle$ with boundary (solid black line) determined by the condition $\langle \hat{n}_z \rangle = 0$.

As for the helical skyrmion lattice the winding number $\deg \hat{\mathbf{n}}$ in each unit cell of this texture depends on the phase shift φ and the magnetisation parameter m . The phase diagram differs however from the one in the helical case: For $m = 0$ the winding number is ± 2 instead of ± 1 and some phase borders run differently. The choice of the chirality via Γ changes the overall sign and the choice of α only rescales the x -axis via $\tilde{m} = \frac{m}{\sqrt{3} \cos \alpha}$. In Fig. 1.6(a) we compute the diagram for $\Gamma = 0$ and $\alpha = \arccos\left(\frac{1}{\sqrt{3}}\right)$, and thus $\tilde{m} = m$, reproducing the result of [Shi+22, Fig. 10]. Analytic expressions for the position of the destructive interference were determined in [Shi+22, Eq. (43)-(45)]. For the net magnetisation we find $\langle \hat{n}_x \rangle = \langle \hat{n}_y \rangle = 0$, while $\langle \hat{n}_z \rangle$ depends on m .

Vortex lattice The last $3q$ -texture we want to compare is constructed as a superposition of three longitudinal spin density waves. Since we do not consider the normalisation, a winding number is not defined. The vector field is in-plane and vanishes at the centre of the vortices.

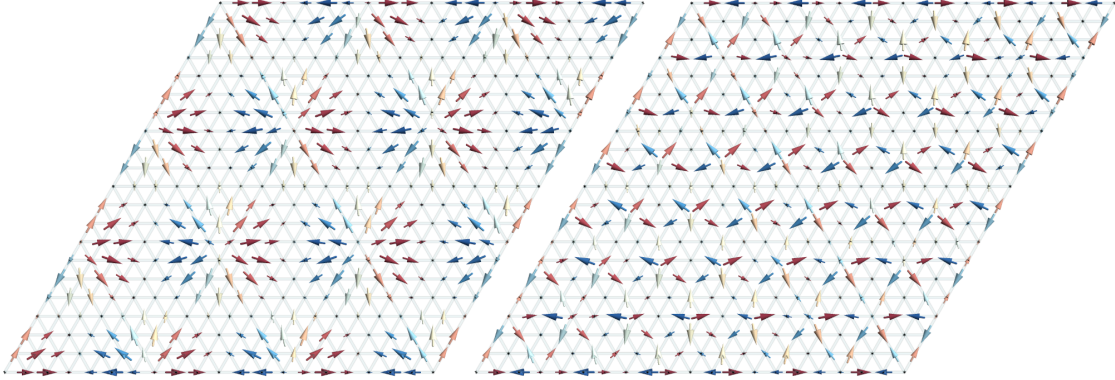


Figure 1.7.: **Vortex lattice.** Superposition of three longitudinal spin density waves with wave vectors summing up to zero. We present two realisations on a two-dimensional triangular lattice with 21×21 sites for $\vartheta = \frac{3}{20}$ (left) and $\vartheta = \frac{7}{20}$ (right).

Instead of the normalisation, we set the amplitude such that the maximum size of the vectors is 1. We also only consider the sinus component with unit vector parallel to $\mathbf{q}_i$ to create longitudinal waves. Since we cannot define a winding number, we set $\varphi_1 = \varphi_2 = \varphi_3 = 0$ and $m = 0$. The resulting vector field has the following explicit form

$$\mathbf{n}(\mathbf{x}) = \sum_{i=1}^3 \frac{1}{3} \hat{\mathbf{q}}_i \sin(\mathbf{q}_i \cdot \mathbf{x}) = \sum_{i=1}^3 \frac{1}{6} (\hat{\mathbf{q}}_i i e^{i\mathbf{q}_i \cdot \mathbf{x}} - \hat{\mathbf{q}}_i i e^{-i\mathbf{q}_i \cdot \mathbf{x}}). \quad (1.25)$$

A commensurate realisation on the triangular lattice is displayed in Fig. 1.7 for two different values of ϑ .

1.3. Winding Number

The winding number, as used in this work, is a property of two-dimensional spin textures that requires an energy barrier to be overcome in order to change.

The concept originates from topology and is applicable to smooth and normalised three-dimensional vector fields on a two-dimensional plane with matching values at its boundary. The unit vector at each point on the plane directs to a point on a two-dimensional sphere, the continuity of the vector field ensures that the mapped out area on the sphere is connected, and the boundary condition requires that the area is closed. The winding number then indicates how many times this area covers or 'winds around' the surface of the sphere. As long as the vector field is varied continuously, the winding number cannot change, as this only results in a shifting and stretching of the area on the sphere. Only discontinuous change, where the area instantaneously (un-)folds through the centre of the sphere, can affect the winding number.

Coming back to the spin texture, which we consider in the continuous field approximation of micromagnetics, such a discontinuous change coincides with a spin flip, which requires the spin on one site to overcome the energy minimised coupling to its neighbours. The outlined concept of the winding number is a special case of the degree of a continuous mapping, which was first defined by Brouwer [Bro11]. It is further related to the total curvature of two-dimensional submanifolds and Chern numbers in two-band systems.

Section Content

We begin this section by giving a general definition of the mapping degree. Next, we illustrate the winding number of the three-dimensional vector field defined by spherical coordinates and draw its connection to the curvature of the sphere. At this point, we also elucidate the relation of the winding number to the Chern number of a simple vector bundle. Using this newly gained intuition, we want to shed some first light on the ideas of non-commutative geometry. Eventually, we look into winding number transitions and make the transitions continuous by applying a regularisation. We observe the change of the winding number expressions explicitly for the case of a single skyrmion.

1.3.1. Degree of Continuous Mapping

The degree of a continuous map between two compact oriented manifolds of the same dimension indicates how often the map wraps the domain manifold around the range manifold. It is therefore an integer number with its sign depending on the orientations, and it remains unaffected by continuous deformations of the map, which makes it a so-called homotopy invariant. In the case that the range manifold is a sphere, the Hopf theorem states, that the mapping degree is the only homotopy invariant of these maps, i.e., if two such maps have the same degree, they are homotopic. This isomorphism between the homotopy classes of maps to the sphere and $\mathbb{Z}$ provides a means of topological classification.

In the following, we define the homotopy of maps in Def. 1.1 and the degree of a continuous map in Def. 1.2, state the Hopf theorem Thm. 1.1, and connect the general form of the mapping degree to the familiar expression for the winding number of a smooth, normalised vector field on the two-dimensional sphere or two-dimensional torus.

We start with the definition of homotopy, which formalises continuous deformations of maps [Dol95, Ch. I Def. 3.3]: Homotopy

Definition 1.1 (Homotopy of maps). Two continuous maps f, g between topological spaces X, Y are called *homotopic*, if there exists a continuous map $H : [0, 1] \times X \rightarrow Y$ such that $H(0, x) = f(x)$ and $H(1, x) = g(x)$. H is called *homotopy*.

Thus, a continuous deformation between two maps means that each intermediate map $H(t, \cdot)$ for $t \in (0, 1)$ is continuous. Being homotopic is an equivalence relation [Dol95, Ch. I Prop. 3.4], and we denote the quotient space of the equivalence classes $[f]$ for functions $f : X \rightarrow Y$ as $[X, Y]$. The most well-studied examples of such quotients are the so-called homotopy groups of the sphere $\pi_n(S^k) := [S^n, S^k]$.

The general definition of the mapping degree requires prior knowledge on homology theory, which can be found in text books such as [Dol95, Ch. III]. In this remark, we only want to give an informal intuition for the concept of the singular homology of topological spaces: If one considers a topological space X , then the k -th homology group $H_k(X; \mathbb{Z})$ is an Abelian group of equivalence classes represented by so-called cycles. The addition of the group is only formal and takes integer coefficients. In simple cases, the cycles can be thought of as embedded closed k -dimensional shapes. The equivalence classes contain all those k -dimensional shapes that only differ by shapes that are the boundary of a $(k + 1)$ -dimensional shape embedded in X . This way $H_k(X; \mathbb{Z})$ detects the $(k + 1)$ -dimensional holes in X with a k -dimensional boundary, since those differentiate the classes. Homology

For example, every circle S^1 embedded in the sphere S^2 is a boundary of a disk D^1 also embedded in the sphere. Thus, the first homology group of the 2-sphere is $H_1(S^2; \mathbb{Z}) = \{0\}$ indicating the absence of 2-dimensional holes. On the contrary, for the torus $T^2 = S^1 \times S^1$ there are two distinct ways to embed a circle, such that they are not a boundary of any embedded disk. Therefore, it is $H_1(T^2; \mathbb{Z}) = \mathbb{Z} \times \mathbb{Z}$ detecting the two 2-dimensional holes of the 2-torus.

A hole with 0-dimensional boundary can be thought of as a gap between path-connected components. The zeroth homology group $H_0(X; \mathbb{Z})$ is therefore the free Abelian group with one generator for each component. If X is a connected manifold it is path-connected and, thus, has only a single component, which results in $H_0(X; \mathbb{Z}) \cong \mathbb{Z}$. If X is a closed, connected, oriented n -dimensional manifold, then the top homology group $H_n(X; \mathbb{Z})$ is $\mathbb{Z}$ as well. Loosely, since X is closed, connected and oriented, the only hole with an n -dimensional boundary is the hole inside X and the choice of orientation implies the choice of a generator of this group. This generator is the so-called fundamental class, which we denote by $[X]$.

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Mapping degree

With these preliminary considerations, we can define the degree of a continuous map [Dol95, Ch. VIII Def. 4.2]: Let X, Y be closed, connected, oriented n -dimensional manifolds. Then, a continuous map $f : X \rightarrow Y$ induces a homomorphism f_* between the homology groups $H_n(X; \mathbb{Z})$ and $H_n(Y; \mathbb{Z})$, which maps the generator $[X]$ to an integer multiple of the generator $[Y]$. This factor coincides with how often X wraps around Y and is therefore the degree of f .

Definition 1.2 (Degree of a continuous map). Let X, Y be closed, connected, oriented n -dimensional manifolds. Let $[X], [Y]$ denote a generator of $H_n(X; \mathbb{Z}), H_n(Y; \mathbb{Z})$, then the degree of a continuous map $f : X \rightarrow Y$ is given by

$$f_*[X] = \deg f [Y].$$

By definition, it follows that the degree is a homotopy invariant, as homotopic maps induce the same homomorphisms of homology groups. In the case of smooth manifolds, any continuous map between them is homotopic to a smooth map, and we can derive an explicit coordinate-free expression:

Let $f : X \rightarrow Y$ be a smooth map between closed, connected, orientable, smooth manifolds and ω be an n -form on Y . We have

$$\langle f_*[X], [\omega] \rangle = \langle [X], f^*[\omega] \rangle \quad (1.26)$$

$$\Rightarrow \deg f \int_Y \omega = \int_X f^* \omega. \quad (1.27)$$

Hopf theorem

The homotopy invariance of the degree implies, that two homotopic maps have the same degree, but in general two maps with the same degree do not need to be homotopic. This is, however, the case with a suitable choice of the range manifold Y . For continuous maps to the n -sphere, the degree is the only homotopy invariant, which makes these maps easy to classify as given by the Hopf theorem [MW65, p. 51]:

Theorem 1.1 (Hopf theorem). *Let X be an n -dimensional closed, connected, oriented manifold, S^n the n -sphere, and $f, g : X \rightarrow S^n$ continuous maps. Then $\deg f = \deg g$ if and only if f and g are homotopic.*

Smooth vector field

For $n = 2$ and $Y = S^2 \subset \mathbb{R}^3$, Eq. (1.27) takes the familiar form of the winding number of a normalised smooth vector field: Let $\mathbf{n} : X \rightarrow S^2 \subset \mathbb{R}^3$ be a smooth three-dimensional vector field on the two-dimensional closed, connected, oriented, smooth manifold X . If we denote the volume form of S^2 by ω_{S^2} , then we have $\int_{S^2} \omega_{S^2} = \text{vol}(S^2) = 4\pi$ on the left hand-side of Eq. (1.27) and $\mathbf{n}^* \omega_{S^2} = \frac{1}{2} \epsilon_{ijk} n_i dn_j \wedge dn_k$ on the right hand-side, and thus in local coordinates

$$\deg f = \frac{1}{8\pi} \int_X \epsilon_{ijk} n_i dn_j \wedge dn_k \quad (1.28)$$

$$= \frac{1}{4\pi} \int_X d\mathbf{x} \cdot (\partial_{x_1} \mathbf{n} \times \partial_{x_2} \mathbf{n}). \quad (1.29)$$

The most important domains X for our purpose are the 2-sphere S^2 and the 2-torus T^2 . *Torus and sphere* In both cases $[T^2, S^2] \cong \mathbb{Z}$ and $[S^2, S^2] \cong \mathbb{Z}$ have a group structure. Both domains occur for spin textures with matching values at their boundaries in the following way: We model a spin texture as a normalised smooth three-dimensional vector field on a two-dimensional plane and identify the points on the boundary at which the vectors match up. This way, we obtain a closed two-dimensional manifold. If we have a vector field with a constant value on the boundary of the plane, then we can use the one-point compactification to identify it with a vector field on S^2 . If we, however, have a periodic vector field, each unit cell has periodic boundary conditions and can be identified with the torus T^2 . The former is the case for a single skyrmion in a constant magnetic background, and the latter is the case of a skyrmion lattice (or any other multi-q texture in two dimensions). Now we know from the Hopf theorem that spin textures with the same winding number can always be continuously deformed into each other.

1.3.2. Intuition from Spherical Coordinates

Homotopy invariants, such as the winding number, are the key concept for topological endeavours in solid state physics. Indeed, many invariants can be viewed as winding number of some sort. The winding number of a unit normal vector field on a surface is equal to its total curvature and measures the genus of the surface. Also, the first Chern number of a complex line bundle, which is the integral over some curvature, can be expressed as the winding number of a vector field as well. To visualise this, we want to consider these different concepts for the most accessible example of a vector field with winding number 1: The spherical coordinates map, that conveniently also describes the unit normal field of a sphere.

Let $\Sigma = ([0, \pi] \times [0, 2\pi]) / \sim$ be the plane spanned by the polar and azimuthal angle φ, θ as depicted in Fig. 1.8. We can identify it with S^2 by contracting the black and the blue line to a single point each (respectively, North and South Pole) and glue the remaining border together along the red line: $(0, \varphi) \sim (0, 0)$ (black line) and $(\pi, \varphi) \sim (\pi, 0)$ (blue line) for all $\varphi \in [0, 2\pi]$ and $(\theta, 0) \sim (\theta, 2\pi)$ (along red line) for all $\theta \in [0, \pi]$.

Spherical coordinates

Then, the vector field $\mathbf{s}$ given by the spherical coordinates

$$\mathbf{s} : \Sigma \rightarrow S^2 \subset \mathbb{R}^3, \quad (\theta, \varphi) \mapsto \begin{pmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ \cos \theta \end{pmatrix} \quad (1.30)$$

defines a smooth map between the two closed surfaces Σ and S^2 . The scalar-valued integrand $\mathbf{s} \cdot (\partial_\theta \mathbf{s} \times \partial_\varphi \mathbf{s}) = \sin \theta$ from Eq. (1.29) is simply the differential solid angle given by the Jacobi determinant of the map $\mathbf{s}$. Therefore, the integral simply yields the surface area $\text{vol}(S^2) = 4\pi$ of the unit sphere, and we obtain the winding number $\text{deg } \mathbf{s} = 1$.

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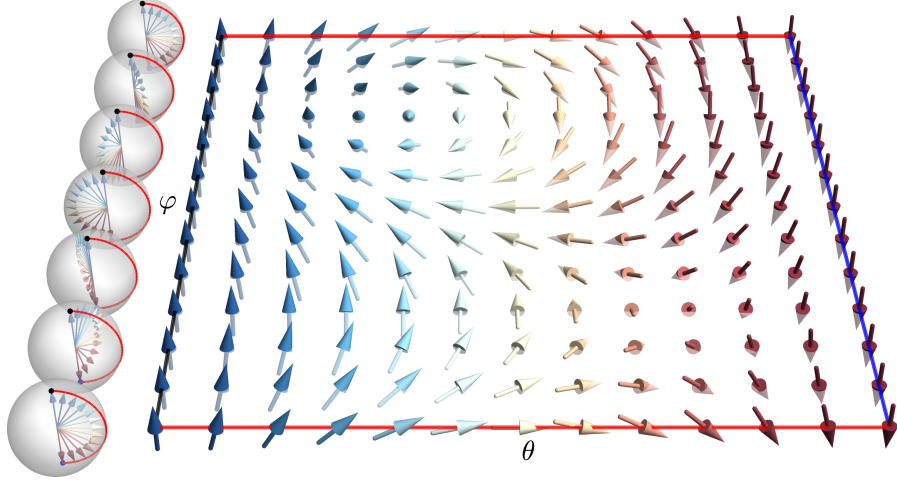


Figure 1.8.: The vector field defined by spherical coordinates on the plane Σ spanned by the polar angle θ and azimuthal angle φ . The spheres in the left hand-side visualise how the vector field wraps once around the sphere S^2 .

Continuous deformations

Any continuous change of the vector field $\mathbf{s}$ leaves this value unaffected: By continuity every rotation of a vector at one point needs to be followed by the vectors in their neighbourhood and the area on the target sphere stays the same. Even a spacial back and forth movement which would target the same area on the sphere, would cover it an odd number of times with alternating signs, such that these contributions compensate each other. Formally, one would say that the sum of the orientation's sign over the preimages of any of the map's regular values is equal to the degree of the map, as proven in [Fra11, Thm. 8.17]. This is sometimes used as the definition for the degree as done in [MW65, p. 27].

Curvature

If we consider $\mathbf{s}$ as the unit vector field on $\Sigma \cong S^2$ as depicted in Fig. 1.9, the integrand $\mathbf{s} \cdot (\partial_\theta \mathbf{s} \times \partial_\varphi \mathbf{s})$ is also a measure for how much infinitesimally neighbouring vectors are tilted against each other and, therefore, for the sphere's curvature. Indeed, the integral over the curvature, the total curvature, of any closed, orientable surface is equal to the winding number of its unit normal vector field, in this context also known as Gauß map. The total curvature is proportional to the so-called Euler characteristic $\chi(\Sigma)$, which is a purely algebraic quantity and indicates the genus g of the surface Σ , i.e. the number of holes. This is a consequence of the Gauß-Bonnet theorem [Fra11, Thm. 17.21.]

$$\deg \mathbf{s} = \frac{1}{2} \chi(\Sigma) = 1 - g. \quad (1.31)$$

Here, a continuous deformation of $\mathbf{s}$ coincides with a continuous deformation of Σ as submanifold embedded in $\mathbb{R}^3$, which is described by a homeomorphism isotopic to the identity map. Each dent, which locally changes the curvature introduces negative and positive curvature in the neighbourhood cancelling out with each other, such that the global integral over the curvature stays unaffected. Change only occurs, if a new hole is introduced which in turn breaks the continuity of the deformation.

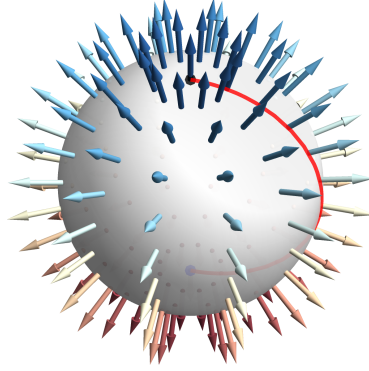


Figure 1.9.: The unit normal field on the sphere Σ obtained from gluing together the plane in Fig. 1.8.

A generalisation of the Gauß-Bonnet theorem is given by the Chern theorem, sometimes also referred to as Chern-Gauß-Bonnet, which is valid for the Euler class of curvature forms in higher-dimensional vector bundles. The mathematical theory on this can be found in [Nak18]. The form $\frac{1}{2\pi}\mathbf{s}^*\omega_{S^2}$ is an instance of an Euler class, in this case of the curvature form of the Levi-Civita connection of the 2-dimensional Riemannian manifold Σ . Similarly, one can consider the Euler class for a curvature form of either an even dimensional real or any complex vector bundle over Σ . It then coincides with the top Chern class.

Chern-Gauß-Bonnet

To construct a simple but non-trivial vector bundle, we consider the following smooth, complex matrix-valued map over Σ :

Vector bundle

$$H : \Sigma \rightarrow M_2(\mathbb{C}), \quad H = \mathbf{s} \cdot \boldsymbol{\sigma}, \quad (1.32)$$

where $\boldsymbol{\sigma}$ denotes the vector of Pauli matrices $\sigma_1, \sigma_2, \sigma_3 \in M_2(\mathbb{C})$. This matrix field is hermitian and has non-degenerate eigenstates ψ_+, ψ_- with respective eigenvalues $+1$ and -1 . If we choose one of the eigenstates, this defines a hermitian complex line bundle (E, B, π, F) :

The base manifold $B = \Sigma$, fibre $F = \mathbb{C}$, total space $E = \{(\mathbf{p}, \psi) \in \Sigma \times \mathbb{C}^2 | H(\mathbf{p})\psi = -\psi\}$ and projection $\pi : E \rightarrow \Sigma, (\mathbf{p}, \psi) \mapsto \mathbf{p}$. It is conveniently embedded in the ambient space $\Sigma \times \mathbb{C}^2$ and has a canonical connection induced by the induced Hermitian norm [BC65].

The canonical connection for embedded bundles can be described globally in terms of a projection P to its fibre: One separates the tangent bundle of the vector bundle E into two components, which are at any point horizontal and vertical to the tangent space of the fibre. As the tangent space of the fibre at any point is the fibre itself, the projection to the eigenspace that belongs to the eigenvalue -1 is the vertical projection. From this, we obtain a covariant derivative $\nabla : \Gamma E \rightarrow \Gamma E \otimes \Omega^1(\Sigma)$, acting on smooth sections on E . Let $\psi \in \Gamma E$, then it is given as $\nabla\psi = Pd\psi$ [Kha13, Ex. 4.1.4.]. We can rewrite it as

Connection

$$\begin{aligned} Pd\psi &= d\psi - dP\psi \\ &= (d - dP + PdP)\psi \end{aligned}$$

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$$= (d - [dP, P])\psi =: (d + A)\psi$$

by using the equalities $\psi = P\psi$, implying $d\psi = dP\psi + Pd\psi$, and $P = P^2$, implying $dPP = dPP + PdPP$ with $PdPP = 0$.

The connection one-form $A = -[dP, P] \in \Omega^1(\Sigma, \text{End}(E))$ determines how much the covariant derivative differs from the exterior derivative of a trivial bundle.

Curvature The curvature two-form for this connection is $\nabla^2\psi = P d(Pd\psi) \in \Omega^2(\Sigma, \text{End}(E))$, which we can rewrite the following way:

$$(PdP) \wedge (d\psi) = (PdP \wedge dP)\psi + (PdPP) \wedge d\psi = (PdP \wedge dP)\psi.$$

The Chern class is then $[\frac{i}{2\pi} \text{tr}(PdP \wedge dP)]$. For the map from Eq. (1.32) the projection P onto the eigenspace with eigenvalue -1 can be easily obtained by rewriting H in terms of projections:

$$H = \mathbb{1}_2 - 2P, \quad P = \frac{1}{2}(\mathbb{1}_2 - \mathbf{s} \cdot \boldsymbol{\sigma})$$

Chern number Now, it is straight forward to check, that the first Chern number, given by the integral over the first Chern class is equal to the winding number of $\mathbf{s}$:

$$\begin{aligned} \frac{i}{2\pi} \int_{\Sigma} \text{tr}(PdP \wedge dP) &= \frac{i}{16\pi} \int_{\Sigma} \text{tr}((\mathbb{1}_2 - s_i \sigma_i)(\sigma_j ds_j) \wedge (\sigma_k ds_k)) \\ &= \frac{i}{16\pi} \int_{\Sigma} \text{tr}(\sigma_j \sigma_k - s_i \sigma_i \sigma_j \sigma_k) ds_j \wedge ds_k \\ &= \frac{i}{16\pi} \int_{\Sigma} (2\delta_{jk} - i2s_i \epsilon_{ijk}) ds_j \wedge ds_k \\ &= \frac{1}{8\pi} \int_{\Sigma} \epsilon_{ijk} s_i ds_j \wedge ds_k = \text{deg } \mathbf{s} \end{aligned}$$

The projection $P = \frac{1}{2}(\mathbb{1}_2 + \mathbf{s} \cdot \boldsymbol{\sigma})$ onto the eigenspace with eigenvector $+1$ carries the first Chern number $-\text{deg } \mathbf{s}$.

Remark 1.3 (Spin- $\frac{1}{2}$ Hamiltonian). In physics, a Hamiltonian with the form of Eq. (1.32) describes a spin- $\frac{1}{2}$ particle in a magnetic field with its direction given by $\mathbf{s}$. This corresponds to a magnetic Dirac monopole at the centre of the sphere Σ [MF14]. The conventional connection coincides with the Berry connection derived from the quantum adiabatic theorem. This was first described by Berry [Ber84] and interpreted in terms of fibre bundle geometry by Simon [Sim83]. An extensive introduction to this can be found in [Boh+03].

The formulation of the adiabatic theorem of quantum mechanics in terms of the projection is due to Kato [Kat50] and was adopted for the connection by Avron et al. [ASS83]. An accessible overview on this can be found in [BT13]. More details on this are discussed in Chap. 2.2 and Chap. 2.3.1, where the electronic transport is treated in terms of fibre bundle geometry and geometric phases.

1.3.3. Intuition for Non-commutative Geometry

There is a well established correspondence between geometry and commutative algebra, which allows us to express the examples of the last section in purely algebraic terms. The topology of any compact Hausdorff space X is fully encoded in the algebra $C(X)$ of complex continuous functions on X , which is an unital commutative C^* -algebra.

In fact, there exists an isomorphism between any commutative C^* -algebra A and the algebra $C_0(\hat{A})$ of complex continuous functions vanishing at infinity over the locally compact Hausdorff space $\hat{A}$ given by the spectrum of A , i.e., the space of characters of A . This is known as the Gelfand-Naimark theorem (Thm. 3.2), which we will discuss in more detail in the introduction to C^* -algebras in Chap. 3. It follows, that any homeomorphism invariant on X can be expressed as an algebraic invariant of the algebra $C(X)$. The idea of non-commutative geometry is, that these algebraic methods are still applicable to algebras which are now longer commutative. In that case, these algebras do not correspond to well-defined geometric spaces, but are often formally associated with fictitious non-commutative spaces. They often appear in physics as operator algebras describing e.g. the phase space in quantum mechanics or the Brillouin zone in the quantum Hall effect.

In the last example of the previous section, a vector bundle and a connection were given by a projection in a matrix-valued function algebra over its base manifold. More generally, by a theorem of Serre and Swan [Ser55; Swa62], the category of complex vector bundles on a compact Hausdorff space X is equivalent to the category of finite projective modules over the algebra $C(X)$ of continuous complex functions on X . The corresponding invariants are the ones of topological K -theory such as the Chern numbers.

In this section, we want to introduce the ideas of non-commutative geometry in the commutative case and reformulate the topological invariants of the last section in this language. The author discussed this example aimed at the Gauß-Bonnet theorem before in his Master's thesis as an introduction to cyclic cocycles [Pra20]. It was first stated by Connes in his introduction [Con94, Intro. C], and we refer to the lecture notes of André F. Reyes-Lega [Rey16] for technical details.

At first, we need to introduce some tools of non-commutative geometry in a simplified form: Let us consider an algebra $\mathcal{A}$ with a trilinear form $\tau : \mathcal{A} \times \mathcal{A} \times \mathcal{A} \rightarrow \mathbb{C}$, such that:

Trilinear form

$$(1) \quad \tau(a_0, a_1, a_2) = \tau(a_2, a_0, a_1),$$

$$(2) \quad \tau(a_0 a_1, a_2, a_3) - \tau(a_0, a_1 a_2, a_3) + \tau(a_0, a_1, a_2 a_3) - \tau(a_3 a_0, a_1, a_2) = 0,$$

for all $a_0, a_1, a_2, a_3 \in \mathcal{A}$. From this we can easily construct a homotopy invariant: For any algebra $\mathcal{A}$ over $\mathbb{R}$ or $\mathbb{C}$ with a trilinear form τ , such that (1) and (2) are satisfied, and any idempotent element $e = e^2 \in \mathcal{A}$, the scalar $\tau(e, e, e)$ stays constant under deformation of e among the idempotents of $\mathcal{A}$. We can demonstrate this statement for a Banach algebra $\mathcal{A}$ (thus having an associative and continuous multiplication operation) and a smooth family of idempotents $t \mapsto e_t = e_t^2$.

Lemma 1.2. $\tau(e_t, e_t, e_t)$ does not depend on t

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Proof: We can use the Leibniz rule for derivations with respect to t because the multiplication is continuous with respect to the Banach norm. We obtain, $\dot{e}_t = \dot{e}_t^2 = \dot{e}_t e_t + e_t \dot{e}_t$ and, thus,

$$0 = e_t \dot{e}_t - e_t \dot{e}_t = e_t \dot{e}_t e_t + e_t^2 \dot{e}_t - e_t \dot{e}_t = e_t \dot{e}_t e_t$$

We can rewrite $\dot{e}_t$ by using $x_t := [\dot{e}_t, e_t]$ as $[x_t, e_t]$ since

$$[x_t, e_t] = [\dot{e}_t, e_t] e_t - e_t [\dot{e}_t, e_t] = \dot{e}_t e_t - 2e_t \dot{e}_t e_t + e_t \dot{e}_t = \dot{e}_t.$$

Then, the statement follows

$$\begin{aligned} \frac{d}{dt} \tau(e_t, e_t, e_t) &= 3\tau([x_t, e_t], e_t, e_t) = 3(\tau(x_t e_t, e_t, e_t) - \tau(e_t x_t, e_t, e_t)) \\ &= 3(\tau(x_t, e_t^2, e_t) - \tau(x_t, e_t, e_t^2) + \tau(e_t x_t, e_t, e_t) - \tau(e_t x_t, e_t, e_t)) = 0. \end{aligned}$$

□

As long as there is a smooth curve $t \mapsto e_t$ connecting two idempotent elements in the subspace of idempotents of $\mathcal{A}$, the corresponding scalar given by the trilinear map is independent of their specific choice. Since every continuous curve is homotopic to a smooth one, this gives us a homotopy invariant.

Function algebra

To obtain invariants of Σ , we want to apply this lemma to the algebra $\mathcal{A} = C^\infty(\Sigma)$ of all smooth functions on Σ , which is a dense subalgebra of $C(\Sigma)$. For it, a trilinear form is given by $\tau(f_0, f_1, f_2) = \int_{\Sigma} f_0 df_1 \wedge df_2$. For every smooth map $f : \Sigma \rightarrow \mathbb{R}^3$ it yields the oriented volume of the submanifold $M \subset \mathbb{R}^3$ (with coordinates x_0, x_1, x_2) which is bounded by the map's image $\partial M := f(\Sigma)$:

$$\int_{\Sigma} f_0 df_1 \wedge df_2 = \int_{\Sigma} f^*(x_0 dx_1 \wedge dx_2) = \int_{f(\Sigma)} x_0 dx_1 \wedge dx_2 = \int_M dx_0 \wedge dx_1 \wedge dx_2$$

We need to check, whether τ satisfies the conditions:

Lemma 1.3. *Let $\mathcal{A} = C^\infty(\Sigma)$, then $\tau(f_0, f_1, f_2) = \int_{\Sigma} f_0 df_1 \wedge df_2$ satisfies (1) and (2).*

Proof: (1) Since $\partial\Sigma = \emptyset$, it follows that:

$$\begin{aligned} \tau(f_0, f_1, f_2) &= \int_{\Sigma} f_0 df_1 \wedge df_2 = \int_{\Sigma} -d(f_0 f_2 df_1) + \int_{\Sigma} f_2 df_0 \wedge df_1 \\ &= \int_{\partial\Sigma} f_0 f_2 df_1 + \tau(f_2, f_0, f_1) = \tau(f_2, f_0, f_1). \end{aligned}$$

(2)

$$\begin{aligned} &\tau(a_0 a_1, a_2, a_3) - \tau(a_0, a_1 a_2, a_3) + \tau(a_0, a_1, a_2 a_3) - \tau(a_3 a_0, a_1, a_2) \\ &= \int_{\Sigma} (f_0 f_1 df_2 \wedge df_3 - f_0 f_1 df_2 \wedge df_3 - f_0 f_2 df_1 \wedge df_3 + f_0 f_2 df_1 \wedge df_3 \\ &\quad + f_0 f_3 df_1 \wedge df_2 - f_3 f_0 df_1 \wedge df_2) = 0 \end{aligned}$$

□

However, since $\mathcal{A} = C^\infty(\Sigma)$ is commutative and Σ is connected, there are no non-trivial idempotents in $\mathcal{A}$ for the construction of an invariant. Instead, we can consider the non-commutative algebra $M_2(\mathcal{A}) = \mathcal{A} \otimes M_2(\mathbb{C})$ of 2×2 -matrices with values in $\mathcal{A}$. An element of this algebra was also the starting point for the construction of the vector bundle we had before. The trilinear form τ canonically extends to a trilinear form τ_2 on this algebra:

$$\tau_2(f_0 \otimes \mu_0, f_1 \otimes \mu_1, f_2 \otimes \mu_2) := \left(\int_{\Sigma} f_0 df_1 \wedge df_2 \right) \text{tr}(\mu_0 \mu_1 \mu_2),$$

with $f_0, f_1, f_2 \in \mathcal{A}$, $\mu_0, \mu_1, \mu_2 \in M_2(\mathbb{C})$ and $\text{tr}(\cdot)$, the trace on $M_2(\mathbb{C})$. It canonically fulfils the conditions due to the cyclicity of the trace.

Next, we need a meaningful idempotent element of $M_2(C^\infty(\Sigma))$ which is a smooth map from Σ to the space of idempotents of $M_2(\mathbb{C})$. Such idempotents can be decomposed into a real linear combination of the unit matrix $\mathbb{1}_2$ and the three *Pauli matrices* $\sigma_1, \sigma_2, \sigma_3$ which span the real vector space of self-adjoint 2×2 -matrices. With the choice of a $\mathbb{R}^3$ vector $\mathbf{n}$ of unit length, we can construct self-adjoint idempotent matrices as $e = \frac{1}{2}(\mathbb{1}_2 + \mathbf{n} \cdot \boldsymbol{\sigma})$:

$$\begin{aligned} e^2 &= \frac{1}{4}(\mathbb{1}_2^2 + 2\mathbf{n} \cdot \boldsymbol{\sigma} + (\mathbf{n} \cdot \boldsymbol{\sigma})^2) = \frac{1}{4}(\mathbb{1}_2 + 2\mathbf{n} \cdot \boldsymbol{\sigma} + n_1^2 \sigma_1^2 + n_2^2 \sigma_2^2 + n_3^2 \sigma_3^2) \\ &= \frac{1}{4}(\mathbb{1}_2 + 2\mathbf{n} \cdot \boldsymbol{\sigma} + \underbrace{(n_1^2 + n_2^2 + n_3^2)}_{=1} \mathbb{1}_2) = \frac{1}{2}(\mathbb{1}_2 + \mathbf{n} \cdot \boldsymbol{\sigma}) = e \end{aligned}$$

Therefore, we can simply choose the projection $P = \frac{1}{2}(\mathbb{1}_2 - \mathbf{s} \cdot \boldsymbol{\sigma})$ as for the definition of the line bundle and its connection.

The smooth deformation invariance of the first Chern number defined in last section and by extension also the Euler characteristic and winding number follows therefore from the algebraic considerations of Lemma 1.2:

Lemma 1.4. $\tau_2(P, P, P) = -2\pi i \deg \mathbf{s} = 4\pi i \chi(\Sigma)$

Proof:

$$\tau_2(P, P, P) = \int_{\Sigma} \text{tr}(P dP \wedge dP)$$

□

This value is invariant under a smooth change of P in its path connected component of the subspace of idempotents of $M_2(C^\infty(\Sigma))$, which translates to a smooth variation of the map $\mathbf{s} : \Sigma \rightarrow S^2$. In fact, the map $e \mapsto \tau_2(e, e, e)$ defines an invariant of K-theory, which is an additive map of $K_0(\mathcal{A})$ to the complex numbers. This is the case, since all finite modules over an algebra $\mathcal{A}$ are given by the image of an idempotent element belonging to a matrix algebra over $\mathcal{A}$. Using the homotopy invariance one can eliminate the ambiguity of the specific choice of the idempotent element out of the stable equivalence class of finite ranked projections belonging to K_0 [Con94, Intro. C].

1. Magnetic Textures

The trilinear form τ is an instance of a cyclic cocycle, where condition (1) amounts to the cyclic permutation property and condition (2) corresponds to the vanishing of the Hochschild boundary and thus to the cocycle property. The trilinear form τ_2 is the *cup product* $\tau \# \text{tr}$ of τ and the matrix trace tr , and thus a cyclic cocycle as well.

1.3.4. Winding Number Transitions and Regularisation

While the winding number is invariant under continuous deformation of the vector field, there are many situations in which continuous parameter manipulation can lead to discontinuous change. A common example are normalised superpositions of spin textures, where variation of the linear coefficients or relative shifts in real space may cause destructive interference, which in turn causes a singularity in the normalised texture. We refer to the corresponding points in parameter space as critical points p_c and to the points of the destructive interference in real space as critical positions $\mathbf{x}_c$.

When passing these parameter points, the winding number changes instantly by an integer value equal to the charge of the singularity. To avoid working with singularities, one can use a regularisation procedure, which changes the target manifold from S^2 to $\mathbb{R}^3$. In that case, the regularised texture deforms continuously along a path through p_c and the expression for the winding number yields continuous values between the integer winding numbers.

In this section, we argue that a winding number transition for a normalised vector field $\hat{\mathbf{n}}$ over a two-dimensional surface M can generally be achieved by a single additional real parameter $t \in \mathbb{R}$ and that there is a finite discrete set of critical points $(\mathbf{x}_c, t_c) \in M \times \mathbb{R}$. Then, we will show, that the winding number changes precisely by the charge of the singularity, i.e. the winding number of the vector field continued in $M \times \mathbb{R}$ on an arbitrary small sphere around $(\mathbf{x}_c, t_c)$. We visualise this using the simple case of the single skyrmion transitioning to the ferromagnet. Eventually, we introduce a simple regularisation procedure and demonstrate for the single skyrmion explicitly how it induces a continuous transition of the winding number.

*Winding number
transitions*

From the viewpoint of the first Chern number of a two-band system as in Sec. 1.3.2, we can reason about the existence of critical parameter points, by investigating the degeneracy of hermitian 2×2 -matrices. Neumann and Wigner [NW93] demonstrated, how in general for a hermitian matrix three real parameters are sufficient to make two eigenvalues coincide. With the matrix-valued map $H = \mathbf{n} \cdot \boldsymbol{\sigma}$ this coincides with the roots of $\mathbf{n} : M \rightarrow \mathbb{R}^3$, which are singularities of $\hat{\mathbf{n}} = \frac{\mathbf{n}}{\|\mathbf{n}\|}$. Therefore, one additional real parameter $t \in \mathbb{R}$ needs to exhibit critical points.

When passing these points, the winding number may jump discontinuously. The precise change in winding number corresponds to the monopole charge of the singularity in 3-dimensional hyperspace composed of real space and parameter space $\mathbb{R}$. This can be illustrated by a brief line of differential geometric arguments as inspired by Jean Bellissard's method to calculate the change in Chern number at band crossings [Bel95].

First, we start by considering the expressions for the winding number and the monopole charge. The parameter dependent winding number is given by

Monopole charge

$$\deg \hat{\mathbf{n}}_t = \frac{1}{4\pi} \int_M \hat{\mathbf{n}}_t^* \omega_{S^2}.$$

Now, we extend the definition of the spin vector field $\hat{\mathbf{n}}_t : M \rightarrow S^2$ to the full hyperspace $\hat{\mathbf{N}} : M \times \mathbb{R} \rightarrow S^2$. Let $\Sigma \subset M \times \mathbb{R}$ be a two-dimensional closed submanifold in hyperspace diffeomorphic to S^2 surrounding exactly one discontinuity point of the vector field. The monopole charge of this point is given by

$$n_{\text{sing}} = \frac{1}{4\pi} \int_{\Sigma} \hat{\mathbf{N}}^* \omega_{S^2}.$$

To demonstrate, that the change in winding number is precisely the monopole charge of the transition, we construct a hypersurface in $M \times \mathbb{R}$ with winding number 0 that can be partitioned in the ball Σ and the surface M before and after the transition:

Hypersurface

Let the vector field $\hat{\mathbf{N}}$ have a discontinuity point at $(\mathbf{x}_c, t_c) \in M \times \mathbb{R}$ and let D be a small open neighbourhood of $\mathbf{x}_c$ in M diffeomorphic to the unit disk in $\mathbb{R}^2$. Let further γ be the oriented boundary of D in M and $M_D = M \setminus D$ be the surface M with a hole at D around $\mathbf{x}_c$. The boundary at this hole is thus $\partial M_D = -\gamma$. Let $-M_D$ be a copy of M_D with opposite orientation. Finally, choose $\epsilon > 0$ such that there is no further singularity of the vector field in the interval $[t_c - \epsilon, t_c + \epsilon] \in S^1$.

Now, we connect the two surfaces M_D and $-M_D$ in hyperspace at $t_c \pm \epsilon$, respectively, by gluing a tube around $(\mathbf{x}_c, t_c)$ along to boundaries of the holes. We obtain the surface

$$\hat{M}(\epsilon) = \left((M_D \times \{t_c - \epsilon\}) \cup (\gamma \times [t_c - \epsilon, t_c + \epsilon]) \cup (-M_D \times \{t_c + \epsilon\}) \right) / \sim, \quad (1.33)$$

where we identify the points along $\gamma \times \{t_c - \epsilon\}$ and as well along $\gamma \times \{t_c + \epsilon\}$ to glue these three surfaces together to one closed, oriented submanifold in the hyperspace. A visualisation is given in Fig. 1.10(b) for the transition of a single skyrmion to the ferromagnetic background.

Now everything is set up. We can compute the winding number of $\hat{\mathbf{N}}$ over the surface $\hat{M}(\epsilon)$ which gives us an integer

Partition

$$\frac{1}{4\pi} \int_{\hat{M}(\epsilon)} \hat{\mathbf{N}}^* \omega_{S^2} \in \mathbb{Z}.$$

As a homotopy invariant it stays the same for $\epsilon \rightarrow 0$, since we cut out the discontinuity point of the vector field. $\hat{M}(0)$ is nothing else than two copies of M_D with opposite orientation and the vector field on it has the same parameter $t = 0$. Thus, the winding number integral needs to yield 0:

$$\frac{1}{4\pi} \int_{\hat{M}(0)} \hat{\mathbf{N}}^* \omega_{S^2} = \frac{1}{4\pi} \int_{M_D \times \{t_c\}} \hat{\mathbf{N}}^* \omega_{S^2} + \frac{1}{4\pi} \int_{-M_D \times \{t_c\}} \hat{\mathbf{N}}^* \omega_{S^2} = 0$$

1. Magnetic Textures

Therefore, the integral over $\hat{M}(\epsilon)$ has to vanish as well. Similarly, since the vector field is continuous at $t = t_c \pm \epsilon$ the integrals over $D \times \{t_c - \epsilon\}$ and $-D \times \{t_c - \epsilon\}$ as well as $D \times \{t_c + \epsilon\}$ and $-D \times \{t_c + \epsilon\}$ cancel respectively. Now, we split the integral back into three parts along γ and glue back in the oppositely oriented disks D . Consequently, we have the integral over M at $\{t_c - \epsilon\}$ plus the integral over the cylinder surface around the singularity (homeomorphic to Σ) minus the integral over M at $\{t_c + \epsilon\}$ equal 0:

$$\begin{aligned}
0 &= \frac{1}{4\pi} \int_{\hat{M}(\epsilon)} \hat{\mathbf{N}}^* \omega_{S^2} \\
&= \frac{1}{4\pi} \int_{M_D \times \{t_c - \epsilon\}} \hat{\mathbf{N}}^* \omega_{S^2} + \frac{1}{4\pi} \int_{\gamma \times [t_c - \epsilon, t_c + \epsilon]} \hat{\mathbf{N}}^* \omega_{S^2} + \frac{1}{4\pi} \int_{-M_D \times \{t_c + \epsilon\}} \hat{\mathbf{N}}^* \omega_{S^2} \\
&= \frac{1}{4\pi} \int_M \hat{\mathbf{n}}_{t_c - \epsilon}^* \omega_{S^2} + \frac{1}{4\pi} \int_{\Sigma} \hat{\mathbf{N}}^* \omega_{S^2} - \frac{1}{4\pi} \int_M \hat{\mathbf{n}}_{t_c + \epsilon}^* \omega_{S^2} \\
&= \deg \hat{\mathbf{n}}_{t_c - \epsilon} + n_{\text{sing}} - \deg \hat{\mathbf{n}}_{t_c + \epsilon}
\end{aligned}$$

This proves, that the winding number of the vector field changes by the monopole charge at passing the phase position of the singularity.

Single skyrmion transition

We want to give a simple example that can serve a toy model for more complex magnetic transitions. For this, we consider the isolated skyrmion as introduced in Sec. 1.2.2 with vorticity 1 and helicity 0 parameterised in polar coordinates $\rho \in [0, 1]$, $\phi \in [0, 2\pi]$ by

$$\mathbf{n}_{\text{sk}}(\rho, \phi) = \left(\sqrt{1 - n_z(\rho)^2} \cos \Phi(\phi), \sqrt{1 - n_z(\rho)^2} \sin \Phi(\phi), n_z(\rho) \right)^T$$

where the azimuthal angle of the vector direction $\Phi(\phi) = \phi$ is equal to the azimuthal angle of the polar coordinates, and the z -component $n_z(\rho) = (2\rho - 1)$ only depends on the radius, such that the texture is that of a ferromagnet for radius $\rho = 1$. If we then identify the circle at $\rho = 1$ with one point, the surface $M = \{(\rho \cos(\theta), \rho \sin(\theta)) \in \mathbb{R}^2 | \rho \in [0, 1], \phi \in [0, 2\pi]\} / \sim$ with $S^1 \sim (1, 0)$ is a closed manifold homeomorphic to S^2 . One has $\|\mathbf{n}_{\text{sk}}(\mathbf{p})\| = 1$ for all $\mathbf{p} \in M$, thus $\mathbf{n}_{\text{sk}} : M \rightarrow S^2$ and a topological charge $\deg \mathbf{n}_{\text{sk}} = -1$. We construct a linear interpolation to the ferromagnet by

$$\mathbf{n}(\rho, \phi, t) = (1 - t)\mathbf{n}_{\text{sk}}(\rho, \phi) + t\hat{\mathbf{e}}_z. \quad (1.34)$$

By design, destructive interference occurs for $t = \frac{1}{2}$ at the origin. At this position the normalisation $\hat{\mathbf{n}}$ has a singularity accompanied by a spin flip from $-\hat{\mathbf{e}}_z$ to $\hat{\mathbf{e}}_z$. The image of the vector field is no longer all of S^2 , but just part of the upper hemisphere as depicted in Fig. 1.10(a). For $t \rightarrow \frac{1}{2}$ from below, the pre-image of the lower hemisphere shrinks to the origin. Then, the flip collapses the lower hemisphere instantly onto the upper while preserving its opposite orientation, such that the winding number integral for $t > \frac{1}{2}$ is zero. For $t \rightarrow 1$ the image area then shrinks to the North Pole.

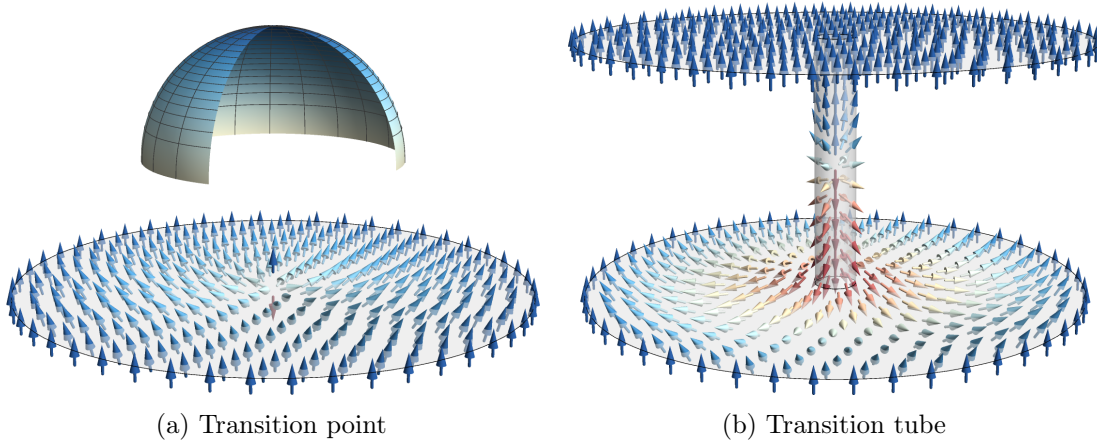


Figure 1.10.: **Transition from single skyrmion to ferromagnet** (a) depicts the vector field at the critical parameter $t = \frac{1}{2}$ with singularity at $(0, 0)$. Above and below are the origin vectors for $t = \frac{2}{5}$ and $t = \frac{4}{5}$ to emphasise the singular nature. The half sphere indicates (3 quarters of) the image of the vector field. (b) depicts the transition along a tube around the singularity. It is visible that the vector field flips its sign at $(0, 0, \frac{1}{2})$.

In Fig. 1.10(b) we visualise the surface $\hat{M}(0.5)$ as defined in Eq. (1.33). If we deform the tube including its caps into a sphere around $(0, 0, \frac{1}{2})$ we can see that the charge of the singularity is 1 since the vector field points outside the sphere and can be deformed to be normal on it. This is the situation we had before in Fig. 1.9.

In general, if we have such a singularity, the normalisation procedure is undefined at $\mathbf{x}_c$ and no matter which choice will be made to redefine $\hat{\mathbf{n}}(\mathbf{x})$, the resulting function will be discontinuous at the singularities $\mathbf{x} = \mathbf{x}_c$. In practice, we can regularise the singularity by making the choice

Regularisation

$$\hat{\mathbf{n}} = \frac{\mathbf{n}}{\|\mathbf{n}\|} \longrightarrow \frac{\mathbf{n}}{\|\mathbf{n}\| + \eta} = \hat{\mathbf{n}}_\eta, \quad (1.35)$$

with $\eta > 0$. It is then guaranteed that $\lim_{\eta \rightarrow 0+} \hat{\mathbf{n}}_\eta = \hat{\mathbf{n}}$ for all $\mathbf{x} \neq \mathbf{x}_c$.

For the simple example of the single skyrmion morphing to the ferromagnet the regularised transition can be worked out exactly [Pra+24]. We regularise the transition texture $\hat{\mathbf{n}}$ from Eq. (1.34) following Eq. (1.35) before we calculate the winding number according to formula Eq. (1.29). Because of the simple polar form of the skyrmion, the winding density $\hat{\mathbf{n}}_\eta \cdot (\partial_\rho \hat{\mathbf{n}}_\eta \times \partial_\phi \hat{\mathbf{n}}_\eta)$ is angular independent and the integrals can be evaluated analytically for the full transition.

*Regularised
single skyrmion
transition*

In Fig. 1.11 (a)-(c) we depict the image of the regularised vector field in $\mathbb{R}^3$ for $\eta = 10^{-1}$ along the transition. The winding number integral yields the (negative oriented) surface area of this closed image manifold in relation to the surface area of S^2 . From this it becomes clear, that it changes continuously in the interval $[-1, 0]$. Fig. 1.11(d) shows this transition for different values of η .

1. Magnetic Textures

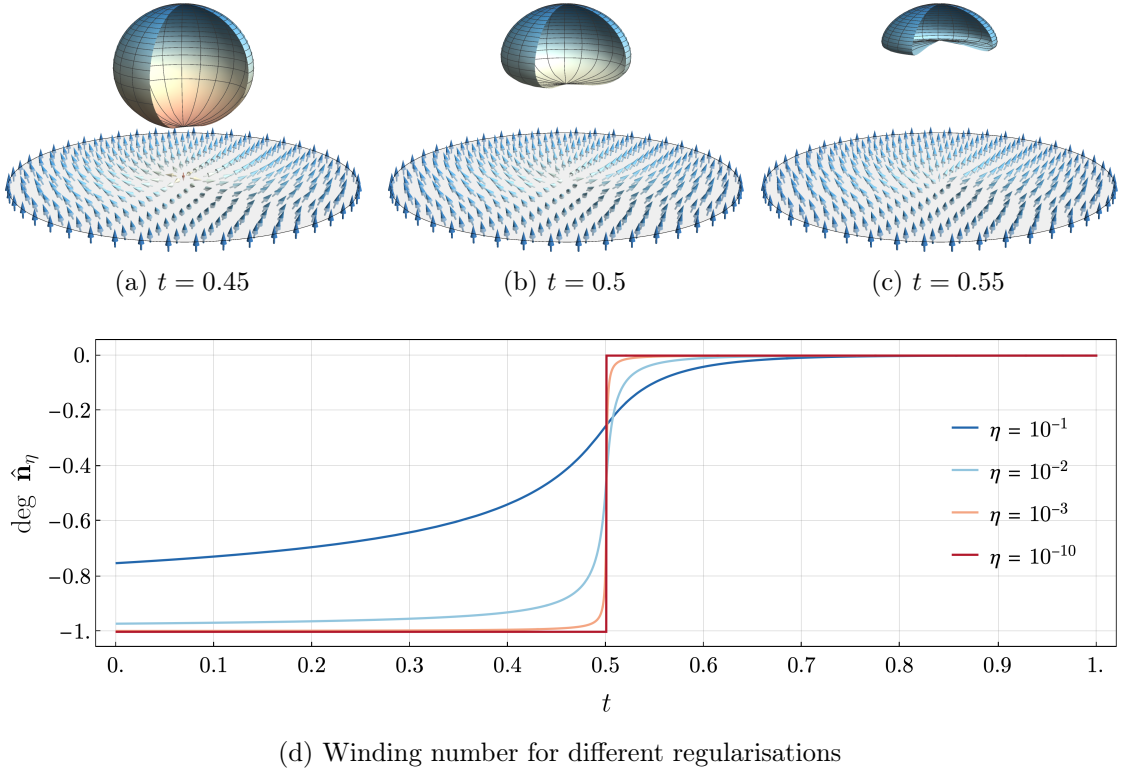


Figure 1.11.: **Regularised transition from single skyrmion to ferromagnet.** We depict the vector field with $\eta = 10^{-1}$ right before (a), during (b), and after (c) the former critical point. The surface above indicates the image of the vector field. With the regularisation it is a closed surface in $\mathbb{R}^3$. The curves (d) indicate the regularised winding number for different η during the transition.

Universal function

Let $t_c(\eta)$ denote the value of t for which $\deg \hat{\mathbf{n}}_\eta$ has depleted to the value of 0.5. As the notation indicates, the value of $t_c(\eta)$ generally depends on η . However, we still recover $t_c(\eta) \rightarrow t_c$ in the limit $\eta \rightarrow 0$. Analytically, we find the asymptotic scaling behaviour [Pru88; XP13]

$$\deg \hat{\mathbf{n}}_\eta(t) \sim F\left((t - t_c)\left(\frac{\eta}{\eta_0}\right)^{-\kappa}\right), \quad \text{for } \eta \rightarrow 0^+,$$

with $\eta_0 = 1$, $\kappa = 1$. F is the universal scaling function of the transition [Pra+24], explicitly given by

$$F(x) = -\frac{1}{2} \left(1 - \frac{x}{1 + \frac{4x^2}{1+4|x|}} \right).$$

Moreover, one finds

$$\lim_{\eta \rightarrow 0^+} \deg \hat{\mathbf{n}}_\eta(t) = \Theta(t_c - t),$$

for all $t \neq 0.5$.

1.3. Winding Number

In summary, the example demonstrates the manner in which topological invariants associated with a normalised multi- q texture in real space, such as the winding number, can undergo a discontinuous change as a function of the texture parameters [HOM21; Shi+22]. This is due to the fact that the texture ceases to be continuous at the critical point, such that the topological degree is not defined. The discontinuous transition can be converted into a continuous one, albeit at the cost of temporarily leaving the function space $C(S^2, S^2)$ in favour of $C(S^2, \mathbb{R}^3)$. This enables the possibility of a continuous change of the mapping degree.

2 | Electronic Properties

We study the electronic properties of materials hosting multi- q textures in a tight-binding model for spin-1/2 electrons with magnetic nearest-neighbour hopping of constant strength λ_{hop} , and exchange coupling of strength λ_{xc} between the electron spin and the magnetisation texture in the strong coupling regime $\lambda_{\text{xc}}/\lambda_{\text{hop}} \gg 1$.

It is not inherently obvious why this model provides an appropriate description for any real physical system. Therefore, we want to justify and motivate its usage by introducing the prevalent quantum mechanical considerations for the electronic system, the commonly used formalisms for its description, and the frequently studied physical phenomena.

In particular, we seek to clarify how interacting many particle systems can be addressed by a discretised effective single electron model, and how the topological properties of the electronic states can be accurately captured.

While the electronic properties of a material depend on numerous interactions between the electrons and the nuclei, one can find an effective model for non-interacting electrons that adequately reproduces the behaviour with interactions. This can be done following the principles of Hohenberg-Kohn-Sham functional density theory, and even be augmented to include the spin degree of freedom. The effective non-interacting model can then be expressed as a single electron Hamiltonian given by an unbounded Hilbert space operator.

*Electronic
system*

For the C^* -algebraic formalism it is convenient to work with bounded operators on a discrete Hilbert space, which can be interpreted as elements belonging to an algebra of physical observables. Moreover, for discrete models there exist canonical finite volume approximations for numerical computation. Therefore, we consider the tight-binding approximation for which the Hamiltonian from the continuum model in d dimensions is approximated by

$$H = - \sum_{\langle \mathbf{i}, \mathbf{j} \rangle \in \mathbb{Z}^{2d}} \lambda_{\text{hop}}(\mathbf{i}, \mathbf{j}) |\mathbf{i}\rangle \langle \mathbf{j}| + \lambda_{\text{xc}} \sum_{\mathbf{i} \in \mathbb{Z}^d} \boldsymbol{\sigma} \cdot \mathbf{n}(\mathbf{x}_{\mathbf{i}}) |\mathbf{i}\rangle \langle \mathbf{i}|.$$

In the first term $\langle \mathbf{i}, \mathbf{j} \rangle$ restricts the sum to the nearest neighbours between which hopping of electrons takes place with transition amplitude given by a transfer integral evaluated to $\lambda_{\text{hop}}(\mathbf{i}, \mathbf{j})$. It consists of a constant hopping parameter $\lambda_{\text{hop}} > 0$ and a complex phase factor $e^{i\Gamma_A(\mathbf{i}, \mathbf{j})}$ picked up from the magnetic vector potential along the path. The second term describes the coupling of the spin of the electron to the smooth magnetic texture $\mathbf{n} : \mathbb{R}^d \rightarrow \mathbb{R}^3$ with coupling strength λ_{xc} and $\boldsymbol{\sigma}$ denoting the vector $(\sigma_1, \sigma_2, \sigma_3)$ of Pauli matrices. We assume that the transition to the tight-binding model preserves the electronic state topology of the lower part of the energy spectrum as has been demonstrated for similar cases.

2. Electronic Properties

Furthermore, we disregard spin-orbit coupling as it is not relevant for our purpose. For instance, in large skyrmion systems spin-orbit coupling is small in comparison with the dominant ferromagnetic interaction, while for small scale skyrmion systems, such as found in Gd-compounds, it is negligible due to orbital freezing [MNA21].

Phenomena

Our focus lies on particular physical phenomena that arise from the non-collinearity or non-coplanarity of the multi- q textures and are connected to topological properties of the electronic states. Those comprise the (quantised) topological Hall effect and the orbital magnetisation generated by the motion of the electrons through the spin texture. Both of them are caused by bulk properties of the solids and can be expressed as Brillouin zone integrals involving the momentum-space Berry curvature. In Chap. 3, we derive the non-commutative version of these formulas that are valid for lattice incommensurate multi- q textures and external magnetic fields with irrational magnetic flux. Moreover, in Chap. 4, we derive the canonical finite-volume approximations that allow us to evaluate them numerically.

Chapter content

We begin this chapter in Sec. 2.1 with a breakdown of the quantum mechanical description of charged particles with spin in the presence of an electromagnetic field. Then, we introduce the general situation in realistic solids that can be treated with density functional theory, and work our way back to an effective one-particle description. From it, we eventually derive the tight-binding model studied in this dissertation.

Before we discuss the physical phenomena under consideration, we delve into the fundamental principles of geometric phases in Sec. 2.2. Thereby, we also introduce Bloch theory as the framework for constructing the Brillouin zone and the momentum-space Berry curvature. Next, we introduce the concept of Hall effects and elaborate on their relation to the topology of the Brillouin zone in Sec. 2.3. We focus in particular on the quantised topological Hall effect, which is expected to arise in the short-pitched multi- q magnets in the strong coupling limit. Finally, in Sec. 2.4, we present the approach of the modern theory of orbital magnetisation and relate it to the expressions evaluated in the results chapters.

2.1. Electronic System

The behaviour of electrons in a solid is contingent on numerous factors originating from the interactions between themselves and the nuclei, as well as external electromagnetic fields. Many electronic properties can be adequately described through approximations to simplified models. For the purpose of studying the topology of the electronic states in this dissertation, we employ a tight-binding model which describes a discrete lattice approximation.

Discrete Models

While single-particle and many-particle quantum mechanical models in the continuum are described by unbounded Hilbert space operators, the tight-binding approximation produces a bounded operator on a discrete Hilbert space. As we seek to study the topology of the electronic spectrum via algebraic methods, we aim to construct an algebra containing all observables obtained from the Hamiltonian and its translates through holomorphic functional calculus. Bounded Hamiltonians themselves are part of this

algebra as their domain does not change under multiplication. Moreover, discrete lattice models possess convenient finite approximations that can be used for numerical evaluation.

In this section, we give an overview of how to describe electrons from a non-relativistic quantum mechanical viewpoint. For this, we begin with the description of a single electron in a magnetic field. We introduce the Schrödinger equation for a quantum particle and discuss the energy terms in the Hamilton operator of a massive particle with charge and spin affected by an electromagnetic field. Subsequently, we present the more general setting of many interacting electrons and their treatment with Density Functional Theory (DFT). From it, we obtain an effective one-particle Hamiltonian with the same form as in the first part. Finally, we perform a tight-binding approximation to a discrete lattice system in order to derive the bounded tight-binding Hamilton operator, which is the subject of scrutiny in the ensuing chapters.

Section content

2.1.1. Single Electron Hamiltonian

The behaviour of a single quantum particle is contingent on the potential landscape surrounding it. For a charged particle, such as the electron, there exist supplementary interactions with electromagnetic fields that also couple to the spin degrees of freedom. A non-interacting gas of particles can be reasonably well described by the individual particles, which renders this model relevant for the description of many electrons as well. In the following, we present the minimal non-relativistic quantum mechanical description of a single electron in a scalar potential and an electromagnetic field.

The time evolution of a quantum particle is described by the time-dependent Schrödinger equation

Time evolution

$$i\hbar \frac{\partial}{\partial t} |\psi_t\rangle = H |\psi_t\rangle,$$

a linear, partial differential equation, where $\hbar$ denotes the Planck constant, H the Schrödinger operator acting on a Hilbert space $\mathcal{H}$, and $t \in \mathbb{R} \mapsto |\psi_t\rangle \in \mathcal{H}$ the time dependent state of the particle. By Stone's theorem [Hal13, Chap. 10.2], if H is self-adjoint, there exists a strongly continuous 1-parameter group uniquely solving the related initial value problem.

For a non-relativistic charge- and spin-less particle of mass m , the Schrödinger operator can be obtained by quantising the Hamilton function of a classical particle of mass m

Hamilton operator

$$h : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}, \quad (\mathbf{x}, \mathbf{p}) \mapsto \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}),$$

where the first term describes the kinetic energy of the particle and the second term the static, scalar potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$. For this, one replaces the position and momentum coordinate functions $\mathbf{x}, \mathbf{p} \in \mathbb{R}^d$ by unbounded, essentially self-adjoint, linear operators $\hat{\mathbf{x}}, \hat{\mathbf{p}}$ on $\mathcal{H}$ with commutation relation $[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij} \mathbf{1}$. Quantisation is generally ambiguous, inter alia, because the coordinate functions commute and the operators do not. There exists various different quantisation procedures [AE05]. Fortunately, since we do not deal

2. Electronic Properties

with mixed polynomials of coordinate functions this does not concern us. The obtained Schrödinger operator is commonly referred to as Hamilton operator or Hamiltonian

$$H = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}}).$$

Here, $V(\hat{\mathbf{x}})$ is understood as a multiplication operator in the sense of functional calculus. In general, this Hamiltonian is an unbounded operator but depending on the properties of the scalar potential V it can be made essentially self-adjoint, i.e., with a unique self-adjoint extension.

*Electromagnetic
potential*

The additional presence of an electromagnetic field with a magnetic vector potential $\mathbf{A} \in C(\mathbb{R} \times \mathbb{R}^d, \mathbb{R}^3)$ and an electric scalar potential $\phi \in C(\mathbb{R} \times \mathbb{R}^d, \mathbb{R})$ affects quantum particles if they have an electric charge q . Its influence is analogous to the Lorentz force in classical mechanics. We obtain

$$H = \frac{1}{2m} (\hat{\mathbf{p}} - q\mathbf{A}(t, \hat{\mathbf{x}}))^2 + q\phi(t, \hat{\mathbf{x}}) + V(\hat{\mathbf{x}}).$$

Spin

In order to further incorporate the influence of the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ on the spin of the particle, we require an additional term. This term can be deduced heuristically, but also arises from the non-relativistic approximation of the relativistic quantum theory described by the Dirac equation. The resulting Schrödinger equation for non-relativistic charged particles with spin $\frac{1}{2}$, mass m , and charge q is also known as Pauli equation. The corresponding (Pauli) Hamiltonian is given by

$$H = \frac{1}{2m} (\hat{\mathbf{p}} - q\mathbf{A}(t, \hat{\mathbf{x}}))^2 + q\phi(t, \hat{\mathbf{x}}) + V(\hat{\mathbf{x}}) + g \frac{q\hbar}{4m} \boldsymbol{\sigma} \cdot \mathbf{B}(t, \hat{\mathbf{x}}), \quad (2.1)$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)^T$ denotes the Pauli matrices as components of a vector and $g \approx 2$ denotes the g-factor describing the strength of the spin magnetic moment as introduced in Chap. 1.1.1. We implicitly treat any scalar expression, such as the first three terms, as scalar 2×2 matrices with respect to the spin degrees of freedom.

Spinor

Remark 2.1 (Spinor representation). The reason for the non-relativistic spin coupling term and spin operators to feature the Pauli matrices as representation of $\mathfrak{su}(2)$ originates from the representation theory of the Lorentz group and the Clifford algebra of Minkowski space. In this remark, we want to give an outline of this relationship:

The Schrödinger equation is not manifestly invariant under Lorentz transformation and therefore incompatible with special relativity. Indeed, Lorentz invariance is incompatible with any scalar description of fermions (spin- $\frac{1}{2}$ particles). Instead, they are described by the relativistic Dirac equation which is a linear first-order partial differential equation for a spinor field $\Psi : \mathbb{R}^{1,3} \rightarrow \mathbb{C}^4$ on flat Minkowski space $\mathbb{R}^{1,3}$. Spinor fields are similar to complex vector fields, however, they transform covariantly under the action of a certain double covering of the Lorentz group, the Spin group, instead of the orthogonal group. This accounts for their characteristic property to change sign under a 2π spacial rotation and justifies their interpretation as 'square roots' of vector fields.

The proper orthochronous Lorentz group $\text{SO}^+(1, 3)$ (restricted to preserve the orientation of space and direction of time) has the double cover $\text{SL}(2, \mathbb{C})$ with Lie algebra $\mathfrak{sl}(2, \mathbb{C}) \cong \mathfrak{so}(3, 1)$. Any irreducible $\mathbb{C}$ -linear representation of $\mathfrak{sl}(2, \mathbb{C})$ can be classified as a $(2m + 1)$ -dimensional spin- m representation for $m \in \frac{1}{2}\mathbb{Z}$. From the 2-dimensional $\mathbb{C}$ -linear spin- $\frac{1}{2}$ representation and its complex conjugate, we can construct a 4-dimensional $\mathbb{R}$ -linear representation, that generates a projective representation of the Lorentz group via the exponential map for Lie groups. We obtain the so-called bispinor representation $(\frac{1}{2}, 0) \oplus (0, \frac{1}{2})$. Spinors of the corresponding representation space are known as bispinors consisting of two 2-dimensional Weyl spinors which transform separately under the representations $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$ [Hal15].

The irreducible representations of the Lie algebra of the Lorentz group are related to the representations of the Clifford algebra over Minkowski space $\text{Cl}(1, 3)$ [Ham17]. Therefore, both can be expressed on the same representation space. The generators of this Clifford algebra appear in the Dirac operator in order to make its square equal to the Klein-Gordon operator. They can be chosen of the form

$$\gamma_0 = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} \quad \text{and} \quad \gamma_j = \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix} \quad j = 1, 2, 3,$$

with the Pauli matrices σ_i . Since the 4-dimensional bispinors from the shared representation space can be decomposed into two 2-dimensional Weyl spinors, the Dirac equation can be expressed in terms of Pauli matrices acting on these spinors. In the non-relativistic limit one of the Weyl spinors is smaller than the other by order of $\frac{v}{c}$ and can be neglected. The two equations reduce to a single equation in the form of Eq. (2.1) [Bih17, Chap. A].

2.1.2. Solid State Hamiltonian

A solid-state system consists of many interacting particles, that shape its electronic structure. A system of interacting electrons cannot be solved exactly with conventional methods, however, by density-functional theory (DFT) it is possible to exactly map it to a system of non-interacting electrons in an effective potential depending on the electron density. The non-interacting problem can be solved exactly in a self-consistent way to obtain the interacting ground-state energy and density. Then, we can factorise the non-interacting many particle Schrödinger equation to obtain an effective one-electron Hamiltonian with the effective potential.

In the following, we want to give a brief overview over DFT and DFT for spin-polarized systems to motivate the one-electron effective model studied in this dissertation. For this we follow mainly the lecture notes [Fou16], [Bih17], and [Blü17].

For the most general description of electron dynamics in quantum mechanical terms we use the Schrödinger equation of the many-particle system:

Many particles

$$\frac{d}{dt} |\Psi\rangle = H |\Psi\rangle.$$

2. Electronic Properties

Here, the Schrödinger operator H contains the kinetic terms of the electrons and nuclei, the electron-electron, electron-nuclei, and nuclei-nuclei interaction potentials, and external potentials. The first approximation one puts into place is the so-called Born-Oppenheimer approximation [BO27]: The movement of the nuclei is neglected, and the nuclei are assumed to stay in their equilibrium position. This casts the electrons into a static external potential. The resulting many-electron Schrödinger equation

$$(T + V_{ee} + V_{en} + E_{nn})\Psi = E\Psi$$

contains the kinetic term of the interacting electrons, the electron-electron interaction potential by the mutual Coulomb repulsion, the static electron-nucleon interaction potential, and the static nucleon-nucleon energy.

Hohenberg-Kohn

Solving such an interacting many-electron system is still incredibly expensive. One of the most successful approaches is the so-called density-functional theory (DFT), which is based on two central theorems discovered by Hohenberg and Kohn [HK64]. They found that for N particles in an external potential $V(\mathbf{r})$, the many-body wave function Ψ and the potential $V(\mathbf{r})$ in a non-degenerate ground state are uniquely determined by the particle density distribution

$$n(\mathbf{r}) = \int d\mathbf{r}_2 \cdots \int d\mathbf{r}_N \Psi^*(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N).$$

Furthermore, there exists an energy functional $E[n(\mathbf{r})]$ of that density which is stationary to variations around the ground state [Bih17, Chap. 3.2].

Consequently, the ground state energy and electron density can be determined by minimising such an energy functional. The Hohenberg-Kohn energy functional

$$E[n(\mathbf{r})] = \int V_{\text{ext}}(\mathbf{r})n(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \iint \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' + G[n(\mathbf{r})]$$

consists of the external potential, the Coulomb interaction energy, and the functional $G[n(\mathbf{r})]$ containing all other contributions. The objective at this stage is to determine or approximate $G[n(\mathbf{r})]$ which is independent of the external potential.

Kohn-Sham

This can be facilitated by mapping the interacting system to a non-interacting system with the same density distribution in the ground state [Bih17, Chap. 3.2]. That is the central approach of Kohn-Sham theory [KS65], in which one extracts the kinetic energy T_0 of the non-interacting electron system from $G[n(\mathbf{r})]$:

$$E_{\text{xc}}[n(\mathbf{r})] = G[n(\mathbf{r})] - T_0[n(\mathbf{r})].$$

The resulting functional is known as the exchange-correlation energy functional. With it, one can construct an equation for the stationarity of the full energy functional, while ensuring particle conservation. Recasting it into the form of an effective single-electron position-space Schrödinger equation by expressing the kinetic energy in terms of wave functions ϕ_i yields the Kohn-Sham equations

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \frac{\delta E_{\text{xc}}[n(\mathbf{r})]}{\delta n(\mathbf{r})} \right] \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r}). \quad (2.2)$$

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The last term is also referred to as exchange-correlation potential V_{xc} . Since it depends on the electron density $n(\mathbf{r}) = \sum_{i=1}^N |\phi_i(\mathbf{r})|^2$ the Kohn-Sham equations require to be solved self-consistently. This entails, solving the equations for the exchange-correlation potential of an initial density, calculating a new density from the solution, and repeating the procedure iteratively until a stationary density is found. With it, we obtain a model for non-interacting electrons in an effective potential that also describes the interacting electrons.

To include the spin of the electrons, we can replace the scalar particle density by a hermitian 2-dimensional spin-density matrix $\mathbf{n}(\mathbf{r})$ as pioneered by Barth and Hedin [BH72]. Its components can be defined by the field operators ψ_α for particle of spin α by

Spin-dependence

$$n_{\alpha\beta}(\mathbf{r}) = \langle \Psi | \psi_\beta^\dagger \psi_\alpha | \Psi \rangle.$$

The Kohn-Sham equation Eq. (2.2) with single electron wave functions ϕ_i^α with $\alpha = +, -$ then takes the form [Blü17, Chap. 4.1]

$$\left[\left(-\frac{\hbar^2}{2m} \nabla^2 + \sum_\alpha \int \frac{n_{\alpha\alpha}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \right) \mathbb{1}_{2 \times 2} + V_{\text{ext}}(\mathbf{r}) + \frac{\delta E_{xc}[\mathbf{n}(\mathbf{r})]}{\delta \mathbf{n}(\mathbf{r})} \right] \begin{pmatrix} \phi_i^+(\mathbf{r}) \\ \phi_i^-(\mathbf{r}) \end{pmatrix} = \epsilon_i \begin{pmatrix} \phi_i^+(\mathbf{r}) \\ \phi_i^-(\mathbf{r}) \end{pmatrix}.$$

Again, the exchange-correlation potential depends on $n_{\alpha\beta}(\mathbf{r}) = \sum_{i=1}^N \phi_i^{\alpha\dagger} \phi_i^\beta$ which warrants a self-consistent treatment. The density can be expanded in terms of a scalar and vectorial part using the identity matrix and the Pauli matrices which span the space of 2×2 matrices:

$$\mathbf{n}(\mathbf{r}) = \frac{1}{2} (n(\mathbf{r}) \mathbb{1}_{2 \times 2} + \boldsymbol{\sigma} \cdot \mathbf{m}(\mathbf{r})).$$

Here, $n(\mathbf{r})$ denotes the charge density and $\mathbf{m}(\mathbf{r})$ the magnetisation density. The external potential V_{ext} and the exchange-correlation potential V_{xc} are now also 2×2 matrices and can be decomposed in the same way in terms of a scalar potential and a magnetic field:

$$V_{\text{ext}} = V_{\text{ext}} \mathbb{1}_{2 \times 2} + \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{ext}}(\mathbf{r}) \quad \text{and} \quad V_{xc} = V_{xc} \mathbb{1}_{2 \times 2} + \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}_{xc}(\mathbf{r}),$$

where $\mu_B = \frac{e\hbar}{2m_e}$ denotes the Bohr magneton. For the exchange-correlation components it is

$$V_{xc} = \frac{\delta E_{xc}[n(\mathbf{r}), \mathbf{m}(\mathbf{r})]}{\delta n(\mathbf{r})} \quad \text{and} \quad \mathbf{B}_{xc}(\mathbf{r}) = \frac{\delta E_{xc}[n(\mathbf{r}), \mathbf{m}(\mathbf{r})]}{\delta \mathbf{m}(\mathbf{r})}.$$

Thus, we can express the Kohn-Sham one-electron Hamiltonian in the form

$$H_{KS} = \frac{1}{2m} (\hat{\mathbf{p}} - e\mathbf{A}_{\text{ext}}(\hat{\mathbf{x}}))^2 + V_{\text{eff}}(\hat{\mathbf{x}}) + \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{eff}}(\hat{\mathbf{x}}) \quad (2.3)$$

similar to Eq. (2.1), with effective potential $V_{\text{eff}}(\hat{\mathbf{x}}) := \sum_\alpha \int \frac{n_{\alpha\alpha}(\mathbf{r}')}{|\hat{\mathbf{x}} - \mathbf{r}'|} d\mathbf{r}' + V_{\text{ext}}(\hat{\mathbf{x}}) + V_{xc}(\hat{\mathbf{x}})$ and effective magnetic field $\mathbf{B}_{\text{eff}}(\hat{\mathbf{x}}) := \mathbf{B}_{\text{ext}}(\hat{\mathbf{x}}) + \mathbf{B}_{xc}(\hat{\mathbf{x}})$.

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2.1.3. Tight-binding Hamiltonian

The tight-binding method is a technique to approximately solve a one-particle Schrödinger equation using a bounded Hamiltonian on a discrete lattice. The latter is obtained by choosing a basis of localised atomic-like wave functions and projecting the full continuous Hamiltonian onto their subspace. This renders it bounded, which is a prerequisite for the C^* -algebraic approach delineated in Chap. 3. Tight-binding models have been employed with great success in the description of topological insulators. The fundamental premise is the supposition that the spectrum of the tight-binding Hamiltonian manifests the same topological features as the lowest part of the energy spectrum from its continuum model. This was recently confirmed to be the case for models in strong constant magnetic fields perpendicular to a two-dimensional crystal in the strong binding regime [SW22]. Following [Fou16], we want to differentiate between semi-empirical and ab-initio tight-binding methods.

In the following, we sketch a tight-binding approximation of a magnetic single electron Hamiltonian in the form discussed in the preceding sections. We then proceed to discuss the assumptions made in order to obtain this model. We further remark upon recent developments in rigorous verification of the preservation of the topological features during the tight-binding reduction. Eventually, we present the tight-binding Hamiltonian considered in this dissertation. For more details, we refer to [Fou16; SW22].

*Continuum
Hamiltonian*

Let us consider the single electron continuum Hamiltonian of the form

$$H = \frac{1}{2m}(\hat{\mathbf{p}} - e\mathbf{A}_{\text{ext}}(\hat{\mathbf{x}}))^2 + V(\hat{\mathbf{x}}) + \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{eff}}(\hat{\mathbf{x}})$$

with periodic crystal potential V , static effective magnetic field $\mathbf{B}_{\text{eff}}$, and vector potential $\mathbf{A}_{\text{ext}}$ for an external constant magnetic field $\nabla \times \mathbf{A}_{\text{ext}} = \mathbf{B}_{\text{ext}}$ which we consider unrelated to $\mathbf{B}_{\text{eff}}$. H is an unbounded operator on $\mathcal{H} = \mathbb{C}^2 \otimes L^2(\mathbb{R}^d)$.

*Localised wave
function*

We assume that the electrons are localised around the atomic lattice sites of a d -dimensional lattice labelled by $\mathbb{Z}^d$. Let $\phi(\mathbf{r})$, $|\phi(\mathbf{r})|^2 = 1$, denote the lowest energy eigenfunction (s -orbital) with energy eigenvalue ϵ of the Hamiltonian

$$H_0 = \frac{1}{2m}(\hat{\mathbf{p}} - e\mathbf{A}_{\text{ext}}(\hat{\mathbf{x}}))^2 + V_0(\hat{\mathbf{x}})$$

for an electron in the spherical potential V_0 of one isolated atom. Note that $\phi(\mathbf{r})$ is, however, not an eigenfunction of the Hamiltonian with the full crystal potential V . We assume that the full potential can be expressed as

$$V(\mathbf{r}) = \sum_{\mathbf{m} \in \mathbb{Z}^d} V_{\mathbf{m}}(\mathbf{r}) = \sum_{\mathbf{m} \in \mathbb{Z}^d} V_0(|\mathbf{r} - \mathbf{r}_{\mathbf{m}}|),$$

with V_0 the local potential at the origin site. We assume that the $V_{\mathbf{m}}$ have non-overlapping support.

We can construct the wave function $\phi_{\mathbf{m}} \in L^2(\mathbb{R}^d)$ at lattice site $\mathbf{m} \in \mathbb{Z}^d$ as a translation of the wave function $\phi_0 \equiv \phi$ at the origin site with position $\mathbf{r}_0 = 0$. Since ordinary translations do not commute with the magnetic momentum operator in the kinetic term, we use the magnetic translations

$$\phi_{\mathbf{m}}^A(\mathbf{r}) = \hat{V}_{\mathbf{m}}^A \phi(\mathbf{r}) = e^{-i\Gamma_{A'}([\mathbf{r}, \mathbf{r}-\mathbf{r}_{\mathbf{m}}])} \phi(\mathbf{r} - \mathbf{r}_{\mathbf{m}})$$

with $\Gamma_{A'}([\mathbf{r}, \mathbf{r} - \mathbf{r}_{\mathbf{m}}]) := \frac{e}{\hbar} \int_{[\mathbf{r}, \mathbf{r}-\mathbf{r}_{\mathbf{m}}]} A' = 2\pi(\mathbf{r} \wedge_{\Phi} \mathbf{r}_{\mathbf{m}}).$

The phase is evaluated along the straight line from $\mathbf{r}$ to $\mathbf{r} - \mathbf{r}_{\mathbf{m}}$, and in the symmetric gauge it can be expressed as matrix product with the antisymmetric flux matrix Φ : $\mathbf{x} \wedge_{\Phi} \mathbf{y} = \frac{1}{2} \mathbf{x}^T \Phi \mathbf{y}$. More details on the magnetic translations can be found in Chap. 3.1.2. A' denotes the modified magnetic vector potential (as a 1-form) such that $dA' = -B_{\text{ext}}$ [Bro64; Zak64]. The modified form allows the magnetic translations to commute with $\hat{\mathbf{p}} - e\mathbf{A}_{\text{ext}}(\hat{\mathbf{x}})$. For A_{ext} in the symmetric gauge, it is given by $A' = -A_{\text{ext}}$.

The phase functions $\phi_{\mathbf{m}}^A$ are the eigenfunctions with eigenvalue ϵ of the magnetically translated Hamiltonian

$$H_{\mathbf{m}}^A = \hat{V}_{\mathbf{m}}^A H_0 \hat{V}_{\mathbf{m}}^{A-1} = \frac{1}{2m} (\hat{\mathbf{p}} - e\mathbf{A}_{\text{ext}}(\hat{\mathbf{x}}))^2 + V_{\mathbf{m}}(\hat{\mathbf{x}}) \quad \text{with} \quad V_{\mathbf{m}}(\mathbf{r}) = \hat{V}_{\mathbf{m}}^{A'} V_0(\mathbf{r}) \hat{V}_{\mathbf{m}}^{A'-1}.$$

We project the Hamiltonian H onto the subspace spanned by the normalised wave functions $\phi_{\mathbf{i}}^A$, $\mathbf{i} \in \mathbb{Z}^d$, to obtain the tight-binding Hamiltonian H^{TB} on $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$ with components

$$H_{\mathbf{ij}}^{TB} := \langle \phi_{\mathbf{i}}^A | H | \phi_{\mathbf{j}}^A \rangle \in M_2(\mathbb{C}).$$

Here, the scalar product is evaluated for all components of the spin space separately. If the local wave functions overlap, they are not orthogonal with respect to the L^2 scalar product. Nevertheless, they can be orthogonalised, and we can identify their linear span with $\ell^2(\mathbb{Z}^d)$. For the diagonal components of the tight-binding Hamiltonian, we obtain

$$\begin{aligned} & \langle \phi_{\mathbf{i}}^A | \frac{1}{2m} (\hat{\mathbf{p}} - e\mathbf{A}_{\text{ext}}(\hat{\mathbf{x}}))^2 + V(\hat{\mathbf{x}}) | \phi_{\mathbf{i}}^A \rangle \\ &= \int d\mathbf{r} \phi_{\mathbf{i}}^A(\mathbf{r})^* \left(\frac{1}{2m} (-i\hbar\nabla - e\mathbf{A}_{\text{ext}}(\mathbf{r}))^2 + V_{\mathbf{i}}(\mathbf{r}) \right) \phi_{\mathbf{i}}^A(\mathbf{r}) = \epsilon \\ \text{and} \quad & \langle \phi_{\mathbf{i}}^A | \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{eff}}(\hat{\mathbf{x}}) | \phi_{\mathbf{i}}^A \rangle = \int d\mathbf{r} \phi_{\mathbf{i}}^A(\mathbf{r})^* \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{eff}}(\mathbf{r}) \phi_{\mathbf{i}}^A(\mathbf{r}) \approx \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{eff}}(\mathbf{r}_{\mathbf{i}}), \end{aligned}$$

where we used the locality of the lattice potentials and assumed that the effective magnetic field $\mathbf{B}_{\text{eff}}$ varies slowly in comparison to the support of the localised wave functions. For the off-diagonal elements we find

$$\begin{aligned} & \langle \phi_{\mathbf{i}}^A | \frac{1}{2m} (\hat{\mathbf{p}} - e\mathbf{A}_{\text{ext}}(\hat{\mathbf{x}}))^2 + V(\hat{\mathbf{x}}) | \phi_{\mathbf{j}}^A \rangle \\ &= \int d\mathbf{r} \phi_{\mathbf{i}}^A(\mathbf{r})^* \left(\frac{1}{2m} (-i\hbar\nabla - e\mathbf{A}_{\text{ext}}(\mathbf{r}))^2 + V_{\mathbf{i}}(\mathbf{r}) + V_{\mathbf{j}}(\mathbf{r}) \right) \phi_{\mathbf{j}}^A(\mathbf{r}) \end{aligned}$$

2. Electronic Properties

$$\begin{aligned}
&= \int d\mathbf{r} e^{-2\pi i \mathbf{r} \wedge_{\Phi} (\mathbf{r}_j - \mathbf{r}_i)} \phi(\mathbf{r} - \mathbf{r}_i)^* \left(\epsilon + V_0(\mathbf{r} - \mathbf{r}_j) \right) \phi(\mathbf{r} - \mathbf{r}_j) \\
&= e^{-2\pi i \mathbf{r}_i \wedge_{\Phi} (\mathbf{r}_j - \mathbf{r}_i)} \int d\mathbf{r} e^{-2\pi i \mathbf{r} \wedge_{\Phi} (\mathbf{r}_j - \mathbf{r}_i)} \phi(\mathbf{r})^* \left(\epsilon + V_0(\mathbf{r} - (\mathbf{r}_j - \mathbf{r}_i)) \right) \phi(\mathbf{r} - (\mathbf{r}_j - \mathbf{r}_i)) \\
&=: -e^{-2\pi i \mathbf{r}_i \wedge_{\Phi} \mathbf{r}_j} \lambda_{\text{hop}} =: -\lambda_{\text{hop}}(\mathbf{i}, \mathbf{j}).
\end{aligned}$$

Here, we used the assumptions that the external magnetic field $\mathbf{B}_{\text{ext}}$ is constant, that only nearest-neighbour wave functions overlap, that all nearest-neighbour sites have the same distance, and that V_0 is spherical. This renders the expression for the hopping parameter λ_{hop} independent of the position $\mathbf{r}_i$ and the direction to the nearest-neighbour $\mathbf{r}_j - \mathbf{r}_i$.

Because of the presence of the complex phase $e^{-2\pi i \mathbf{r} \wedge_{\Phi} (\mathbf{r}_j - \mathbf{r}_i)}$, λ_{hop} is defined by an oscillatory integral. It can be shown, however, that its integral kernel is positive and has a representation as a non-oscillatory integral [FSW22, Sec. 5]. This makes λ_{hop} a positive real number that describes the quantum mechanical tunnelling amplitude between neighbouring atoms. Moreover, the magnetic phase factor $e^{-2\pi i \mathbf{r}_i \wedge_{\Phi} \mathbf{r}_j}$ is consistent with the one obtained by Peierls substitution method [Pei33; Lut51]. We obtained precisely the hopping term of the Hofstadter Hamiltonian [Hof76].

The only contribution left, stems from the off-diagonal elements of the spin coupling term $\langle \phi_i^A | \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{eff}}(\hat{\mathbf{x}}) | \phi_j^A \rangle$ which we assume vanishes, since the magnetic field varies slowly in space in comparison to the lattice constant and the localised wave functions.

From the considerations above, we obtain a tight-binding approximation of H as a bounded operator on $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$ with the form

$$H^{TB} = - \sum_{\langle \mathbf{i}, \mathbf{j} \rangle \in \mathbb{Z}^{2d}} \lambda_{\text{hop}}(\mathbf{i}, \mathbf{j}) |\mathbf{i}\rangle \langle \mathbf{j}| + \mu_B \sum_{\mathbf{i} \in \mathbb{Z}^d} \boldsymbol{\sigma} \cdot \mathbf{B}(\mathbf{x}_i) |\mathbf{i}\rangle \langle \mathbf{i}| + \epsilon \sum_{\mathbf{i} \in \mathbb{Z}^d} |\mathbf{i}\rangle \langle \mathbf{i}|,$$

where $\langle \mathbf{i}, \mathbf{j} \rangle$ denotes the restriction of the sum to the nearest neighbours and $|\mathbf{i}\rangle$, $\mathbf{i} \in \mathbb{Z}^d$, is an orthonormal basis of $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$. Since we computed the components from a different and non-orthogonal basis $|\phi_j^A\rangle \approx |\mathbf{i}\rangle$, the expressions above receive some corrections from the unitary orthonormalisation transformation. For a rigorous treatment of the tight-binding reduction of a continuum model we refer to [SW22]. If we are not interested in the absolute energy values, we can drop the last term for the analysis of the spectral topology.

*Topological
equivalence*

Remark 2.2 (Spectral and topological properties). In order to study the topological properties of an electronic system using the tight-binding model, we require the latter to capture the same topological features as the underlying continuum model. Tight-binding models have been successfully used for some time for the study of topological insulators, which suggests an affirmative correspondence.

As demonstrated in [SW22], the topological properties are preserved in the case of two-dimensional crystals in the presence of a strong perpendicular magnetic field. In the following, we briefly summarise this result: Let λ linearly scale the strength of the magnetic field and quadratically scale the depth of the spherical atomic potential wells of the Hamiltonian H^λ . Let ρ^λ denote the inter-well hopping coefficient defined as an

overlap integral. Then, the resolvent of the scale-free continuum model converges in the operator norm on $L^2(\mathbb{R}^2)$ to the resolvent of the tight-binding Hamiltonian:

$$\left((\rho^\lambda)^{-1}H^\lambda - z\mathbb{1}\right)^{-1} \rightarrow J^*(H^{\text{TB}} - z\mathbb{1})^{-1}J \quad \text{for } \lambda \rightarrow \infty,$$

with $z \in \mathbb{C} \setminus \sigma(H^{\text{TB}})$ and $J : L^2(\mathbb{R}^2) \rightarrow \ell^2(\mathbb{Z}^2)$ an appropriate partial isometry [SW22, Thm. 3.1]. It can be further demonstrated, that for large λ the topological indices (describing the Hall conductance of the integer quantum Hall effect) in both models are in agreement [SW22, Thm. 3.2].

There are several approaches to obtain a tight-binding model [Fou16]. In the so-called *ab initio* tight-binding method one computes the parameters for an explicit basis set and an effective potential, and proceeds to iteratively calculate the charge density from the tight-binding model until self-consistency is obtained. This way one can solve the DFT equations discussed in the last section.

Semi-empirical model

An alternative is the so-called semi-empirical tight-binding method in which the parameters of the model are treated as adjustable. This has the advantage, that no explicit set of basis functions needs to be chosen. Instead, one simply derives the form of the tight-binding Hamiltonian as done above. The most common approximation for this approach is the form of the effective potential

$$V_{\text{eff}}(\mathbf{r}) = \sum_{\mathbf{i}} V_{\text{eff},\mathbf{i}}(|\mathbf{r} - \mathbf{r}_{\mathbf{i}}|),$$

where $\mathbf{r}_{\mathbf{i}}$ denotes the position of the atom of site $\mathbf{i}$ and $V_{\text{eff},\mathbf{i}}$ is assumed to be spherical and short-ranged. According to DFT calculations, this is a good approximation for many solids [FH89; Fou16].

For the purpose of this dissertation, we study a semi-empirical tight-binding Hamiltonian describing electrons coupled to a multi- q texture $\mathbf{n} \in C(\mathbb{R}^d, \mathbb{R}^3)$ in a constant magnetic field $\mathbf{B}$:

Magnetic multi- q Hamiltonian

$$H = - \sum_{\langle \mathbf{i}, \mathbf{j} \rangle \in \mathbb{Z}^{2d}} \lambda_{\text{hop}}(\mathbf{i}, \mathbf{j}) |\mathbf{i}\rangle \langle \mathbf{j}| + \lambda_{\text{xc}} \sum_{\mathbf{i} \in \mathbb{Z}^d} \boldsymbol{\sigma} \cdot \mathbf{n}(\mathbf{x}_{\mathbf{i}}) |\mathbf{i}\rangle \langle \mathbf{i}|.$$

The hopping parameter $\lambda_{\text{hop}}(\mathbf{i}, \mathbf{j})$ is given by $\lambda_{\text{hop}} e^{i\Gamma_A([\mathbf{i}, \mathbf{j}])}$, and we usually assume $\lambda_{\text{xc}}/\lambda_{\text{hop}} \gg 1$. It is important to note that we consider multi- q textures with length scales approaching the lattice constant, thereby straining the assumption of vanishing off-diagonal terms for the coupling to the spin. Moreover, the influence of the external magnetic field on the spins is not considered separately.

In Chap. 3.4.1 we demonstrate that the above tight-binding Hamilton operator can be interpreted as the representation of an element of the observable C^* -algebra that we construct in Chap. 3.1.

2.2. Geometric Phases

Quantum mechanical states describe physics up to an arbitrary complex phase. However, under adiabatic time-evolution along a closed path on a parameter manifold, an initial energy state changes by a phase with a dynamic and a geometric contribution, the latter of which is gauge invariant and holds physical meaning.

In general, while changing system parameters over time, an initial energy eigenstate transitions into a superposition of all other eigenstates as governed by the Schrödinger equation. The adiabatic approximation of the initial state only changing by a phase is only justified for slowly changing systems and energetically well-separated eigenstates. This evolution describes a kind of parallel transport of the eigenstate along a path, which corresponds to the connection of a line bundle. The geometric contribution to the phase is also commonly referred to as the Berry phase and can be expressed in terms of the Berry connection and its curvature on the parameter manifold.

Section content

In this section, we follow the lecture notes [MF14; Mok17] for a brief introduction to geometric phases in quantum systems. For a textbook account on this subject, we direct the reader to [Boh+03]. At the end of the section, we present the derivation of Bloch theory and the Brillouin zone manifold, which represents one of the most common settings for Berry curvature physics.

Parameter dependence

Let us consider a quantum system described by a parameter-dependent Hamilton operator $H(\lambda)$ on a Hilbert space $\mathcal{H}$ with parameter $\lambda \in M$ from a differentiable manifold M . We assume that the Hamiltonian depends smoothly on λ such that its discrete spectrum $\{\epsilon_n(\lambda)\}$ consists of unique smooth functions on M . The corresponding instantaneous eigenstates $\{|n\lambda\rangle \in \mathcal{H}\}$, satisfying $H(\lambda)|n\lambda\rangle = \epsilon_n(\lambda)|n\lambda\rangle$, can in general only be locally defined as smooth maps on patches $U \subset M$. They are only unique up to a λ dependent $U(1)$ phase factor, which is the freedom to choose a gauge for the description.

Time evolution

Changing the parameter λ needs to be parameterised over time $t \in \mathbb{R}$ by a path $\mathcal{C}$ with $\lambda : [0, T] \rightarrow \mathcal{C} \subset M, t \mapsto \lambda(t)$. We assume this path lies fully in a patch U of M on which the eigenstates are defined smoothly. The time evolution of a state $\psi(t) \in \mathcal{H}$ following this path is governed by the Schrödinger equation

$$i \frac{\partial \psi(t)}{\partial t} = H(\lambda(t)) \psi(t).$$

Adiabatic evolution

Let us assume, that the state $\psi(0)$ at time $t = 0$ is the eigenstate $|n\lambda(0)\rangle$ and its evolution at time t is the eigenstate $e^{-i\alpha_n(t)}|n\lambda(t)\rangle$ of the same energy eigenvalue up to a complex phase. This is known as the adiabatic approximation, where the system remains in the same energy state over its time-evolution. If we expand a general solution of the Schrödinger equation into a superposition of energy eigenstates

$$|\psi(t)\rangle = \sum_m c_m(t) |m\lambda(t)\rangle,$$

we obtain a differential equation for the evolution of its coefficients in the form of

$$\partial_t c_n(t) = -i\epsilon_n(t)c_n(t) - \sum_m c_m(t) \langle n\lambda(t) | \partial_t | m\lambda(t) \rangle.$$

To fulfil the adiabatic assumption with $c_m(0) = c_m(t) = \delta_{nm}$, it is necessary that the factors

$$\langle n\lambda(t) | \partial_t | m\lambda(t) \rangle = \frac{\langle n\lambda(t) | \partial_t H | m\lambda(t) \rangle}{\epsilon_m(t) - \epsilon_n(t)}$$

vanish for $n \neq m$, which requires in particular that the energy eigenvalues $\epsilon_m(t)$ and $\epsilon_n(t)$ stay well separated. The expression on the right-hand side of the equation describes the transition frequency between the states $|n\lambda(t)\rangle$ and $|m\lambda(t)\rangle$. If we parameterise our path more slowly in time, this frequency gets smaller. The adiabatic evolution is therefore only valid for infinitely slow changes of the system over time, and $e^{-i\alpha_n(t)} |n\lambda(t)\rangle$ only approximates a solution of the Schrödinger equation otherwise.

Applying the adiabatic assumption, we can solve the time-evolution equation and obtain the phase $\alpha_n(t)$ for which we find two separate contributions

Berry phase

$$|\psi_n(t)\rangle = e^{-i \int_0^t \epsilon_n(\tau) d\tau} e^{i \int_0^t \langle n\lambda\tau | \partial_\tau | n\lambda\tau \rangle d\tau} |n\lambda(t)\rangle =: e^{-i\alpha_{\text{dyn}}(t)} e^{i\gamma_n(t)} |n\lambda(t)\rangle. \quad (2.4)$$

The first phase α_{dyn} is the dynamic phase and the second phase γ_n the geometric phase, which is also known as the Berry phase after Michael Berry [Ber84] who first discovered it. The integrand of the Berry phase integral is the pullback $\lambda^* \mathcal{A}^n$ of the so-called Berry connection, given by a local connection 1-form

Berry connection

$$\mathcal{A}^n := i \langle n\lambda | \partial_{\lambda_i} | n\lambda \rangle d\lambda_i \in \Omega^1(U, \mathbb{R})$$

on a patch $U \subset M$. Since $|n\lambda\rangle$ is smooth on a given patch of M the same is true for $\mathcal{A}^n$. Switching to an alternative set of eigenstates $\{|n\lambda'\rangle\}$, that differs by a λ dependent phase $e^{i\zeta_n(\lambda)}$, generates an additional contribution

$$\mathcal{A}^{n'} = \mathcal{A}^n - d\zeta_n. \quad (2.5)$$

Consequently, the Berry connection itself is not gauge invariant. Instead, many physical expressions depend on its gauge-invariant exterior derivative, the Berry curvature, which is the local curvature 2-form

Berry curvature

$$\begin{aligned} \Omega^n &:= d\mathcal{A}^n = \partial_{\lambda_i} \mathcal{A}_j^n - \partial_{\lambda_j} \mathcal{A}_i^n d\lambda_i \wedge d\lambda_j \\ &= -2 \operatorname{Im} \langle \partial_{\lambda_i} n\lambda | \partial_{\lambda_j} n\lambda \rangle d\lambda_i \wedge d\lambda_j \in \Omega^2(U, \mathbb{R}). \end{aligned}$$

It is independent of the choice of gauge and can therefore be extended to a global 2-form $\Omega^n \in \Omega^2(M, \mathbb{R})$. Its significance becomes apparent, if we choose a closed path $\mathcal{C}$ in $U \subset M$, such that $\lambda(0) = \lambda(T)$ and therefore $H(0) = H(T)$ and $\epsilon_n(0) = \epsilon_n(T)$. Then, the Berry

2. Electronic Properties

phase only depends on the path $\mathcal{C}$ or, by Stokes theorem, on its enclosing surface $S \subset U$ with $\partial S = \mathcal{C}$:

$$\gamma_n(\mathcal{C}) = \oint_{\mathcal{C}} \mathcal{A}^n = \int_S \Omega^n.$$

If M is a compact, orientable, 2-dimensional Riemannian manifold without boundary, then the integral over the entirety of M defines the Chern number

$$\int_M \Omega^n = C^n \in \mathbb{Z},$$

which is topological invariant of the system.

A useful form of the Berry curvature components in terms of the partial derivatives of the Hamiltonian is given by

$$\Omega_{ij}^n = -2 \operatorname{Im} \sum_{m \neq n} \frac{\langle m\lambda | \partial_{\lambda_i} H(\lambda) | n\lambda \rangle \langle n\lambda | \partial_{\lambda_j} H(\lambda) | m\lambda \rangle}{(\epsilon_n(\lambda) - \epsilon_m(\lambda))^2}.$$

It often appears in linear response theory, such as for electronic transport.

Fibre bundle interpretation

Following Michael Berry's discovery of the Berry phase Barry Simon [Sim83] recognised it as the holonomy in a Hermitian line bundle with connection naturally defined by the adiabatic assumption, which specifies a way of transporting a vector along a curve. The one-dimensional eigenspace at any specific well-separated energy defines a line bundle over the parameter manifold and by embedding the line bundle one obtains a natural Hermitian connection.

Let P denote the orthogonal projection from the ambient trivial vector bundle onto the line bundle, then the curvature is given by $\frac{i}{2\pi} \operatorname{tr}(P dP \wedge dP)$, which is the form we discussed in Chap. 1.3.2 for a two-band system as remarked in Rem. 1.3. For more details we refer to the review article [BT13].

2.2.1. Bloch Theory

Bloch theory describes extended states in a periodic system that can be characterised by a crystal momentum vector from the Brillouin zone. It is one of the most common setups for the theory of Berry curvature. We follow loosely [Bel03, Chap. 2.5] to derive the Bloch theory for a two-dimensional periodic system. A similar derivation by the author for the case of magnetic Bloch functions has been given in [Pra20, Chap. 3.2.3].

Periodic system

Let us consider a two-dimensional system with a periodic potential $V(\mathbf{x})$ with period a in both directions, for instance, in the case of a square crystal lattice. Such a potential is invariant with respect to translations from the lattice translation group $\mathbb{G} = \{n_1 a \hat{\mathbf{e}}_x + n_2 a \hat{\mathbf{e}}_y\}$.

If the Hamiltonian H only contains a kinetic term beside the potential, it commutes with the translation operators $\hat{T}_{\mathbf{v}}$, $\mathbf{v} \in \mathbb{G}$: $[H, \hat{T}_{\mathbf{v}}] = 0$. This implies, there exists a basis

of simultaneous eigenstates of H and $\hat{T}_{\mathbf{v}}$ allowing us to decompose the Hilbert space $\mathcal{H}$ onto eigenspaces of $\hat{T}_{\mathbf{v}}$ on which the so-called Bloch Hamiltonian can be defined.

Irreducible representations of Abelian groups, such as $\mathbb{G}$, can be expressed in terms of their characters. For the translation group $\mathbb{R}^n$ and its subgroups the characters are functions $\eta : \mathbb{R}^n \rightarrow U(1)$ that can be characterised by elements $\mathbf{k}$ of the dual group $\mathbb{R}^{n*} \cong \mathbb{R}^n$ such that $\eta_{\mathbf{k}}(\mathbf{v}) = e^{i\mathbf{k} \cdot \mathbf{v}}$. The dual group of $\mathbb{G}$ is defined as $\mathbb{G}^* := \mathbb{R}^{2*}/G^\perp$ with $G^\perp = \{\mathbf{G} \in \mathbb{R}^2 \mid \mathbf{G} \cdot \mathbf{v} = 2\pi\mathbb{Z} \ \forall \mathbf{v} \in \mathbb{G}\}$. It is isomorphic to the Brillouin zone and contains those vectors $\mathbf{k}$ for which $\eta_{\mathbf{k}} = \eta_{\mathbf{k}'}$ is only satisfied if $\mathbf{k} - \mathbf{k}' \in G^\perp$. This is equivalent to $\mathbf{k} \in \mathbb{R}^2 / \frac{2\pi}{a}\mathbb{Z}^2$. The Brillouin zone $\mathbb{B}$ is therefore homeomorphic to the 2-torus T^2 .

Brillouin zone

With that, we can decompose the Hilbert space into eigenspaces of $\hat{T}_{\mathbf{v}}$, $\mathbf{v} \in \mathbb{G}$, over the Brillouin zone $\mathbb{B}$:

Bloch functions

$$\mathcal{H} = \int_{\mathbf{k} \in \mathbb{B}}^\oplus d^2\mathbf{k} \ \mathcal{H}_{\mathbf{k}} \quad \text{and} \quad H = \int_{\mathbf{k} \in \mathbb{B}}^\oplus d^2\mathbf{k} \ H_{\mathbf{k}}.$$

Any finite collection of states from $\mathcal{H}$ spans a vector bundle over the Brillouin zone.

Let $\psi_{n\mathbf{k}}$, $n \in \mathbb{N}$, $\mathbf{k} \in \mathbb{B}$ denote the eigenfunctions of H and $\hat{T}_{\mathbf{v}}$, $\mathbf{v} \in \mathbb{G}$, with

$$\psi_{n\mathbf{k}}(\mathbf{r} - \mathbf{v}) = \hat{T}_{\mathbf{v}}\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{v}}\psi_{n\mathbf{k}}(\mathbf{r}).$$

We can define a set of lattice periodic eigenfunctions of the translation operator by $u_{n\mathbf{k}}(\mathbf{r}) := e^{i\mathbf{k} \cdot \mathbf{r}}\psi_{n\mathbf{k}}(\mathbf{r})$, such that the phases of the eigenvalues cancel each other. These are energy eigenfunctions of the so-called Bloch Hamiltonian $H_{\mathbf{k}} := e^{i\mathbf{k} \cdot \hat{\mathbf{x}}} H e^{-i\mathbf{k} \cdot \hat{\mathbf{x}}}$ with the form $H_{\mathbf{k}} = \frac{1}{2m}(\hat{\mathbf{p}} - \hbar\mathbf{k})^2 + V(\hat{\mathbf{x}})$ motivating the interpretation of $\mathbf{k}$ as crystal momentum.

The Berry curvature $\Omega^n(\mathbf{k}) = -2 \text{Im} \langle \partial_{k_i} u_{n\mathbf{k}} | \partial_{k_j} u_{n\mathbf{k}} \rangle dk_i \wedge dk_j$ with respect to the Brillouin zone occurs in the theory of electronic transport phenomena such as the Hall conductivity of the quantum Hall effect and the (quantum) anomalous Hall effect, and also in the modern theory of orbital magnetisation, as we will see in Sec. 2.3 and Sec. 2.4.

Berry curvature

$\Omega^n(\mathbf{k})$ possesses some simple symmetry properties: It is antisymmetric under time-reversal $\Omega^n(-\mathbf{k}) = -\Omega^n(\mathbf{k})$ and symmetric under space inversion $\Omega^n(-\mathbf{k}) = \Omega^n(\mathbf{k})$. This implies in particular, that for time-reversal and space-reversal invariant systems, the Berry curvature is zero for every $\mathbf{k}$. Moreover, for all time-reversal systems, the integral of $\Omega^n(\mathbf{k})$ over the entire Brillouin zone is zero. Consequently, for systems with non-zero Hall conductivity, time-reversal symmetry needs to be broken, for instance, by the presence of a magnetic field or magnetisation texture.

2.3. Hall Effects

Hall effects constitute a broad category of phenomena in two-dimensional systems that are characterised by the generation of a voltage perpendicular to an applied current. The prototypical instance is the classical Hall effect, which is induced by a magnetic field permeating the system and scales linearly with the field strength. For low temperatures, it has been observed that the transverse conductivity assumes precise quantised values.

2. Electronic Properties

This can be explained by the topology of the Brillouin zone of the crystal momentum and is known as the (ordinary) quantum Hall effect. Moreover, in the absence of a magnetic field, (quantised) Hall effects occur as a consequence of other phenomena that break time-reversal symmetry, such as spin-orbit coupling or the non-coplanar spin textures. The former gives rise to the anomalous Hall effect, which is linear in the magnetisation, while the latter leads to the topological Hall effect, which depends on the scalar spin chirality of the texture.

Hall resistivity

In Hall experiments, the Hall conductivity σ_{xy} , which is the off-diagonal element of the conductivity tensor σ , cannot be accessed directly. Instead, one can readily measure the components of the resistivity tensor $\rho = \sigma^{-1}$. The transverse Hall resistivity $\rho_{xy} = \frac{-\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}$ can be decomposed into three distinct contributions

$$\rho_{xy} = \rho_{xy}^{\text{HE}} + \rho_{xy}^{\text{AHE}} + \rho_{xy}^{\text{THE}} = R_0 B + R_S M + \rho_{xy}^{\text{THE}}.$$

The first contribution from the classical Hall effect is proportional to the magnetic field strength B with the factor R_0 predominantly dependent on the density of charge carriers. The second contribution is attributed to the anomalous Hall effect and is proportional to the magnetisation M . The coefficient R_S is material-specific and also depends on the longitudinal resistivity ρ_{xx} . The final component is attributed to the topological Hall effect and incorporates all subsequent contributions that occur in the presence of non-coplanar textures.

Section content

We begin this section with a brief introduction to the classical Hall effect. Next, we present the quantum Hall effect and discuss its working principles and how they connect to the momentum-space topology of the Brillouin zone. Subsequently, we provide a brief overview of the quantum anomalous Hall effect. Finally, we discuss the topological Hall effect in the emergent magnetic field picture for weak and strong coupling as well as its quantised version for short-pitched spin textures.

Classical Hall effect

The classical Hall effect was discovered by Edwin Hall in 1878 as a permanent alteration of the charge distribution in a thin gold leaf permeated by a magnetic field [Hal79]. We can explain its working principle in the minimal setting of an ideal gas of fermions with charge $q = \pm e$ confined to the xy -plane and a constant uniform magnetic field $\mathbf{B} \equiv B \hat{\mathbf{e}}_z$ perpendicular to the plane. If we apply a constant current with area density $\mathbf{j} \equiv j \hat{\mathbf{e}}_x$, the particles are affected by the Lorentz force acting perpendicular to the $\mathbf{j}$ and $\mathbf{B}$. Since fermion gases are incompressible, an opposing electric field $\mathbf{E} \equiv E \hat{\mathbf{e}}_y$ arises, that compensates the force density:

$$nq\mathbf{E} + \mathbf{j} \times \mathbf{B} = 0.$$

Here, n denotes the fermion density, i.e., the number of fermions per unit area. Solving this equation for the current density $\mathbf{j}$ yields

$$\mathbf{j} = -\frac{nq}{B} \hat{\mathbf{e}}_z \times \mathbf{E} := \begin{pmatrix} \sigma & 0 \\ 0 & 0 \end{pmatrix} \mathbf{E}$$

where σ denotes the 2×2 conductivity tensor relating the in-plane components of $\mathbf{j}$ and $\mathbf{E}$ to each other. In the chosen coordinate system it is anti-diagonal with elements $\pm\sigma_H$ given by the Hall conductivity

$$\sigma_H = \frac{j}{E} = \frac{nq}{B} =: \nu \frac{e^2}{h} \quad \text{with} \quad \nu = \frac{nh}{qB}.$$

The sign of the charge q determines the sign of the Hall conductivity, which can be used to differentiate positively and negatively charged particles. The size of the conductivity is linear in the filling factor ν , which can be manipulated by altering the magnetic field strength B or the charge carrier density n .

2.3.1. Quantum Hall Effect

The quantum Hall effect describes the quantisation of the Hall conductivity in a constant magnetic field at low temperature. It was first reported by Klaus von Klitzing [KDP80] in 1980 for an electron gas trapped in the inversion layer of a metal-oxide-semiconductor field-effect transistor (MOSFET) with magnetic fields between 15T and 18T at temperatures as low as 1K to 2K and was found to be independent of the sample geometry.

For an electron gas in a constant magnetic field, the electronic spectrum splits into narrow, equidistant Landau levels, which are fully occupied for integer filling factors. However, for a clean system without disorder and localised states, the conductivity cannot be observed as a step function, since the system never resides in between Landau levels over an extended interval of field strengths or charge densities. Instead, the presence of disorder is required, although the states localised by the disorder do not participate in any electronic transport.

In 1981, Robert Laughlin connected the precise value of the plateaus to the real space topology of the setup [Lau81]. Shortly after, in 1982, David Thouless, Mahito Kohmoto, Peter Nightingale, and Marcel den Nijs (TKNN) demonstrated that the Hall conductivity can be expressed as a Brillouin zone integral over the momentum-space Berry curvature [Tho+82; ASS83] which corresponds to the momentum-space Chern number as recognised by Barry Simon [Sim83]. This proved that the quantum Hall effect is determined by a bulk property, even though for finite samples, where the flat Landau levels bend upwards near the edges, the Hall current is carried by edge states. The extension of the Berry curvature description to the case of weak and strong disorder was developed by Jean Bellissard, who first devised the non-commutative C^* -algebraic framework used in this dissertation [Bel86].

In the following, we introduce the ordinary quantum Hall effect, its prerequisites, and its interpretation in the context of momentum space topology. An extended review of the quantum Hall effect is given by the author in [Pra20, Chap. 3.2]. At the end, we comment on the (quantum) anomalous Hall effect.

2. Electronic Properties

Landau levels The Landau Hamiltonian for a free gas of fermions with mass m and charge $q = \pm e$ in the presence of a constant magnetic field with vector potential $\mathbf{A}(\mathbf{x})$ is given by

$$H_L = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{x}}))^2.$$

The energy eigenvalues of this system take quantised values of the form

$$E_n = \hbar \frac{qB}{m} \left(n + \frac{1}{2} \right), \quad n \in \mathbb{N},$$

known as Landau levels. Each Landau level has a unit degeneracy of $n_B = \frac{qB}{h}$ corresponding to the relation between magnetic flux per unit area $\phi = B$ and magnetic flux quantum $\phi_0 = \frac{h}{q}$. Thus, the filling factor $\nu = \frac{nh}{qB}$ can be expressed as the ratio $\frac{n}{n_B}$ between charge carrier density and unit degeneracy.

Localisation The Fermi energy E_F indicates the energy of the highest occupied state at zero temperature. In a clean system as above, it always resides at the highest unfilled Landau level, and as soon as it is fully occupied, it jumps to the next higher one. Since the filling factor changes linearly with n or B , so does the Hall conductivity, and we do not observe extended plateaus.

In the presence of disorder, however, the Landau levels are broadened, and localised states, which do not participate in charge transport, occupy the energy spectrum between the Landau levels. Therefore, the charge carrier density n can increase while the Landau levels below the Fermi energy are fully occupied, such that the Hall conductivity maintains a constant value. The conundrum of the quantised Hall effect is the precise value of the plateaus in integer multiples of $\frac{e^2}{h}$, although the localised states are missing from the Landau levels.

Edge states In a sample with finite width without disorder, the edge acts as a sharp confining potential. This bends the otherwise flat Landau levels upwards such that all Landau levels below the Fermi energy in the bulk cross the Fermi level at the edge. The corresponding Fermi surface states carry currents that can be interpreted as charge carriers skipping orbit to orbit along the edge. The magnetic field imposes a direction of the angular momentum such that these currents on the opposing edges flow in opposite directions. Since the number of edge states is precisely the number of occupied Landau levels, this explains the integer Hall conductivity. However, this argument is difficult to generalise to the disordered case, where the Hall current is carried by the edge states around localised bulk states [Dav97, Chap. 6.5-6.6].

The Laughlin argument Robert Laughlin explained the integer values (in multiples of $\frac{e^2}{h}$) of the Hall conductivity with the gauge invariance of the system and its ability to pump charges [Lau81]. For that, he considered a metallic loop as the sample with the magnetic field normal to the surface. Then, he demonstrated that for filled Landau levels, increasing the magnetic potential by a constant increment, which is equivalent to forcing one flux quantum through the loop,

results in a shift of the centre of the orbits of the electronic states to their neighbours' positions along the width of the loop. This can be conceptualised as pumping one electron per occupied Landau level through the system, resulting in a potential difference between the edges. The change of the magnetic flux can be induced by applying a current to the loop.

This property needs to be preserved in the presence of impurities, which bind down localised states from the Landau levels. For the localised states, the gauge transformation only results in a change of phase as they do not extend along the loop. Therefore, the remaining delocalised states in the Landau level need to compensate this by carrying more current.

David Thouless, Mahito Kohmoto, Peter Nightingale, and Marcel den Nijs (TKNN) connected the quantised Hall conductivity to the momentum space topology of the electronic spectrum in terms of the Berry curvature [Tho+82]. Their motivation was the following: By Laughlin's argument, if a Landau level splits into sublevels separated by an energy gap, each of them should contribute an integer amount to the Hall conductivity while the total contribution of the Landau levels remains unchanged. To solve this seeming paradox, they explicitly derived the Hall currents of the sublevels.

TKNN

Splitting of the Landau levels is, for instance, achieved in the presence of a periodic potential and the number of sublevels corresponds to the numerator of the reduced ratio of magnetic flux quanta per the potential's unit cells. Let $V(x, y)$ denote such a potential with period $a, b \in \mathbb{R}$ in x - and y -direction, and let the magnetic flux per unit cell be $\phi = \frac{l}{m}\phi_0 = abB$. We can construct Bloch functions similar to those in Sec. 2.2.1. However, due to the magnetic field, the translation generator representing the lattice translation group $\mathbb{G}$ no longer commute. This is resolved by switching to a supercell with an integer number of flux quanta and the corresponding magnetic lattice group $\mathbb{G}^A$ for which the magnetic translation operators $\hat{V}^A$ commute:

$$\begin{aligned}\hat{V}^A(v\hat{\mathbf{e}}_x)\hat{V}^A(w\hat{\mathbf{e}}_y) &= e^{i\Gamma_B(\langle \hat{\mathbf{x}}, \hat{\mathbf{x}} - v\hat{\mathbf{e}}_x, \hat{\mathbf{x}} - v\hat{\mathbf{e}}_x - w\hat{\mathbf{e}}_y \rangle)} \hat{V}^A(v\hat{\mathbf{e}}_x + w\hat{\mathbf{e}}_y) \\ &= e^{i\frac{e}{2\hbar}vwB} \hat{V}^A(v\hat{\mathbf{e}}_x + w\hat{\mathbf{e}}_y) = e^{i\frac{e}{\hbar}vwB} \hat{V}^A(w\hat{\mathbf{e}}_y)\hat{V}^A(v\hat{\mathbf{e}}_x).\end{aligned}$$

This is the case for $\frac{vw}{abm} \in \mathbb{Z}$ since the magnetic field strength can be expressed as $B = \frac{2\pi\hbar}{abq} \frac{l}{m}$ in terms of the flux per unit cell. The magnetic translation group consists consequently only of the elements

$$\mathbb{G}^A = \{n_1 am\hat{\mathbf{e}}_x + n_2 b\hat{\mathbf{e}}_y \mid n_1, n_2 \in \mathbb{Z}\} \subset \mathbb{G} \subset \mathbb{R}^2 \quad \text{for} \quad \frac{\phi}{\phi_0} = \frac{l}{m}, \quad l, m \in \mathbb{N}.$$

Then, the construction of the magnetic Brillouin zone $\mathbb{B}^A$ with Bloch functions $\psi_{n\mathbf{k}}$ precedes analogous to the non-magnetic case presented in Sec. 2.2.1 with the difference that the eigenfunctions of the Bloch Hamiltonian are only periodic up to a magnetic phase

$$u_{n\mathbf{k}}(\mathbf{r}) = e^{-i\Gamma_{A'}([\mathbf{r}, \mathbf{r} - \mathbf{v}])} u_{n\mathbf{k}}(\mathbf{r} - \mathbf{v}) \quad \forall \mathbf{v} \in \mathbb{G}^A.$$

2. Electronic Properties

The Hall conductivity in this setting can be determined from the Bloch Hamiltonian $H_{\mathbf{k}}$ by the Kubo equation from linear response theory [Tho+82]:

$$\begin{aligned}\sigma_H &= \frac{e^2}{h} \sum_n^{\text{occ}} \int_{\mathbb{B}^A} \frac{d^2\mathbf{k}}{2\pi} \left(-2 \text{Im} \sum_m^{\text{unocc}} \frac{\langle u_{n\mathbf{k}} | \partial_{k_i} H_{\mathbf{k}} | u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | \partial_{k_i} H_{\mathbf{k}} | u_{n\mathbf{k}} \rangle}{(E_{n\mathbf{k}} - E_{m\mathbf{k}})^2} \right) \\ &= \frac{e^2}{h} \sum_n^{\text{occ}} \int_{\mathbb{B}^A} \frac{d^2\mathbf{k}}{2\pi} \left(-2 \text{Im} \langle \partial_{k_1} u_{n\mathbf{k}} | \partial_{k_2} u_{n\mathbf{k}} \rangle \right).\end{aligned}$$

We recognise this as the Brillouin zone integral over the Berry curvature which is equal to the sum over the Chern numbers of the occupied states

$$\sigma_H = \frac{e^2}{h} \sum_n^{\text{occ}} C_n.$$

For our purpose, we can reformulate the integral in terms of Fermi projections $P_{\mathbf{k}} = \sum_n^{\text{occ}} |u_{n\mathbf{k}}\rangle \langle u_{n\mathbf{k}}|$ onto the occupied states, for which we obtain

$$\sigma_H = \frac{e^2}{h} \int_{\mathbb{B}^A} \frac{d^2\mathbf{k}}{2\pi} i \text{tr} \left(P_{\mathbf{k}} [\partial_{k_1} P_{\mathbf{k}}, \partial_{k_2} P_{\mathbf{k}}] \right)$$

as verified in App. A1. This expression is in the same form as the formula for the first Chern numbers, we derive in Chap. 3.3.2 for the C^* -algebra of physical observable we construct in Chap. 3.1.

The presumed paradox studied by TKKN was then resolved by their discovery that the Chern numbers carried by the subbands of the Landau levels follow a Diophantine equation, which enforces that the individual contributions add up to 1 for each full level.

Non-commutative geometry

In order to define the Chern numbers in the presence of disorder, which breaks translation invariance such that the Brillouin zone cannot be constructed as a well-defined manifold, Jean Bellissard applied techniques from the newly developed mathematical field of non-commutative geometry [Bel86; BES94]. In this framework, he was able to prove the integrality result for weak and strong disorder by connecting it to an index theorem. Even the correspondence between the edge states currents in finite samples and the bulk topology can be proven in the presence of disorder in the non-commutative framework [PS16]. This principle is known as the bulk-boundary correspondence.

2.3.1.1. Quantum anomalous Hall Effect

The anomalous Hall effect depends on the magnetisation of the material in combination with spin-orbit coupling, and therefore persists even in the absence of an external magnetic field. Its quantised version can be described by the momentum space Berry curvature, just as the ordinary quantum Hall effect. In the following, we provide a short outline following [Nag+10].

Shortly after his discovery of the classical Hall effect, Edwin Hall reported a one order of magnitude larger Hall effect in ferromagnetic irons such as Ni and Co [Hal81]. All contributions to this stronger Hall conductivity that depend on the magnetisation are conflated into the so-called anomalous Hall effect [Nag+10]. The intrinsic contribution attributed to the Berry curvature over all occupied states is dominant in metallic ferromagnets with moderate conductivity, while the extrinsic contribution attributed to impurity scattering prevails in highly conductive ferromagnets.

Anomalous Hall effect

In two-dimensional systems at low temperature with the Fermi energy within a gap between Bloch bands, the intrinsic anomalous Hall conductivity is quantised in multiples of $\frac{e^2}{h}$ analogous to the quantum Hall effect. An explicit setup featuring this so-called quantum anomalous Hall effect was first proposed by Frederick Haldane [Hal88] in the form of a tight-binding model on a honeycomb lattice with nearest and next-nearest neighbour hopping. Subsequently, Charles Kane and Eugene Mele [KM05b; KM05a] demonstrated that the circumstances in this model can be induced by spin-orbit interaction. From the symmetry considerations in Sec. 2.2.1, we know that non-zero Chern numbers require systems with broken time-reversal symmetry. This condition is met in the context of spin-orbit coupling. Insulators with non-zero Chern number within a band gap are called topological insulators or Chern insulators. They manifest a quantised Hall effect fully carried by surface states in the absence of an external magnetic field [PS16].

Quantum anomalous Hall effect

2.3.2. Topological Hall Effect

In the presence of non-coplanar spin textures, a Hall effect arises that is related to the scalar spin chirality. Since it does not depend on spin-orbit coupling, it can be considered separate from the anomalous Hall effect and is referred to as the topological Hall effect due to its occurrence in topological spin textures such as skyrmion crystals.

If the spins of the conduction electrons are strongly coupled to a smooth texture, one can assume adiabaticity and the scalar spin chirality can be interpreted as a real space Berry curvature or emergent magnetic field: The spins align with the texture while traversing the material and accumulate a Berry phase. For weak coupling or rapidly varying textures, the adiabatic assumption fails since the electrons cannot adjust their spins to the local magnetisation. Nevertheless, there still exists a topological Hall effect that is related to the scattering of electrons. For small-scale skyrmion lattices in the strong coupling limit, a crossover from the real to the momentum space curvature is expected, which leads to a quantum anomalous Hall effect that can be interpreted as a quantised topological Hall effect.

In the following, we give an overview of the various concepts related to the topological Hall effect. For the strong coupling limit, we derive the emergent magnetic field, and for the weak coupling limit, we introduce the non-adiabatic contributions. At the end, we present the quantised topological Hall effect predicted for small-scale skyrmion crystals in the strong coupling limit, which is the regime studied in this dissertation.

The coupling energy term for the spins of the conduction electrons favours the alignment with the magnetic texture. Therefore, in the strong coupling limit with smooth spin

Strong coupling regime

2. Electronic Properties

textures, the electron spin fully aligns with the magnetisation vectors. We can thus assume adiabaticity, implying that the electrons stay in their spin state and only gather a phase from following the texture while traversing the material. This is a Berry phase of the real space Berry curvature that can be expressed in terms of the continuous scalar spin chirality $\hat{\mathbf{n}} \cdot (\partial_x \hat{\mathbf{n}} \times \partial_y \hat{\mathbf{n}})$, and that can also be interpreted as a fictitious emergent magnetic field [Göb+18].

*Emergent
magnetic field*

Indeed, if we consider a co-moving frame of reference for the electron spin aligned to the magnetisation texture, the kinetic term of the electron Hamiltonian obtains a contribution resembling a magnetic vector potential. We can illuminate this procedure in the minimal model of the one electron Hamiltonian

$$H = \frac{\hat{\mathbf{p}}^2}{2m} - J\hat{\mathbf{n}}(\hat{\mathbf{x}}) \cdot \boldsymbol{\sigma}$$

in the presence of a smooth magnetisation texture $\hat{\mathbf{n}} : \mathbb{R}^2 \rightarrow S^2$ with coupling constant J . Switching to the reference frame of the electron with spin in z -direction can be achieved by a unitary transformation

$$U^\dagger(\mathbf{x})(\hat{\mathbf{n}}(\mathbf{x}) \cdot \boldsymbol{\sigma})U(\mathbf{x}) = \sigma_z.$$

If we parameterise the texture in polar coordinates as $\hat{\mathbf{n}}(\theta, \phi)$, then such a unitary transformation is given by $U(\theta, \phi) = \hat{\mathbf{n}}(\theta/2, \phi) \cdot \boldsymbol{\sigma} =: \mathbf{m} \cdot \boldsymbol{\sigma}$. From this, we obtain the transformed Hamiltonian

$$U^\dagger(\hat{\mathbf{x}})HU(\hat{\mathbf{x}}) = \frac{1}{2m} \left(\hat{\mathbf{p}}^2 - i\hbar U^\dagger(\hat{\mathbf{x}}) \nabla U(\hat{\mathbf{x}}) \right)^2 - J\sigma_z,$$

with additional term

$$i\hbar U^\dagger \nabla U =: \mathbf{A}^x \sigma_x + \mathbf{A}^y \sigma_y + \mathbf{A}^z \sigma_z \quad (2.6)$$

being an $\mathfrak{su}(2)$ -valued gauge field [NBK18]. In the adiabatic approximation, we neglect the coupling of different spin channels given by the off-diagonal components in spin space with $\mathbf{A}^x, \mathbf{A}^y$. Instead, we only consider the diagonal spin space components, that can be interpreted as a spin-dependent vector potential with real space components

$$A_i^\pm := \pm A_i^z = \pm \frac{\hbar}{e} (\mathbf{m} \times \partial_i \mathbf{m})_z,$$

where the sign is opposite for opposite spin states. The corresponding effective magnetic field has the field strength

$$B_z^\pm = (\nabla \times \mathbf{A}^\pm)_z = \pm \frac{\hbar}{2e} \hat{\mathbf{n}} \cdot (\partial_x \hat{\mathbf{n}} \times \partial_y \hat{\mathbf{n}}),$$

which we recognise as proportional to the continuous scalar spin chirality and thus the skyrmion density in skyrmionic crystals.

Accordingly, the magnetic flux for a spin texture with an isolated skyrmion in a ferromagnetic background is given by

$$\Phi^\pm = \int_{\mathbb{R}^2} d^2\mathbf{x} B_z^\pm = \pm \frac{\hbar}{2e} \int_{\mathbb{R}^2} d^2\mathbf{x} \hat{\mathbf{n}} \cdot (\partial_x \hat{\mathbf{n}} \times \partial_y \hat{\mathbf{n}}) = \pm 2\pi \frac{\hbar}{e} \deg \hat{\mathbf{n}}.$$

Hence, the topological Hall effect in the strong coupling limit can be used to detect skyrmions and scales linearly with the skyrmion density.

If the coupling is weak or the magnetic texture varies too rapidly in space for the electron spin to adjust, the adiabatic assumption is invalid [NBK18; NK19]. Nevertheless, also in the weak coupling limit a topological Hall effect exists. However, for its description the off-diagonal components from Eq. (2.6) that induce spin-flip transitions cannot be neglected. Since the $\mathfrak{su}(2)$ -valued gauge field was produced by a pure gauge transformation with vanishing field strength/curvature $dA + \frac{1}{2}[A, A] = 0$, they produce the same field as the adiabatic component

Weak coupling

$$B_z^{xy} = A_x^y A_y^x - A_x^x A_y^y = \frac{\hbar}{2e} \hat{\mathbf{n}} \cdot (\partial_x \hat{\mathbf{n}} \times \partial_y \hat{\mathbf{n}}).$$

The magnetisation breaks the $SU(2)$ gauge symmetry to $U(1)$, such that the projected gauge field $\mathbf{A}^\pm$ has finite field strength [NBK18].

The topological Hall conductivity behaves differently in the different regimes depending on the strength of the exchange coupling J , the length scale of the spin texture q^{-1} , the electron scattering time τ , and the mean free path $l = v_F \tau$, with the Fermi velocity v_F of the electrons. For instance, the effective field can be non-local in the diffusive regime, where the effective field arises from the effective spins that the electron encounters in their diffusive motion. For a skyrmion lattice, this results in a topological Hall effect that decreases in strength as the skyrmion density increases, which stands in stark contrast to the case of the strong coupling limit.

The topological Hall effects in the different regimes can be studied by various methods, such as through perturbation theory or in terms of spin gauge fields [NBK18], as introduced above. For more details on the weak coupling theory, we refer to [NK19].

For short-pitched skyrmion lattices in the strong coupling regime, such as the ones studied in this dissertation, the dominant descriptor changes from the real space to the momentum space Berry curvature [MNA21]. While the topological Hall conductivity increases with the skyrmion density in the real space picture, the magnetic Brillouin zone becomes larger for smaller skyrmion sizes which decreases the number of occupied bands contributing in the momentum space picture. Consequently, the extreme values are expected in the crossover region, where both Berry curvatures play a crucial role.

*Skyrmion
size-dependence*

In [MNA21], the optimum skyrmion size λ_{sk}^* is determined in terms of the lifetime τ of the itinerant electrons (proportional to the mean free path) and the coupling constant J . They find it proportional to $\sqrt{\tau}$ and in a wide range of τ and J , where adiabaticity holds, about ten times the lattice constant a , i.e. $q^* = \frac{2\pi}{\lambda_{\text{sk}}^*} \sim 0.1 \frac{2\pi}{a}$.

2. Electronic Properties

2.3.2.1. Quantised topological Hall Effect

For small-scale skyrmion lattices, the topological Hall effect is determined by the momentum-space Berry curvature, and a formation of gaps is induced in the electronic spectrum. Therefore, a quantisation of the Hall conductivity is expected.

The quantised topological Hall conductivity can be studied for an effective tight-binding model in which the hopping term receives a phase from the emergent magnetic vector potential generated by the spin texture. Investigations of the conditions to realise this effect suggest that the quantised effect would occur in skyrmion crystals even with strong disorder at room temperature [HEN15]. The quantised topological Hall effect can be mapped onto the classical quantum Hall effect by making the emergent magnetic field homogeneous and thereby assigning the electronic gapped states to Landau levels [Göb+17b; Göb+17a].

Below we introduce the effective tight-binding model from which the quantised topological Hall effect emerges and discuss its characteristic properties.

Quantisation

When the length scale of a multi- q spin texture approaches the lattice constant of its host material, the interference between periodicities of the lattice and the texture can lead to the formation of gapped energy states. Since the topological Hall conductivity in this regime is best described by the momentum-space Berry curvature that integrates over the Brillouin zone to a Chern number, it is expected to be quantised for fully occupied levels with Fermi energy inside spectral gaps. This can be modelled by the tight-binding Hamiltonian

Effective model

$$H = - \sum_{\langle \mathbf{i}, \mathbf{j} \rangle \in \mathbb{Z}^2 \times \mathbb{Z}^2} \lambda_{\text{hop}}^{\mathbf{i}\mathbf{j}} |\mathbf{i}\rangle \langle \mathbf{j}| \lambda_{\text{xc}} \sum_{\mathbf{i} \in \mathbb{Z}^2} \boldsymbol{\sigma} \cdot \mathbf{n}(\mathbf{x}_{\mathbf{i}}) |\mathbf{i}\rangle \langle \mathbf{i}|$$

on the Hilbert space $\mathbb{C}^2 \otimes \ell(\mathbb{Z}^d)$, where $\lambda_{\text{hop}}^{\mathbf{i}\mathbf{j}}$ denotes the transfer integral between nearest sites $\mathbf{i}$ and $\mathbf{j}$, λ_{xc} denotes the coupling strength, and $\boldsymbol{\sigma}$ denotes the vector of Pauli matrices. Switching to the co-moving frame for the texture $\mathbf{n}(\theta, \phi)$ as for the continuous case discussed above, leads to effective hopping parameters

$$\lambda_{\text{hop}}^{\text{eff}}(\mathbf{i}, \mathbf{j}) = \lambda_{\text{hop}}^{\mathbf{i}\mathbf{j}} U^\dagger(\mathbf{x}_{\mathbf{i}}) U(\mathbf{x}_{\mathbf{j}}) \longrightarrow \lambda_{\text{hop}}^{\text{eff}}(\mathbf{i}, \mathbf{j}) = \lambda_{\text{hop}} e^{ia_{\mathbf{i}\mathbf{j}}} \cos\left(\frac{\theta_{\mathbf{i}\mathbf{j}}}{2}\right)$$

$$\text{with } a_{\mathbf{i}\mathbf{j}} = \arctan\left(\frac{-\sin(\phi_{\mathbf{i}} - \phi_{\mathbf{j}})}{\cos(\phi_{\mathbf{i}} - \phi_{\mathbf{j}}) + \cot\left(\frac{\theta_{\mathbf{i}}}{2}\right) \cot(\theta_{\mathbf{j}})}\right) \quad \text{and} \quad \lambda_{\text{hop}} \in \mathbb{R},$$

where $\theta_{\mathbf{j}}$ and $\phi_{\mathbf{i}}$ denote the polar and azimuthal angles of the spin direction at site $\mathbf{i}$, $\theta_{\mathbf{i}\mathbf{j}}$ denotes the angle between the spins at $\mathbf{i}$ and $\mathbf{j}$, and the arrow symbolises the projection onto the component parallel to the spin direction [HEN15]. The effective tight-binding Hamiltonian has the form

$$H = \sum_{\langle \mathbf{i}, \mathbf{j} \rangle \in \mathbb{Z}^2 \times \mathbb{Z}^2} \lambda_{\text{hop}}^{\text{eff}}(\mathbf{i}, \mathbf{j}) |\mathbf{i}\rangle \langle \mathbf{j}|,$$

similar to the Hofstadter Hamiltonian for the ordinary quantum Hall effect.

Studying the model introduced above, one finds gaps forming in the low energy regime between well separated bands with respective Chern number -1 [HEN15]. In contrast to the Landau levels they are not flat, but warped and even overlap in the regime of large electron density, which leads to the vanishing of the Hall plateaus.

Properties

In order to determine under which conditions the quantised topological Hall effect occurs in a skyrmion crystal, one needs to consider the effects of finite temperature, disorder, and finite exchange coupling on the Hall conductivity [HEN15]: The temperature scale is given by the size of the gaps. Focusing on the lowest gap, one finds it visibly affecting the Hall conductivity even at room temperature. Furthermore, strong disorder does not extinguish the Hall conductivity up to a disorder potential strength larger than the hopping constant λ_{hop} . Finally, the strong coupling limit is already reached at about $\lambda_{\text{xc}}/\lambda_{\text{hop}} > 3$, with plateaus observable for $\lambda_{\text{xc}}/\lambda_{\text{hop}} > 1$.

Adiabatically passing from the inhomogeneous, space-dependent, emergent magnetic field to the uniform average has no singularities and therefore preserves the topological properties of the states. This maps the gapped energy states to the flat Landau levels of the ordinary quantum Hall effect.

Unconventional behaviour

Using this approximation allows for the study of other influences, such as the topology of the structural lattice [Göb+17b; Göb+17a]. As such, at the van Hove singularity of the density of states, the Hall conductivity exhibits an unconventional behaviour: The bands below and above the van Hove singularity carry different Chern numbers, and the band at the van Hove singularity carries the entire compensating contribution to the vanishing overall Chern number for a fully occupied system.

We corroborate this unconventional behaviour in Chap. 5.2 and also find it exhibited by all real and momentum space Chern numbers. In particular, we find the band at the van Hove singularity to carry the entire contribution to the real space first Chern number that describes the real space winding of the electronic states.

In [Göb+17a, Sec. 3.4], an approximation for the energy dependence of the Hall conductivity is proposed, which has the Chern number coinciding with the skyrmion winding number for the bands below the van Hove singularity. However, our results challenge this approximation rule: For some areas of the parameter range of the studied textures, we find the momentum space Chern number vanishing while the winding number is preserved or even increased, as presented in Chap. 5.3.

2.4. Orbital Magnetisation

The motion of electrons gives rise to a magnetic field. For electrons in the orbits of free atoms, the emerging orbital magnetic moment contributes substantially to the overall magnetic moment. However, in solid-state systems, the situation is often different. The presence of electric crystal fields from the surrounding atoms lift the degeneracies in the system, thereby quenching the total orbital angular momentum present in the many-electron ground state. Nevertheless, if the one-electron Hamiltonian that describes a system exhibits broken time-reversal symmetry, it is possible for orbital magnetisation to arise in both finite and infinite samples.

2. Electronic Properties

Finite system

In finite systems, such as atoms and molecules, the orbital magnetisation can be calculated in a straightforward manner. The velocity operator $\hat{\mathbf{v}} = -\frac{i}{\hbar}[\hat{\mathbf{r}}, H]$ is defined as the commutator of the position operator $\hat{\mathbf{r}}$ and the Hamiltonian H of the system. From it the angular momentum operator $\hat{\mathbf{L}} = m_e \hat{\mathbf{r}} \times \hat{\mathbf{v}}$ can be defined easily. Therefore, the orbital magnetisation $\mathbf{M}_{\text{orb}}$, which is defined as the total orbital moment $\mathbf{m}_{\text{orb}}$ per unit volume V , is computed from the sum of the expectation values of $\hat{\mathbf{r}} \times \hat{\mathbf{v}}$ over all electronic eigenstates $|\psi_n\rangle$ of H with occupation number f_n :

$$\mathbf{M}_{\text{orb}} = -\frac{e}{2V} \sum_n f_n \langle \psi_n | \hat{\mathbf{r}} \times \hat{\mathbf{v}} | \psi_n \rangle. \quad (2.7)$$

This is analogous to the classical magnetic dipole moment as defined in Eq. (1.1).

Infinite system

For infinite systems, the computation is much more intricate. The eigenstates of the Hamiltonian H are extended states for which the position operator is not well-defined. This conundrum was resolved in 2005 through a variety of approaches from a semi-classical ansatz with Berry phase corrections [XSN05] over Wannier representation calculations of local and itinerant contributions [Tho+05; Cer+06] to perturbation theory calculations at finite temperature [Shi+07]. The results obtained culminate in the so-called *modern theory of orbital magnetisation in solids*, which treats orbital magnetisation as an electronic bulk property expressed as a gauge-invariant Brillouin zone integral over occupied Bloch functions.

Many challenges of the perturbational approach can be circumvented in the algebraic framework used in this dissertation, as demonstrated in [ST13] and discussed in Chap. 3.4.3.

Section content

In this section, we present the Wannier representation approach to the orbital magnetisation in periodic insulators and its heuristic extension to multi-band insulators, Chern insulators, and metals. This allows us to identify the local and itinerant circulation contributions. Subsequently, we briefly introduce the perturbation theory approach and its challenges. For an overview article we refer to [Tho11].

2.4.1. Wannier Representation Approach

The contributions to the orbital magnetisation can be calculated from an orthonormal basis of localised orbitals such as given by the Wannier representation. One finds a contribution from the local circulation of Wannier functions in the bulk and a second contribution from the currents carried by Wannier functions near the surface, which can be expressed as a gauge-invariant bulk property as well.

In the following, we present the local circulation and itinerant circulation contributions derived from the Wannier representation approach. From them, we obtain a Bloch theory expression for the orbital magnetisation of single-band insulators which can be extended to multi-band insulators, Chern insulators, and metals. In doing so, we follow [Tho11] and refer to the primary sources [Tho+05; Cer+06] for more details.

In the Wannier representation approach, we start with considering a finite sample from which we transition to an infinite periodic system. Localised orthonormal orbitals $|\phi_i\rangle$ inside the sample away from the surface are thereby associated with bulk Wannier functions $|\mathbf{R}\rangle$, with lattice vector $\mathbf{R}$. For insulators with vanishing Chern invariant they are exponentially localised which allows for the calculation of well-defined expectation values of the position operator.

LC and IC contributions

Let us consider first a single occupied band in a two-dimensional system. Replacing the wave functions in the finite expression in Eq. (2.7) with the Wannier function $|0\rangle$ in the home unit cell with volume V_0 results in the following contribution to the orbital magnetisation:

$$\mathbf{M}_{\text{orb}}^{LC} = -\frac{e}{2V_0} \langle 0 | \hat{\mathbf{r}} \times \hat{\mathbf{v}} | 0 \rangle.$$

This can be interpreted as the density of the magnetic moment arising from the Wannier function rotating around its centre.

A second contribution arises from the itinerant current at the boundary of a finite sample. While the bulk band in an insulating crystal generally carries no current, the Wannier-like functions near the surface carry a substantial net current with velocity $\mathbf{v}_n = \langle \phi_n | \hat{\mathbf{v}} | \phi_n \rangle$ at the Wannier centre $\mathbf{r}_n = \langle \phi_n | \hat{\mathbf{r}} | \phi_n \rangle$. Its contribution to the total magnetisation is given by

$$\mathbf{M}_{\text{orb}}^{IC} = -\frac{e}{2V_0} \sum_n \mathbf{r}_n \times \mathbf{v}_n,$$

It is important to emphasise that the Wannier-like orbitals themselves perform a centre-of-mass movement around the surface, which then generates the current. This itinerant circulation contribution can be expressed as a bulk property, such as the local circulation contribution [Tho+05].

Coming back to the extended states in the thermodynamic limit given by the Bloch representation $|\psi_{\mathbf{k}}\rangle$ with wave vector $\mathbf{k}$, we can express the contributions as Brillouin zone integrals. The Wannier functions in a periodic solid are defined in terms of the cell-periodic part of the Bloch functions $|u_{\mathbf{k}}\rangle = e^{-i\mathbf{k}\cdot\mathbf{r}} |\psi_{\mathbf{k}}\rangle$ such that

Bloch representation

$$|\mathbf{R}\rangle = \frac{V_0}{(2\pi)^2} \int d^2\mathbf{k} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})} |u_{\mathbf{k}}\rangle.$$

This requires the quantisation of the magnetic flux to an integer number of flux quanta per (super-)unit cell, such that $\mathbf{k}$ is a good quantum number. Then, the $|u_{\mathbf{k}}\rangle$ are eigenstates of the Hamiltonian $H_{\mathbf{k}} \equiv e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}}$ with eigenvalue $E_{\mathbf{k}}$. We obtain [Tho+05]

$$\mathbf{M}_{\text{orb}} = \mathbf{M}_{\text{orb}}^{LC} + \mathbf{M}_{\text{orb}}^{IC} = \frac{e}{2\hbar} \text{Im} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \langle \partial_{\mathbf{k}} u_{n\mathbf{k}} | \times (H_{\mathbf{k}} + E_{n\mathbf{k}}) | \partial_{\mathbf{k}} u_{n\mathbf{k}} \rangle.$$

Both contributions are individually gauge invariant and invariant with respect to shifts of the zero energy of the Hamiltonian. Such a shift generates a contribution proportional to $\int d^2\mathbf{k} \Omega_{\mathbf{k}} = 2\pi C$ with Berry curvature $\Omega_{\mathbf{k}}$ and Chern number C , which was assumed to be zero.

2. Electronic Properties

Extension

The above result can be extended to multi-band insulators and (heuristically) also to insulators with non-zero Chern number and even metals [Cer+06]. Several occupied bands are included straightforwardly by summing over the band index n . We denote the Bloch functions of band n by $|\psi_{n\mathbf{k}}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} |u_{n\mathbf{k}}\rangle$. This also implies multiple Wannier functions $|n\mathbf{R}\rangle$ in each unit cell. With these Bloch function we can also define the multi-band Berry curvature

$$\begin{aligned}\boldsymbol{\Omega}_{n\mathbf{k}} &= i \langle \partial_{\mathbf{k}} u_{n\mathbf{k}} | \times | \partial_{\mathbf{k}} u_{n\mathbf{k}} \rangle = -\text{Im} \langle \partial_{\mathbf{k}} u_{n\mathbf{k}} | \times | \partial_{\mathbf{k}} u_{n\mathbf{k}} \rangle \\ \Omega_{n\mathbf{k}}^z &= \Omega_{12}^n = -2 \text{Im} \langle \partial_{k_1} u_{n\mathbf{k}} | \partial_{k_2} u_{n\mathbf{k}} \rangle\end{aligned}$$

and Chern number

$$\mathbf{C} = \frac{1}{2\pi} \sum_n^{\text{occ}} \int d^2\mathbf{k} \boldsymbol{\Omega}_{n\mathbf{k}}.$$

Heuristically, we can counteract the contribution from a shift of the Hamiltonian's zero energy in systems with non-zero Chern number, by subtracting the corresponding term (twice, to account for the Hamiltonian and the eigenvalue). This way one obtains the expression [Cer+06]

$$\mathbf{M}_{\text{orb}} = \frac{e}{2\hbar} \text{Im} \sum_n^{\text{occ}} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \langle \partial_{\mathbf{k}} u_{n\mathbf{k}} | \times (H_{\mathbf{k}} + E_{n\mathbf{k}} - 2\mu) | \partial_{\mathbf{k}} u_{n\mathbf{k}} \rangle, \quad (2.8)$$

where μ denotes the chemical potential. This heuristic can be justified by the other approaches, which arrive at the same expression for Chern insulators and metals.

*Chemical
potential
dependence*

For (Chern) insulators with the chemical potential inside a spectral gap the derivative of the orbital magnetisation with respect to the chemical potential is proportional to the Chern number

$$\frac{d\mathbf{M}_{\text{orb}}}{d\mu} = \frac{e}{\hbar} \frac{\mathbf{C}}{2\pi}.$$

This relationship can be interpreted in terms of the chiral edge states of a finite sample cut from a two-dimensional Chern insulator [Cer+06, Chap. II.F.]:

The orbital magnetisation corresponds via $\nabla \times \mathbf{M}_{\text{orb}} = \mathbf{j}$ to a macroscopic current at the edge of the sample. The intensity $I = M_{\text{orb}}^z$ of this current is therefore related to the Chern number $\frac{dI}{d\mu} = \frac{e}{\hbar} C^z$. If the chemical potential is raised by $d\mu$, this fills $\frac{dk}{2\pi}$ states per unit length, and the intensity of the current increases by $dI = v \frac{e}{\hbar} \frac{dk}{2\pi}$ with group velocity $v = \frac{d\mu}{dk}$. This implies that C^z counts the difference in the number of chiral edge channels with positive and negative circulation.

The orbital magnetisation is a bulk property that stays valid in the thermodynamic limit of the infinite system without a boundary and that can be evaluated by adopting toroidal boundary conditions. The interpretation is therefore in line with the bulk-boundary correspondence between bulk characteristics and surface currents, well known for the quantum Hall effect and topological insulators [PS16, Preface].

One consequence of the multi-band case is that the local and itinerant contributions in the form above are no longer separately gauge invariant, whilst their sum maintains this property. Nevertheless, they can be regrouped into two gauge invariant contributions, as shown in [Cer+06, Chap. II.D.], that can be separately experimentally determined by gyromagnetic and magneto-optical experiments as derived in [SV08]. The regrouping involves expressing the components in terms of traces of the ground-state projector

*Fermi
projections*

$$P_{\mathbf{k}} = \sum_n^{\text{occ}} |u_{n\mathbf{k}}\rangle \langle u_{n\mathbf{k}}|$$

and its derivatives $\partial_{k_i} P_{\mathbf{k}}$ with respect to $\mathbf{k}$. As demonstrated in App. A2, we obtain for the z -component

$$M_{\text{orb}}^z = \frac{e}{\hbar} \text{Im} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \text{tr}(P_{\mathbf{k}} \partial_{k_1} P_{\mathbf{k}} H \partial_{k_2} P_{\mathbf{k}} + H P_{\mathbf{k}} \partial_{k_1} P_{\mathbf{k}} \partial_{k_2} P_{\mathbf{k}} - 2\mu P_{\mathbf{k}} \partial_{k_1} P_{\mathbf{k}} \partial_{k_2} P_{\mathbf{k}}).$$

This is the same form occurring in Eq. (3.69) from the C^* -algebraic approach presented in Chap. 3.4.3. This connection has also been drawn before in [ST13, Sec. 5].

2.4.2. Perturbation Theory Approach

The orbital magnetisation can be defined as the response of the free energy to changes in the magnetic field. Using perturbation theory, one can derive the orbital magnetisation formula of modern theory, which extends its validity to finite temperatures, strong magnetic fields, spin-orbit coupling, and even interacting electrons. The caveat of this approach is the control issue of perturbation theory for unbounded vector potentials such as the one of the magnetic field. This can be circumvented by using periodic magnetic fields and going to the long wave length limit as done in [Shi+07]. Another approach is the C^* -algebraic framework as presented in Chap. 3.4.3.

In the following, we present the thermodynamic definition of orbital magnetisation as the derivative of the free energy density with respect to the magnetic field. Subsequently, we will briefly discuss the approach using periodic magnetic fields following [Shi+07] and the extent of this description.

The orbital magnetisation (density) in quantum many-body theory is defined as the derivative of the grand thermodynamical potential $\Omega = E - TS - \mu N$ with respect to the magnetic field $\mathbf{B}$:

*Thermodynamic
definition*

$$\mathbf{M}_{\text{orb}} = -\frac{1}{V} \left(\frac{\partial \Omega}{\partial \mathbf{B}} \right)_{T, \mu}.$$

Here, V denotes the volume of the system, E the inner energy, T the temperature, S the entropy, N the number of particles, and μ the chemical potential. The magnetic field $\mathbf{B}$ is thought to only couple to the orbital motion of the electrons but not to their spin. For the computation, one starts with an auxiliary quantity in terms of the potential $K = E - \mu N$:

$$\tilde{\mathbf{M}}_{\text{orb}} = -\frac{1}{V} \left(\frac{\partial K}{\partial \mathbf{B}} \right)_{T, \mu}.$$

2. Electronic Properties

It relates back to the full orbital magnetisation through the relation

$$\frac{\partial(\beta \mathbf{M}_{\text{orb}})}{\partial \beta} = \tilde{\mathbf{M}}_{\text{orb}} \quad (2.9)$$

for $\beta = \frac{1}{kT}$. At $T = 0$, we have $\tilde{\mathbf{M}}_{\text{orb}} = \mathbf{M}_{\text{orb}}$.

*Perturbation
theory*

For a uniform magnetic field the orbital magnetisation operator is non-local. Therefore, in [Shi+07] a magnetic field with infinitely slow spatial variation $\mathbf{B}(\mathbf{r}) = B \cos(qy) \hat{\mathbf{e}}_z$ is employed. Then, the auxiliary orbital magnetisation is obtained as the linear order coefficient from an expansion of K in B :

$$\delta K(\mathbf{r}) = -\tilde{\mathbf{M}} \cdot \mathbf{B}(\mathbf{r}).$$

At the end of the calculation the limit $q \rightarrow 0$ yields the desired result for a uniform field. At zero temperature this results in precisely the formula in Eq. (2.8).

Generalisation

From the derivation in [Shi+07], one can also obtain a formula for the orbital magnetisation at finite temperatures by using the relation from Eq. (2.9). Moreover, the result is valid for insulators with and without Chern numbers and metals.

The approach can be further generalised to interacting systems in the framework of current and spin-density functional theory [Shi+07]. The finite temperature thermodynamic potential functional is constructed from the effective one-particle Schrödinger equation. Next, the variation of the functional in response to a variation in the magnetic field is evaluated. This leads to the same finite temperature formula as the perturbation of the non-interacting system discussed above.

3 | C*-Algebra Theory of Multi-q Textures

Mathematics is a succession of trivialities. The problem with mathematics is the accumulation of trivialities.

(Jean Bellissard)

The C^* -algebraic viewpoint on the quantum-mechanical operators that describe the observables of an electronic system offers numerous advantages. As such, it allows for the incorporation of arbitrary multi- q textures and arbitrary constant external magnetic fields as well as providing algebraic access to well-established topological invariants, such as the Chern numbers associated with the electronic spectrum, and physical properties, including the anomalous Hall conductivity and orbital magnetisation.

The common approach to study electronic state topology using the geometry of fibre bundles, aka *Berry phase physics*, requires the translation invariance of the Hamiltonian operator making quasi-momentum space a well-defined smooth manifold, the *Brillouin zone* $\mathbb{B}$. We introduced and discussed this framework in the second part of Chapter 2. By Bloch's theorem, physical observables can then be expressed as elements of $\mathcal{K} \otimes C(\mathbb{B})$, the compact operators that depend continuously on the quasi-momentum. As the algebra of continuous functions over the Brillouin zone is commutative, this approach can be equally expressed in terms of so-called commutative geometry.

Advantage over Bloch Theory

Breaking the translation invariance, the observable algebra becomes inherently non-commutative. This is the case for an incommensurate magnetic texture or an irrational number of magnetic flux quanta per unit cell. By analogy with the commutative case, one speaks of the non-commutative Brillouin zone as the fictitious underlying space, and many of the algebraic tools can be applied as before. These are C^* -algebras and their K -theories [Bla98; RLL00] as well as Alain Connes' non-commutative geometry [Con94].

The application of non-commutative geometry to solid-state phenomena was pioneered by Jean Bellissard with his description of the Integer Quantum Hall Effect (IQHE) in the presence of disorder [Bel86; BES94]. For this, he constructed a non-commutative observable algebra to describe an electronic Hamiltonian coupled to an arbitrary constant magnetic field and a disorder potential. He then employed the tools of non-commutative geometry to prove the integrality of the Hall conductivity. For weak disorder, he found the observable algebra isomorphic to the *irrational rotation algebra* or *non-commutative torus* and was even able to prove the integrality in the presence of strong disorder by identifying the Chern character with the index of a Fredholm operator.

Integer Quantum Hall Effect

3. C^* -Algebra Theory of Multi- q Textures

Topological Insulators

Based on Bellissard’s seminal work, non-commutative geometry has been successfully employed in the field of topological insulators for which spin-orbit interaction induces intrinsic properties similar to the IQHE. A comprehensive overview over these methods can be found in the monograph of Emil Prodan and Hermann Schulz-Baldes [PS16]. One of the novelties in their work is the decomposition of the range of the topological invariants using generalised Středa formulas derived from Itô derivatives with respect to the magnetic field. They allow establishing connections between different invariants. Another significant contribution by Hermann Schulz-Baldes and Stefan Teufel [ST13] uses Itô derivatives to derive formulas for the contribution of the conduction electrons to orbital polarisation and orbital magnetisation, generalising the known formulas from Bloch theory. Moreover, Emil Prodan developed an explicit programme for computer implementation based on canonical finite-volume approximations for the non-commutative Brillouin torus [Pro17], which facilitates the numerical evaluation of the topological invariants and formulas. Our work applies these developments to magnetic systems with arbitrary multi- q textures while excluding the incorporation of disorder.

Multi- q Textures

In [Lux+24], we demonstrated that all possible tight-binding Hamiltonians incorporating multi- q magnetic order are representations of a non-commutative torus C^* -algebra as bounded operators on the Hilbert space $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$. In these systems, the non-trivial topology of the spin texture induces topological spectral gaps assuming the role of the magnetic field for the IQHE or the spin-orbit interaction for topological insulators. The algebraic structure then encodes the essential physical properties of electrons in multi- q magnets thereby enabling a complete topological characterisation of electronic states in terms of their Chern numbers. The investigation of the range of the Chern numbers as in [PS16] predicts the scaling behaviour of the Chern numbers with respect to the pitch of the multi- q spin waves. This reveals in particular the fingerprints of the gap labels in the integrated density of states (IDS) of the system and allows for the extraction of a subset of all Chern numbers, such as the top Chern number.

Following the computational programme devised by Emil Prodan, the subsequent work [Pra+24] evaluated the Chern numbers numerically for the case of the $3q$ helical skyrmion lattice, as introduced in Eq. (1.19), and verified the findings extracted from the IDS. A further manipulation of the texture’s real space winding number revealed its relation to the electronic state Chern numbers. The central results are that the entire contribution to the real space Chern number is carried by a single band at the van-Hove singularities, which depend on the lattice geometry, and that the (topological) order parameters of the real space texture affect the electronic state topology. A focus of this work lies in the change of Chern number for which spectral flow coinciding with the topological phase transitions is revealed by employing a regularisation of the texture’s singularities at critical points in parameter space.

Chapter content

This chapter presents a synthesis of the C^* -theory framework of multi- q textures, as developed in the authors’ publications [Lux+24] and [Pra+24], with the additional incorporation of an external magnetic field.

In Sec. 3.1, the physical observable algebra is constructed as a crossed product algebra of the continuous functions on the phase space and the lattice translation group. The

introduction of the magnetic field results additionally in a twisting of the involved group action. On this algebra, a C^* -norm is constructed using covariant representations, thereby arriving at the C^* -algebra completion, which is known as the non-commutative torus.

The subsequent stage in Sec. 3.2 is the establishment of a differential calculus on this algebra comprising a unique trace on the non-commutative torus and a family of $*$ -derivations. For this purpose, we introduce the smooth non-commutative torus, a dense subalgebra of infinitely differentiable elements. At this juncture, we also introduce the Itô derivatives.

With Sec. 3.3, we then proceed to present the fundamental concepts of K -theory for C^* -algebras, together with an exposition of its application to the non-commutative torus. For extracting the Chern numbers, the K -group is paired with cyclic cocycles constructed from the non-commutative torus algebra. These are key concepts from non-commutative geometry, as cyclic cohomology is designed to serve as the natural receptacle for the Chern character in K -homology. For the decomposition of the Chern numbers, we expand the generalised Středa formulas and obtain a formula for higher gap labelling.

Eventually, in Sec. 3.4, we rewrite the tight-binding Hamiltonian into its canonical form as a representation of an element from the observable algebra. We present the explicit decomposition of the Chern numbers in the multi- q systems in terms of the pitch of the multi- q spin waves and the magnetic flux per unit cell. Moreover, we use the Itô derivatives to present the derivation of the formula for the orbital magnetisation.

C^* -algebra Foundations

To begin this chapter, we need to establish the concept of C^* -algebras and its significance for operator analysis and quantum mechanics as well as topology. C^* -algebras are designed to be abstractions for bounded operator algebras on complex Hilbert spaces and as such have a long history in quantum physics [MN36].

C^ -algebras*

The mathematical appeal of these algebras stems from the fact that their algebraic properties are closely related to the topology of their spectra [GN43] and, thus, to the topology of the spectra of their elements. This relationship is preserved for dense subalgebras which are stable under holomorphic calculus, so-called *pre- C^* -algebras*, which provides a framework for the construction of operators like the resolvent and the spectral (Fermi) projection, making them particularly suitable for modelling algebras of physical observables.

The underlying objects for which we can define the C^* -structure are *Banach algebras* over a field: complete normed vector spaces $(A, \|\cdot\|)$ with an associative bilinear product such that

Definition

$$\|ab\| \leq \|a\|\|b\| \quad \forall a, b \in A \quad (\text{submultiplicative}).$$

3. C^* -Algebra Theory of Multi-q Textures

If we have a complex Banach algebra with an anti-multiplicative and anti-linear involution $*$, we call it a Banach $*$ -algebra [Ric14, Def. 2.4.1]:

Definition 3.1 (B^* -algebra). A *Banach $*$ -algebra* or B^* -algebra is a Banach algebra A over $\mathbb{C}$ together with an involution $*$ such that for any $a, b \in A$ and $\alpha \in \mathbb{C}$:

- (i) $(a^*)^* = a$ (*involution*),
- (ii) $(a + b)^* = a^* + b^*$ (*additive*),
- (iii) $(\alpha a)^* = \bar{\alpha} a^*$ (*conjugate homogeneous*),
- (iv) $(ab)^* = b^* a^*$ (*anti-multiplicative*).

For the C^* -structure, we demand an additional property concerning the compatibility of involution and norm [Ric14, Def. 2.4.3]:

Definition 3.2 (C^* -algebra). A C^* -algebra is a B^* -algebra A such that

$$\|a^* a\| = \|a\|^2 \quad \forall a \in A.$$

One significant implication of this property is that any C^* -algebra has at most one norm satisfying it [Ric14, Cor. 2.4.9]. The prototypical example of a C^* -algebra is the complex algebra of all bounded linear operators $\mathcal{B}(\mathcal{H})$ on a complex Hilbert space $\mathcal{H}$ with the operator norm satisfying the C^* -property, whose subalgebras are intended to be abstracted. A norm closed subalgebra of a C^* -algebra which is stable under the involution is a C^* -subalgebra, and a homomorphism $\phi : A \rightarrow B$ between two C^* -algebras that preserves the involution, i.e. $\phi(a^*) = \phi(a)^*$ for all $a \in A$, is called as *$*$ -homomorphism*. Many common concepts from operator theory can be transferred to elements of a C^* -algebra: An element $a \in A$ can be *self-adjoint* ($a = a^*$), *normal* ($aa^* = a^*a$), *unitary* ($aa^* = \mathbf{1} = a^*a$) (provided that A is unital), or an *orthogonal projection* ($a = a^2 = a^*$).

Representations

The connection back from the abstraction to bounded linear operators on a Hilbert space is given by *representations* of the C^* -algebras [Ric14, Def. 2.5.10]:

Definition 3.3 (Representation of a C^* -algebra). A *representation* of a C^* -algebra A is a pair $(\mathcal{H}, \pi)$, where $\mathcal{H}$ is a Hilbert space and $\pi : A \rightarrow \mathcal{B}(\mathcal{H})$ is a $*$ -homomorphism. This representation is called *faithful* if π is injective, and *non-degenerate* if for any $\psi \in \mathcal{H} \setminus \{0\}$ there exists $a \in A$ such that $\pi(a)\psi \neq 0$.

This connection receives special significance by the construction of the *Gelfand-Naimark-Segal* (GNS) representation [GN43] through which any C^* -algebra can be embedded as a C^* -subalgebra of the algebra of bounded linear operators on some Hilbert space [Kha13, Thm. A.4]:

Theorem 3.1 (Gelfand-Naimark-Segal representation). *Every C^* -algebra is isomorphic to a C^* -subalgebra of the algebra of bounded operators on a Hilbert space.*

The proof of this statement can be conducted explicitly by the GNS construction and is based on the concepts of states and left regular representations. An instructive sketch of the proof can be found in [Kha13, A.2].

The significance for the study of topology comes from the close link of algebraic and topological properties in C^* -algebras. A commutative C^* -algebra $C(X)$ of complex-valued continuous functions on a compact Hausdorff space X encodes all topological properties of X and the *Gelfand-Naimark Theorem* [GN43] extends this duality to all commutative C^* -algebras:

Topology

Theorem 3.2 (Gelfand-Naimark Theorem). *The category of locally compact Hausdorff spaces and continuous proper maps is equivalent to the opposite of the category of commutative C^* -algebras and proper C^* -morphisms.*

This can be understood by the *Gelfand transform* $\Gamma : A \rightarrow C_0(\hat{A})$ [Kha13, Chap. 1.1.2], which provides an isomorphism between any commutative C^* -algebra A with *spectrum* $\hat{A}$, which is locally Hausdorff [Ric14, Prop. 2.3.4], and the commutative algebra $C_0(\hat{A})$ of complex-valued continuous functions on $\hat{A}$ that vanish at infinity. The spectrum $\hat{A}$ of a commutative algebra A is the space of all *characters* τ , i.e. non-zero homomorphisms from A to $\mathbb{C}$. It is closely related to the notion of the *spectrum of an element* $\sigma_A(a) = \{\lambda \in \mathbb{C} \mid a - \lambda 1 \text{ is not invertible in } A\}$ for an element a from an unital Banach algebra A by the following relation valid for any element a in an unital commutative Banach algebra A [Ric14, Prop 2.3.2]:

$$\sigma_A(a) = \{\tau(a) \mid \tau \in \hat{A}\}.$$

Non-commutative topology refers to the study of non-commutative algebras with similar generalised algebraic methods and, thus, the formal study of the topology of "non-commutative locally compact spaces". The central tool for this is operator K -theory which generalises topological K -theory. Instead of classifying stable isomorphism classes of complex vector bundles over compact Hausdorff spaces, it classifies stable isomorphism classes of finitely generated projective modules over C^* algebras [Kha13, Chap. 1.2]. By the Serre-Swan theorem [Ser55; Swa62] these classifications coincide in the case of commutative algebras.

3.1. Non-commutative Torus

Non-commutative torus is the name for a non-commutative C^* -algebra which generalises the commutative algebra of continuous functions on a torus. It is the archetype for a non-commutative space as it can be visualised in 2 dimensions by the Kronecker foliation of the 2-dimensional real torus $T^2 = \mathbb{R}^2/\mathbb{Z}^2$. The foliation is given by lines of constant, irrational slope $dx = \theta dy$, $\forall x, y \in \mathbb{R}/\mathbb{Z}$ with $\theta \in (0, 1) \setminus \mathbb{Q}$ [CM08, Chap. 6]. Each leaf, which is a continuous injection of the non-compactified real line, is a dense subset in the 2-torus T^2 and does not inherit the subspace topology. The transversal $T = \{y = 0\}$ to the foliation is isomorphic to the circle S^1 , and any two of its points belong to the

Non-commutative space

3. C^* -Algebra Theory of Multi- q Textures

same leaf, if they differ by an integer multiple of θ . The corresponding quotient space $S^1/\theta\mathbb{Z}$ which identifies the points on the same leaf is the underlying space for the non-commutative torus. The non-commutative algebra describing it, is generated by the unitary $V(\alpha) = e^{2\pi i\alpha}$, $\alpha \in S^1$, that generates the algebra $C(S^1)$ of continuous functions on S^1 , together with a second unitary U , such that

$$UV = \lambda VU \quad \text{with} \quad \lambda = e^{2\pi i\theta}.$$

Their universal unital C^* algebra is the non-commutative torus. In non-commutative geometry, it is one of the most intensively studied cases, offering an accessible example for the application of a range of tools.

Quantum mechanics The relevance to physics begins already with the *canonical commutation relation* (CCR) $[q, p] = i\hbar\mathbb{1}$ in quantum mechanics. The one-parameter unitary groups $U_t = e^{itp}$, $V_s = e^{isq}$ generated by the unbounded position and momentum operators q and p obey the Weyl form of the CCR: $U_t V_s = e^{ihts} V_s U_t$. This is another realisation of the defining relation for unitaries which generate the non-commutative torus [Dav96, Chap. 6]. We will demonstrate, that relations of the same form are introduced through the presence of a multi- q spin textures as in Eq. (3.20) or a constant magnetic field as in Eq. (3.22).

K-Theory The most general algebra which contains the tight-binding Hamiltonian coupled to arbitrary magnetic fields and even completely generic, continuous textures $\mathbf{n} \in C(\mathbb{R}^d, \mathbb{R}^3)$ is the full algebra of bounded operators $\mathcal{B}(\mathcal{H})$ on the Hilbert space $\mathcal{H}$. Unfortunately, it is too large to study the topology of the system using K -theory as its K -groups are trivial, i.e. $K_i(\mathcal{B}(\mathcal{H})) = 0$, $i = 0, 1$ [RLL00, Ex. 3.3.3]. By restricting the system to constant magnetic fields and to the class of multi- q textures, as introduced in Chap. 1.2.3, one can construct a C^* -algebra, the non-commutative torus, which is isomorphic to a sufficiently small subalgebra. Its K -group is the same as for the algebra of functions over the torus $K_i(C(T^n)) = \mathbb{Z}^{2^{n-1}}$ [RLL00, Ex. 11.3.4], which coincides with the topological K -group of the torus $K^i(T^n)$ [RLL00, Chap. 3.3.7]. The restriction has this effect, because the vector fields of multi- q textures can be thought of as a composition of maps [Lux+24]:

$$\mathbb{R}^d \xrightarrow{\omega} T^r \xrightarrow{\mathbf{n}} \mathbb{R}^3$$

with ω defined as in Eq. (1.8) and where $\mathbf{n}$ is a continuous function. Leveraging the fundamental property that translations on the electronic lattice can be compensated by continuous shifts of the multi- q texture, as described by the natural action of the lattice translation group from Eq. (1.10), one can give a very compact essential description of the algebra of physical observables. This property is known as *covariance* and is built into the algebraic structure of so-called crossed product algebras [Ped18, Ch. 7] [Wil07].

Section Content Therefore, although the non-commutative torus can be defined as the universal unital C^* -algebra for commutation relations of unitaries, in the following, it is constructed as a twisted crossed product C^* -algebra. For this, the crossed product between the algebra of continuous functions on the torus and the group of lattice translations is introduced, and its C^* -completion is constructed from the norm given by the covariant representations as bounded operators on a Hilbert space.

3.1.1. Crossed Product Algebra

A crossed product algebra is constructed from a C^* -algebra acted on by a locally compact group. It is closely related to the semi-direct product of groups and the non-commutativity of the algebra is completely dependent on the group action. In general, the crossed product algebra does not inherit the properties of a C^* -algebra, which require the completion under a suitable norm. In the following, we are only going to consider the discrete and Abelian lattice group $G = \mathbb{Z}^d$ acting on the commutative algebra $C(T^r)$ of complex functions over the torus which describes the phases of the multi- q texture's spin waves. The action is twisted by the presence of a constant magnetic field.

In the discussion of multi- q systems coupled to lattice electrons in Chap. 1.2.3.1, we defined the natural action τ of the lattice translation group $\mathbb{Z}^d$ on the phase functions $\omega \in C^\infty(\mathbb{R}^d, T^r)$ with Eq. (1.10). From this, we can define a corresponding continuous action of $\mathbb{Z}^d$ on the algebra $C(T^r)$ of complex-valued continuous functions on the r -torus given via $*$ -automorphisms

Group action

$$\alpha: \mathbb{Z}^d \rightarrow \text{Aut}(C(T^r)), \mathbf{m} \mapsto \alpha_{\mathbf{m}} \quad (3.1)$$

$$(\alpha_{\mathbf{m}} f)(\varphi) \equiv f(\tau_{-\mathbf{m}} \varphi) = f(\varphi - 2\pi\theta\mathbf{m}), \quad (3.2)$$

which we will use to build the crossed product algebra. By denoting the abstract generators of $\mathbb{Z}^d$ by $t_1, \dots, t_d$, we can express $\mathbb{Z}^d$ with the presentation

Group algebra

$$\mathbb{Z}^d = \langle t_1, \dots, t_d \mid t_i t_j = t_j t_i \rangle.$$

In the following, we employ a multi-index notation and write $t^{\mathbf{m}} = t_1^{m_1} \dots t_d^{m_d}$ for $\mathbf{m} \in \mathbb{Z}^d$. With it, we can express the underlying complex vector space of the group algebra $\mathbb{C}\mathbb{Z}^d$ generated by the set $\mathbb{Z}^d$ as finite linear combinations $\sum_{\mathbf{m} \in \mathbb{Z}^d} c_{\mathbf{m}} t^{\mathbf{m}}$ with $c_{\mathbf{m}} \in \mathbb{C}$. Its unital involutive algebra structure is inherited from the group structure by linear extension of

$$t^{\mathbf{a}} t^{\mathbf{b}} = t^{\mathbf{a}+\mathbf{b}} \quad \text{and} \quad (t^{\mathbf{m}})^* = t^{-\mathbf{m}}.$$

The underlying vector space of the crossed product of the C^* -algebra $C(T^r)$ and the group $\mathbb{Z}^d$ is then defined as the $\mathbb{C}$ -linear tensor product $C(T^r) \otimes \mathbb{C}\mathbb{Z}^d$ with a typical element a in the form of

Vector space

$$a = \sum_{\mathbf{m} \in \mathbb{Z}^d} f_{\mathbf{m}} \otimes t^{\mathbf{m}}. \quad (3.3)$$

The complex coefficients now have flourished into continuous complex functions on T^r : $f_{\mathbf{m}} \in C(T^r)$. Still, only finitely many $f_{\mathbf{m}}$ are different from zero.

To obtain the algebraic structure on $C(T^r) \otimes \mathbb{C}\mathbb{Z}^d$ that is characteristic for the crossed product, we declare

Crossed product

$$(f_1 \otimes t^{\mathbf{m}_1})(f_2 \otimes t^{\mathbf{m}_2}) = f_1 \alpha_{\mathbf{m}_1}(f_2) \otimes t^{\mathbf{m}_1 + \mathbf{m}_2}.$$

We then obtain a natural anti-multiplicative and anti-linear involution constructed from the involutions of $C(T^r)$ and $\mathbb{C}\mathbb{Z}^d$:

$$\begin{aligned} (f \otimes t^{\mathbf{m}})^* &= ((f \otimes t^{\mathbf{0}})(1 \otimes t^{\mathbf{m}}))^* = (1 \otimes t^{\mathbf{m}})^*(f \otimes t^{\mathbf{0}})^* = (1 \otimes t^{-\mathbf{m}})(f^* \otimes t^{\mathbf{0}}) \\ &= \alpha_{-\mathbf{m}}(f^*) \otimes t^{-\mathbf{m}}. \end{aligned}$$

3. C^* -Algebra Theory of Multi- q Textures

We denote the resulting algebraic crossed product algebra by $C_c(\mathbb{Z}^d, C(T^r), \alpha)$. Then, for any two elements $a, b \in C_c(\mathbb{Z}^d, C(T^r), \alpha)$ we have

$$\begin{aligned} ab &= \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}}, \\ a^* &= \sum_{\mathbf{m} \in \mathbb{Z}^d} \alpha_{\mathbf{m}}(a_{-\mathbf{m}}^*) \otimes t^{\mathbf{m}}. \end{aligned}$$

Twisted action This presentation is in particular useful once we twist the group action with respect to the flux of the magnetic field permeating the system. For this, we consider a *strictly continuous 2-cocycle* $\gamma : \mathbb{Z}^d \times \mathbb{Z}^d \rightarrow \mathcal{U}(C(T^r))$ with values in the *unitary group* of the *multiplier algebra* of $C(T^r)$ and refer to (α, γ) as *twisted action*.

Remark 3.1 (Multiplier algebra). The multiplier algebra $\mathcal{M}(A)$ of a C^* -algebra A is the maximal C^* -algebra containing A as an essential ideal. It is equipped with the strict topology generated by the semi-norms $\|x\|_a = \|ax\| + \|xa\|$ for $a \in A$ [Bla98, Chap. 12.1]. The unitary group refers to the unitary C^* -subalgebra of the multiplier algebra.

Since $C(T^r)$ is already unital it is $\mathcal{M}(C(T^r)) = C(T^r)$ and the strict topology of $\mathcal{M}(C(T^r))$ coincides with the norm topology. The unitary group $\mathcal{U}(C(T^r))$ is thus given by $C(T^r, S^1)$, the continuous functions with values on the unit circle. The *2-cocycle condition* demands

$$\gamma(\mathbf{l} + \mathbf{m}, \mathbf{n})\gamma(\mathbf{l}, \mathbf{m}) = \theta_1[\gamma(\mathbf{m}, \mathbf{n})]\gamma(\mathbf{l}, \mathbf{m} + \mathbf{n}) \quad \text{for } \mathbf{l}, \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d, \quad (3.4)$$

where θ denotes a continuous action in terms of automorphisms on $\mathcal{U}(C(T^r))$. For any Abelian C^* -algebra A the only automorphisms on $C_0(\hat{A})$ are implemented as compositions with homeomorphisms of the underlying locally compact space [MPR05, Chap. 2.1]. This is the case for $\alpha_{\mathbf{m}}$ on $C(T^r)$ being implemented as composition with $\tau_{-\mathbf{m}}$. The 2-cocycle condition is equivalent to γ being in the kernel of the coboundary map from group cohomology as defined in [MPR05, Chap. 2.3]. The cocycle γ is further called *normalised* if $\gamma(\mathbf{m}, 0) = \gamma(0, \mathbf{m}) = 1$ for all $\mathbf{m} \in \mathbb{Z}^d$.

Magnetic cocycle The magnetic field does not depend on the phases of the multi- q texture, and, thus, we only need a continuous normalised 2-cocycle $\mathbb{Z}^d \times \mathbb{Z}^d \rightarrow S^1$ that adheres to $\gamma(\mathbf{l} + \mathbf{m}, \mathbf{n})\gamma(\mathbf{l}, \mathbf{m}) = \gamma(\mathbf{m}, \mathbf{n})\gamma(\mathbf{l}, \mathbf{m} + \mathbf{l})$ for $\mathbf{l}, \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d$. This is satisfied by

$$\gamma(\mathbf{m}, \mathbf{n}) = e^{2\pi i(\mathbf{m} \wedge_{\Phi} \mathbf{n})} \quad \text{with} \quad \mathbf{m} \wedge_{\Phi} \mathbf{n} = \frac{1}{2} \sum_{i,j=1}^d \Phi_{ij} m_i n_j, \quad (3.5)$$

where Φ is a real antisymmetric $(d \times d)$ -dimensional matrix with entries from $[0, 1]$ describing the magnetic flux quanta per unit cell of a constant magnetic field. We will circle back to this choice for the cocycle in the next section when it comes to Hilbert space representations.

The twisted crossed product structure is given by

Twisted crossed product

$$ab = \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge_{\Phi} \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}}, \quad (3.6)$$

$$a^* = \sum_{\mathbf{m} \in \mathbb{Z}^d} \alpha_{\mathbf{m}}(a_{-\mathbf{m}}^*) \otimes t^{\mathbf{m}}, \quad (3.7)$$

with the algebra denoted by $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$. Here, it is important to distinguish between the group elements which commute and the algebra elements which do not commute. For the generators of the group $\mathbb{Z}^d$ **as algebra elements** Eq. (3.6) implies

$$t_i t_j := (1 \otimes t_i)(1 \otimes t_j) = e^{2\pi i \Phi_{ij}} (1 \otimes t_j)(1 \otimes t_i) =: e^{2\pi i \Phi_{ij}} t_j t_i, \quad (3.8)$$

and

$$t^{\mathbf{m}} t^{\mathbf{n}} = e^{4\pi i (\mathbf{m} \wedge_{\Phi} \mathbf{n})} t^{\mathbf{n}} t^{\mathbf{m}} = e^{2\pi i (\mathbf{m} \wedge_{\Phi} \mathbf{n})} t^{\mathbf{m}+\mathbf{n}}. \quad (3.9)$$

For consistency, the multi-index notation needs to be $t^{\mathbf{m}} = e^{2\pi i \frac{1}{2} \sum_{i < j}^d \Phi_{ij} m_i m_j} t_1^{m_1} \dots t_d^{m_d}$.

While this description would already be sufficient to feature a wide class of tight-binding model Hamiltonians H , the same cannot be said for their many physical properties encoded in the resolvent $(z - H)^{-1}$ for $z \in \mathbb{C}$, which is not representable as an element of $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$. Therefore, we need a meaningful completion of the algebraic crossed product to a larger set of observables. This is given by the C^* -completion, which requires first the introduction of covariant Hilbert space representations for the construction of a suitable norm.

3.1.2. Covariant Representation

A covariant representation for a crossed product algebra entails a representation of the C^* -algebra and a unitary representation of the group on the same Hilbert space such that the group action is given through conjugation with the corresponding operators. In the case of a twisted action, the group representation becomes a generalised projective unitary representation. A covariant representation can be used to construct a representation of the (twisted) crossed product algebra.

First, we will introduce the notion of a (twisted) C^* -dynamical system and its covariant representation. Then, we will construct an explicit representation as multiplication and translation operators, which requires some care for the magnetic translation representation with respect of the gauge of the vector potential and the integrability of the cocycle. Finally, we will compose a family of representations for the (twisted) crossed product algebra.

3. C^* -Algebra Theory of Multi-q Textures

*Twisted
 C^* -dynamical
system*

The mathematical objects $C(T^r), \mathbb{Z}^d, \alpha, \gamma$ we introduced in the last section amount to a so-called twisted C^* -dynamical system as defined in [MPR05, Def. 2.1]:

Definition 3.4 (Twisted C^* -dynamical system (A, G, α, γ)). A *twisted C^* -dynamical system* consists of a quadruplet (A, G, α, γ) , where

- (i) A is a C^* -algebra,
- (ii) G is a second countable locally compact group,
- (iii) $\alpha : G \rightarrow \text{Aut}(A)$ is a homomorphism from G to the group of $*$ -automorphisms of A , such that $x \mapsto \alpha_x(a)$ is continuous for all $a \in A$, and
- (iv) γ is a strictly continuous normalised 2-cocycle on G with values in $\mathcal{U}(A)$, the unitary group of the multiplier algebra of A .

A C^* -dynamical system is defined in an analogous manner as the triple (A, G, α) , excluding the stipulation of property (iv).

*Covariant
representation*

A covariant representation of a C^* -dynamical system refers to Hilbert space representations of the C^* -algebra and the group, which are compatible with the group action. In case of a twisted group action there is an additional condition on the group representation. A general definition is given by [MPR05, Def. 2.2]:

Definition 3.5 (Covariant representation $(\mathcal{H}, \pi, \rho)$). A (non-degenerate) *covariant representation* of a twisted C^* -dynamical system (A, G, α, γ) consists in a triple $(\mathcal{H}, \pi, \rho)$, where

- (i) $\mathcal{H}$ is a separable Hilbert space,
- (ii) $(\mathcal{H}, \pi)$ is a (non-degenerate) representation of A ,
- (iii) $(\mathcal{H}, \rho)$ is a strongly continuous map from G to $\mathcal{U}(\mathcal{H})$ which satisfies

$$\rho(x)\rho(y) = \pi(\gamma(x, y))\rho(x + y) \quad \forall x, y \in G,$$

- (iv) the following compatibility condition holds

$$\pi(\alpha_x(f)) = \rho(x)\pi(f)\rho(x)^* \quad \forall x \in G, f \in A.$$

Here, ρ is a generalisation of a projective representation, which would be a homomorphism $G \rightarrow \mathcal{U}(\mathcal{H})/\{S^1 \mathbb{1}_{\mathcal{H}}\}$, as $\mathcal{U}(A)$ generally does not yield a constant phase factor. In the case of A commutative, $\mathcal{U}(A)$ contains the functions on the spectrum of A with values in the unit circle S^1 .

3.1. Non-commutative Torus

From a covariant representation $(\mathcal{H}, \pi, \rho)$ of the twisted C^* -dynamical system $(C(T^r), \mathbb{Z}^d, \alpha, \gamma)$ introduced in last section, we can construct a representation $(\mathcal{H}, \pi \rtimes \rho)$ of $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$, known as the *integrated representation*:

$$(\pi \rtimes \rho)(a) = \sum_{\mathbf{m} \in \mathbb{Z}^d} \pi(f_{\mathbf{m}}) \rho(t^{\mathbf{m}}). \quad (3.10)$$

In fact, there exists a bijective correspondence between covariant representations of (twisted) dynamical systems and non-degenerate representations of the corresponding twisted crossed products [Ric14, Thm. 3.4.8., Lem. 5.2.5].

To identify any tight-binding Hamiltonian as a representation of a C^* -algebra element, we require in particular a representation on the physical Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}^d)$. The natural choice for this is known as *Schrödinger representation* and represents the functions in terms of multiplication operators and the translation group elements in terms of translation operators. These representations are familiar from the one-parameter groups generated by the position and momentum operators in quantum mechanics, which we briefly discussed in the introduction of Sec. 3.1. In fact, by the Stone-von Neumann Theorem [Neu31] all representations which fulfil the unitary relations of the non-commutative torus are unitarily equivalent to these operators.

Schrödinger representation

The representation as multiplication operators on $\ell^2(\mathbb{Z}^d)$ is straight-forward for the C^* -algebra $C_b(\mathbb{Z}^d)$ of bounded and continuous complex functions on $\mathbb{Z}^d$, however, for $C(T^r)$ we first need to restrict the functions to specific orbits $\mathbb{Z}^d \varphi$ on T^r as defined in Eq. (1.12). This is done via composition with $\omega(\mathbf{x}_{\bullet}) : \mathbb{Z}^d \rightarrow \mathbb{Z}^d \varphi \subseteq T^r$, $\mathbf{i} \mapsto \omega(\mathbf{x}_{\mathbf{i}}) = \tau_{\mathbf{i}} \varphi$, first embedding the lattice sites into real space and then mapping the real space positions to the corresponding phases of the multi- q textures' spin waves. A faithful representation of $C_b(\mathbb{Z}^d)$ is given by $\pi : C_b(\mathbb{Z}^d) \rightarrow \mathcal{B}(\ell^2(\mathbb{Z}^d))$, such that for any $f \in C_b(\mathbb{Z}^d)$

Multiplication operators

$$\pi(f) = \sum_{\mathbf{i} \in \mathbb{Z}^d} f(\mathbf{i}) |\mathbf{i}\rangle \langle \mathbf{i}|, \quad (3.11)$$

which is clearly an injective $*$ -homomorphism. Then, a family $\{\pi_{\varphi}\}_{\varphi \in T^r}$ of representations is given by $\pi_{\varphi} : C(T^r) \rightarrow \mathcal{B}(\ell^2(\mathbb{Z}^d))$ with $\pi_{\varphi}(f) := \pi(f \circ \omega(\mathbf{x}_{\bullet}))$, such that

$$\pi_{\varphi}(f) = \sum_{\mathbf{i} \in \mathbb{Z}^d} f(\omega(\mathbf{x}_{\mathbf{i}})) |\mathbf{i}\rangle \langle \mathbf{i}| \stackrel{(1.11)}{=} \sum_{\mathbf{i} \in \mathbb{Z}^d} f(\tau_{\mathbf{i}} \varphi) |\mathbf{i}\rangle \langle \mathbf{i}| = \sum_{\mathbf{i} \in \mathbb{Z}^d} (\alpha_{-\mathbf{i}} f)(\varphi) |\mathbf{i}\rangle \langle \mathbf{i}|. \quad (3.12)$$

These are faithful if τ acts ergodic on T^r [Pro17, Prop. 3.8]. This is because $\pi_{\varphi}(f) = 0$ if and only if $f(\tau_{\mathbf{i}} \varphi) = 0$ for all $\mathbf{i} \in \mathbb{Z}^d$. If the action is ergodic for all $\varphi \in T^r$ and the functions are continuous, one must have $f(\varphi) = 0$ everywhere.

Since $C_b(\mathbb{Z}^d)$ is unital, its multiplier algebra is $C_b(\mathbb{Z}^d)$ itself and the unitary subgroup is given by $C_b(\mathbb{Z}^d, S^1)$. This allows us to use the so-called *dual magnetic translations* U^A as representations of the translation group. In most general terms, we can describe a magnetic field as closed continuous field of 2-forms $B \in C(\mathbb{R}^d, \wedge^2 T^* \mathbb{R}^d)$ on real space [MPR05, Chap. 4.1].

Magnetic translations

3. C^* -Algebra Theory of Multi-q Textures

In coordinates, the components $B_{jk} \in C(\mathbb{R}^d, \mathbb{R})$ are continuous real functions on position space with $B_{jk} = -B_{kj}$ and $\partial_j B_{kl} + \partial_l B_{ij} + \partial_k B_{lj} = 0$ (in the distributional sense). The components of the corresponding vector field are given by $B_i = \epsilon_{ijk} B_{jk}$. For the (dual) magnetic translations we express the magnetic field as the exterior derivative $dA = B$ of a continuous field of 1-forms $A \in C(\mathbb{R}^d, T^*\mathbb{R}^d)$, the *vector potential*. Its components $A_i \in C(\mathbb{R}^d, \mathbb{R})$ are continuous real functions on position space as well and $dA = B$ implies $\partial_j A_k - \partial_k A_j = B_{jk}$. For a given B an adequate A is given by the *symmetric gauge* with continuous component functions $A_i \in C(\mathbb{R}^d, \mathbb{R})$

$$A_i(\mathbf{x}) = - \sum_{j=1}^n \int_0^1 ds B_{ij}(s\mathbf{x}) s x_j.$$

The explicit choice of A for a given B is not unique, which is known as *gauge freedom*. The dual magnetic translations are based on the unitary translation operator $\hat{T}_{\mathbf{m}}$ on $\ell^2(\mathbb{Z}^d)$ with $\hat{T}_{\mathbf{m}} |\mathbf{n}\rangle = |\mathbf{n} + \mathbf{m}\rangle$ for $\mathbf{n}, \mathbf{m} \in \mathbb{Z}^d$. They receive an additional phase factor

$$\hat{U}_{\mathbf{m}}^A |\mathbf{n}\rangle = e^{-i\Gamma_A([\mathbf{n}, \mathbf{n} + \mathbf{m}])} |\mathbf{n} + \mathbf{m}\rangle, \quad (3.13)$$

with phase $\Gamma_A([\mathbf{n}, \mathbf{n} + \mathbf{m}])$ denoting the circulation of the vector potential A along the line $[\mathbf{n}, \mathbf{n} + \mathbf{m}]$ between the lattice sites $\mathbf{n}$ and $\mathbf{n} + \mathbf{m}$ embedded in real space:

$$\Gamma_A([\mathbf{n}, \mathbf{n} + \mathbf{m}]) := \frac{e}{\hbar} \int_{[\mathbf{x}_{\mathbf{n}}, \mathbf{x}_{\mathbf{n} + \mathbf{m}}]} A = \frac{e}{\hbar} \sum_{i=1}^d (\mathbf{x}_{\mathbf{m}})_i \int_0^1 dt A_i(\mathbf{x}_{\mathbf{n}} + t\mathbf{x}_{\mathbf{m}}). \quad (3.14)$$

We can express the phase factor as a multiplication operator in the form of Eq. (3.11) and separate it thereby from $\hat{T}_{\mathbf{m}}$:

$$\begin{aligned} \hat{U}_{\mathbf{m}}^A |\mathbf{n}\rangle &= e^{-i\Gamma_A([\mathbf{n}, \mathbf{n} + \mathbf{m}])} |\mathbf{n} + \mathbf{m}\rangle = \sum_{\mathbf{i} \in \mathbb{Z}^d} e^{-i\Gamma_A([\mathbf{i} - \mathbf{m}, \mathbf{i}])} |\mathbf{i}\rangle \langle \mathbf{i} | \mathbf{n} + \mathbf{m} \rangle \\ &= \pi \left(e^{i\Gamma_A([\bullet, \bullet - \mathbf{m}])} \right) \hat{T}_{\mathbf{m}} |\mathbf{n}\rangle \end{aligned}$$

Remark 3.2 (Magnetic translation phase). The explicit form of the phase factor for the dual magnetic translation can be derived from the magnetic momentum operator $\mathbf{p} - e\mathbf{A}$, which is given by the *minimal coupling principle* and generates the unitary group of magnetic translation operators. This can be done in a descriptive way using the *Trotter product formula* [Hal13, Thm. 20.1] as has been presented by the author in [Pra20, Chap. 1.3.3].

For the commutation relation of the dual magnetic translation operators follows

$$\hat{U}_{\mathbf{m}}^A \hat{U}_{\mathbf{n}}^A = \pi \left(e^{i\Gamma_B(\langle \bullet, \bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n} \rangle)} \right) \hat{U}_{\mathbf{m} + \mathbf{n}}^A, \quad (3.15)$$

where the phase $\Gamma_B(< \mathbf{l}, \mathbf{l} + \mathbf{n}, \mathbf{l} + \mathbf{n} + \mathbf{m} >)$ corresponds to the flux of the magnetic field B through the lattice site triangle $< \mathbf{l}, \mathbf{l} + \mathbf{n}, \mathbf{l} + \mathbf{n} + \mathbf{m} >$:

$$\begin{aligned} \Gamma_B(< \mathbf{l}, \mathbf{l} + \mathbf{n}, \mathbf{l} + \mathbf{n} + \mathbf{m} >) &:= \frac{e}{\hbar} \int_{< \mathbf{l}, \mathbf{l} + \mathbf{n}, \mathbf{l} + \mathbf{n} + \mathbf{m} >} B \\ &= \frac{e}{\hbar} \sum_{j,k=1}^d (\mathbf{x}_{\mathbf{n}})_j (\mathbf{x}_{\mathbf{m}})_k \int_0^1 dt \int_0^1 ds s B_{jk}(\mathbf{x}_{\mathbf{l}} + s\mathbf{x}_{\mathbf{n}} + st\mathbf{x}_{\mathbf{m}}). \end{aligned} \quad (3.16)$$

Each translation operators in Eq. (3.15) contributes a phase factor which corresponds to the circulation of the vector potential along one side of the triangle. The relation follows then by *Stokes Theorem* [Fra11, Chap. 3.3] as explicitly carried out in App. A3.

We can interpret this magnetic phase factor as the continuous normalised 2-cocycle $\gamma_B : \mathbb{Z}^d \times \mathbb{Z}^d \rightarrow C(\mathbb{Z}^d, S^1)$ by

Group
cohomology

$$(\mathbf{m}, \mathbf{n}) \mapsto \gamma_B(\bullet; \mathbf{m}, \mathbf{n}) := e^{i\Gamma_B(< \bullet, \bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n} >)}. \quad (3.17)$$

If an action θ is given by automorphisms on $f \in C_b(\mathbb{Z}^d, S^1)$ as $[\theta_{\mathbf{m}} f](\mathbf{n}) = f(\mathbf{n} - \mathbf{m})$, then the 2-cocycle and normalisation conditions are satisfied as shown in App. A4. Now, we can interpret the phase factor of the dual magnetic translation as a 1-cocycle λ^A and demonstrate that the commutation relation in Eq. (3.15) corresponds exactly to γ_B being the coboundary of λ^A . For this, we need to briefly introduce the corresponding group cohomology [MPR05, Chap. 2.3]:

For a C^* -algebra A and an Abelian locally compact group G , we define n -cochains as continuous functions $G^n \rightarrow \mathcal{U}(A)$. The set of all n -cochains $C^n(G; \mathcal{U}(A))$ is an Abelian group itself. Let θ denote a continuous action of G on $\mathcal{U}(A)$. Then, for any $n \in \mathbb{N}$ a coboundary map $\delta^n : C^n(G; \mathcal{U}(A)) \rightarrow C^{n+1}(G; \mathcal{U}(A))$ is given by

$$\begin{aligned} [\delta^n(f)](g_1, \dots, g_n, g_{n+1}) &:= \theta_{g_1} [f(g_2, \dots, g_{n+1})] f(g_1, \dots, g_n)^{(-1)^{n+1}} \\ &\quad \left(\prod_{j=1}^n f(g_1, \dots, g_j + g_{j+1}, \dots, g_{n+1})^{(-1)^j} \right). \end{aligned}$$

The coboundary map δ^n is a group morphism and $\delta^{n+1} \circ \delta^n = 1$ for any $n \in \mathbb{N}$. Then, it is $\text{Im}(\delta^n) \subset \ker(\delta^{n+1})$ and one defines the set of n -cocycles $Z^n(G; \mathcal{U}(A)) := \ker(\delta^n)$, the set of n -coboundaries $B^n(G; \mathcal{U}(A)) := \text{Im}(\delta^{n-1})$, and the cohomology group $H^n(G; \mathcal{U}(A)) := Z^n(G; \mathcal{U}(A)) / B^n(G; \mathcal{U}(A))$ which contains the cohomology classes.

The coboundary $\delta^1(\lambda)$ of a 1-cochain $\lambda \in C^1(G; \mathcal{U}(A))$ takes the form

$$[\delta^1(\lambda)](g_1, g_2) = \lambda(g_1) \theta_{g_1}(\lambda(g_2)) \lambda(g_1 + g_2)^{-1},$$

and the coboundary $\delta(\gamma)$ of a 2-cochain $\gamma \in C^2(G; \mathcal{U}(A))$

$$[\delta^2(\gamma)](g_1, g_2, g_3) = \theta_{g_1} [\gamma(g_2, g_3)] \gamma(g_1 + g_2, g_3)^{-1} \gamma(g_1, g_2 + g_3) \gamma(g_1, g_2)^{-1}.$$

3. C^* -Algebra Theory of Multi-q Textures

Thus, $\gamma_B \in Z^2(\mathbb{Z}^d; C_b(\mathbb{Z}^d, S^1))$ is a 2-coboundary if it is of the form $\delta^1(\lambda)$ for some $\lambda \in C^1(\mathbb{Z}^d; C_b(\mathbb{Z}^d, S^1))$. Indeed, the dual magnetic translation representation is constructed with the corresponding 1-cochain $\lambda^A \in C^1(\mathbb{Z}^d; C_b(\mathbb{Z}^d, S^1))$ which has γ_B as its coboundary $\delta^1(\lambda^A) = \gamma_B$. It is given by

$$\lambda^A(\bullet; \mathbf{m}) := e^{i\Gamma_A([\bullet, \bullet - \mathbf{m}])} \quad \text{such that}$$

$$\begin{aligned} \delta^1(\lambda^A)(\bullet; \mathbf{m}, \mathbf{n}) &= e^{i\Gamma_A([\bullet, \bullet - \mathbf{m}])} \theta_{\mathbf{m}}(e^{i\Gamma_A([\bullet, \bullet - \mathbf{n}])}) e^{-i\Gamma_A([\bullet, \bullet - \mathbf{m} - \mathbf{n}])} \\ &= e^{i\Gamma_A([\bullet, \bullet - \mathbf{m}])} e^{i\Gamma_A([\bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n}])} e^{-i\Gamma_A([\bullet, \bullet - \mathbf{m} - \mathbf{n}])} \\ &= e^{i\Gamma_B(\langle \bullet, \bullet - \mathbf{m}, \bullet - \mathbf{m} + \mathbf{n} \rangle)} = \gamma_B(\bullet; \mathbf{m}, \mathbf{n}). \end{aligned}$$

From the coboundary map the same contributions emerge, that appeared from the dual translation operators in the commutation relation in Eq. (3.15). The last equality is again the identity by Stokes theorem shown in App. A3.

Constant magnetic field If we now consider a constant magnetic field B for all $\mathbf{l} \in \mathbb{Z}^d$ the phase assumes the form

$$\begin{aligned} \Gamma_B(\langle \mathbf{l}, \mathbf{l} - \mathbf{m}, \mathbf{l} - \mathbf{m} - \mathbf{n} \rangle) &= \frac{e}{2\hbar} \sum_{j,k=1}^d (\mathbf{x}_{\mathbf{m}})_j (\mathbf{x}_{\mathbf{n}})_k B_{jk} \\ &= \frac{2\pi}{2} \sum_{j,k=1}^d \Phi_{jk} m_j n_k = 2\pi(\mathbf{m} \wedge_{\Phi} \mathbf{n}) \end{aligned}$$

with $\Phi = \frac{1}{\phi_0} D^T B D$, where $\phi_0 = \frac{h}{e}$ is the flux quantum, B is the real antisymmetric $(d \times d)$ -matrix, which contains the components of the magnetic field 2-form B , and D is the real $(d \times d)$ -matrix $D = (\mathbf{a}_1, \dots, \mathbf{a}_d)$, which has the d lattice vectors encoding the real space positions by $\mathbf{x}_{\mathbf{m}} = \sum_j^d m_j \mathbf{a}_j$. Thus, Φ itself is a real antisymmetric $(d \times d)$ -matrix and since it encodes phases for any $\mathbf{m}, \mathbf{n} \in \mathbb{Z}^d$ its entries are equivalent modulo 1 and can thus be chosen in $[0, 1)$. It describes the magnetic flux through the facets of the primitive cells in units of the flux quantum. This form coincides with Eq. (3.5), thus $\gamma_B(\bullet; \mathbf{m}, \mathbf{n}) \equiv \gamma(\mathbf{m}, \mathbf{n})$ for all $\mathbf{m}, \mathbf{n} \in \mathbb{Z}^d$. For the vector potential in the symmetric gauge follows $A_i(\mathbf{x}) = -\frac{1}{2} \sum_{j=1}^d B_{ij} x_j$ and thus

$$\begin{aligned} \Gamma_A([\mathbf{n}, \mathbf{n} - \mathbf{m}]) &= -\frac{e}{\hbar} \sum_{i=1}^d (\mathbf{x}_{\mathbf{m}})_i \int_0^1 dt \left(-\frac{1}{2} \sum_{j=1}^d B_{ij} (\mathbf{x}_{\mathbf{n}} - t\mathbf{x}_{\mathbf{m}})_j \right) \\ &= \frac{e}{2\hbar} \sum_{i,j=1}^d (\mathbf{x}_{\mathbf{m}})_i (\mathbf{x}_{\mathbf{n}})_j B_{ij} = 2\pi(\mathbf{m} \wedge_{\Phi} \mathbf{n}). \end{aligned}$$

Therefore, the phase factor of the magnetic translation can be written in the compact form $\lambda^A(\mathbf{m}; \mathbf{n}) = \gamma_B(\mathbf{0}; \mathbf{m}, \mathbf{n}) = e^{2\pi i(\mathbf{m} \wedge_{\Phi} \mathbf{n})}$. This defines a projective unitary representation

$$\begin{aligned} \rho^A : \mathbb{Z}^d &\rightarrow \mathcal{U}(\ell^2(\mathbb{Z}^d))/S^1, \quad \rho^A(\mathbf{m}) |\mathbf{n}\rangle = \hat{U}_{\mathbf{m}}^A |\mathbf{m}\rangle = \pi(\lambda^A(\mathbf{m})) \hat{T}_{\mathbf{m}} |\mathbf{n}\rangle \\ &= e^{2\pi i(\mathbf{m} \wedge_{\Phi} \mathbf{n})} |\mathbf{n} + \mathbf{m}\rangle. \end{aligned}$$

While the constant magnetic field B is independent of the choice of origin and can therefore be treated as constant prefactor, the magnetic potential A is linear. This is why $\lambda^A(\mathbf{m}) \in C_b(\mathbb{Z}^d, S^1)$ needs to be represented as a multiplication operator on $\ell^2(\mathbb{Z}^d)$ using π .

Remark 3.3 (Gauge invariance). It is important to note that although $\lambda^A(\mathbf{m}; \mathbf{n})$ can be expressed in the form $e^{2\pi i(\mathbf{m} \wedge \Phi \mathbf{n})}$ only depending on the gauge invariant magnetic flux matrix Φ , this is a consequence of the choice of symmetric gauge. While the algebraic structure of the twisted crossed product, in contrast, is gauge invariant, a different presentation than Eq. (3.6) can be used in case of a different choice of gauge. In [PS16, Chap. 3] the choice of the symmetric gauge as well as the Landau gauge is discussed. While the former is advantageous for the description of bulk systems, the latter is to be preferred for boundary observables.

The triple $(\ell^2(\mathbb{Z}^d), \pi, \rho^A)$ is a covariant representation of the twisted C^* -dynamical system $(C_b(\mathbb{Z}^d), \mathbb{Z}^d, \theta, \gamma_B)$ and provides us with a family of covariant representations $\{(\ell^2(\mathbb{Z}^d), \pi_\varphi, \rho^A)\}_{\varphi \in T^r}$ for $(C(T^r), \mathbb{Z}^d, \alpha, \gamma)$:

*Covariant
Schrödinger
representations*

- (i) $\mathcal{H} = \ell^2(\mathbb{Z}^d)$ is a separable Hilbert space,
- (ii) $(\ell^2(\mathbb{Z}^d), \pi_\varphi)$ is a non-degenerate representation for $C(T^r)$ with

$$\pi_\varphi(f) = \sum_{\mathbf{n} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n}} f)(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \quad \forall f \in C(T^r),$$

- (iii) $(\ell^2(\mathbb{Z}^d), \rho^A)$ is a projective unitary representation of $\mathbb{Z}^d$ with

$$\rho^A(\mathbf{m}) = \hat{U}_{\mathbf{m}}^A = \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i(\mathbf{m} \wedge \Phi \mathbf{n})} |\mathbf{n} + \mathbf{m}\rangle \langle \mathbf{n}| \quad \forall \mathbf{m} \in \mathbb{Z}^d$$

such that

$$\rho^A(\mathbf{m}) \rho^A(\mathbf{n}) = \pi_\varphi(\gamma(\mathbf{m}, \mathbf{n})) \rho^A(\mathbf{m} + \mathbf{n}) \quad \forall \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d,$$

and

- (iv) the covariance condition is satisfied

$$\pi_\varphi(\alpha_{\mathbf{m}}(f)) = \rho^A(\mathbf{m}) \pi_\varphi(f) \rho^A(\mathbf{m})^* \quad \forall \mathbf{m} \in \mathbb{Z}^d, f \in C(T^r).$$

The commutation relation in (iii) has been confirmed in App. A4 and the covariance condition in (iv) can be verified by the following brief calculation:

$$\begin{aligned} \rho^A(\mathbf{m}) \pi_\varphi(f) \rho^A(\mathbf{m})^* &= \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i(\mathbf{m} \wedge \Phi \mathbf{n})} (\alpha_{-\mathbf{n}} f)(\varphi) e^{-2\pi i(\mathbf{m} \wedge \Phi \mathbf{n})} |\mathbf{n} + \mathbf{m}\rangle \langle \mathbf{n} + \mathbf{m}| \\ &= \sum_{\mathbf{n} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n} + \mathbf{m}} f)(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| = \pi_\varphi(\alpha_{\mathbf{m}}(f)). \end{aligned}$$

3. C^* -Algebra Theory of Multi-q Textures

*Integrated
Schrödinger
representation*

From the family of covariant representations $\{(\ell^2(\mathbb{Z}^d), \pi_\varphi, \rho^A)\}_{\varphi \in T^r}$ we can construct the family $\{\pi_\varphi \rtimes \rho^A\}_{\varphi \in T^r}$ of non-degenerate representations of the twisted crossed product algebra $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ on the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}^d)$ [Pro17, Prop. 3.8] by

$$(\pi_\varphi \rtimes \rho^A)(f \otimes t^{\mathbf{m}}) = \pi_\varphi(f) \rho^A(\mathbf{m}).$$

A generic element $a = \sum_{\mathbf{m} \in \mathbb{Z}^d} f_{\mathbf{m}} \otimes t^{\mathbf{m}}$ of this algebra is then represented by

$$(\pi_\varphi \rtimes \rho^A)(a) = \sum_{\mathbf{n}, \mathbf{m} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n}} f_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A.$$

As shorthand notation we write $\pi_\varphi^\rtimes := \pi_\varphi \rtimes \rho^A$ in the following. The $*$ -homomorphism property of $\pi_\varphi^\rtimes$ depends on the $*$ -algebraic structure of the twisted crossed product defined by Eq. (3.6) and (3.7), and we verify it in App. A5. Analogous to the faithfulness of π_φ , $\pi_\varphi^\rtimes$ is faithful, if τ acts ergodic on T^r [Pro17, Prop. 3.8]. It is $\pi_\varphi^\rtimes(a) = 0$ if and only if $f_{\mathbf{m}}(\tau_{\mathbf{n}}\varphi) = 0$ for all coefficient functions $f_{\mathbf{m}}$ and translations $\mathbf{n} \in \mathbb{Z}^d$, and if the action is ergodic for all $\varphi \in T^r$ and the coefficient functions are continuous, one must have $f_{\mathbf{m}}(\varphi) = 0$ everywhere. The faithfulness of the representation shows that our twisted crossed product algebra does not contain any redundant or unnecessary information about the observables. It is the minimal algebraic structure that describes the essential physical properties of the electronic system: Algebraically distinct observables in $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ will have physically distinct representations on $\mathcal{B}(\mathcal{H})$.

Covariance

The integrated representation satisfies its own version of the covariance condition. Although the translation invariance of a Hamiltonian is broken in the presence of a magnetic field, it can be recovered by changing the representation of the translation group to the magnetic translation operators $\hat{V}_{\mathbf{m}}^A$, $\mathbf{m} \in \mathbb{Z}^d$ [Bro64; Zak64; Flo97]. They commute with the dual magnetic translation operators $\hat{U}_{\mathbf{m}}^A$, $\mathbf{m} \in \mathbb{Z}^d$, and can be expressed in the same form with a modified magnetic vector potential A' such that $dA' = -B$. This depends on the choice of gauge, and in the case of the symmetric gauge it is $A' = -A$, such that

$$\hat{V}_{\mathbf{m}}^A = \hat{U}_{\mathbf{m}}^{-A} = \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i(\mathbf{n} \wedge \Phi \mathbf{m})} |\mathbf{n} + \mathbf{m}\rangle \langle \mathbf{n}|.$$

Thus, we get the following covariance of the representation: A magnetic lattice translation of the representation of a physical observable is compensated by an inverse shift of the phase chosen at the origin of the representation

$$\hat{V}_{\mathbf{m}}^A \pi_\varphi^\rtimes(a) \hat{V}_{\mathbf{m}}^{A^{-1}} = \pi_{\tau_{-\mathbf{m}}\varphi}^\rtimes(a). \quad (3.18)$$

This follow directly from the covariance condition of the covariant representation and the commutation of the magnetic translations with the dual magnetic translations:

$$\begin{aligned} \hat{V}_{\mathbf{m}}^A \pi_\varphi^\rtimes(a) \hat{V}_{\mathbf{m}}^{A^{-1}} &= \sum_{\mathbf{n} \in \mathbb{Z}^d} \hat{U}_{\mathbf{m}}^{-A} \pi_\varphi(a_{\mathbf{n}}) \hat{U}_{\mathbf{m}}^{-A*} \hat{U}_{\mathbf{n}}^A = \sum_{\mathbf{n} \in \mathbb{Z}^d} \pi_\varphi(\alpha_{\mathbf{m}} a_{\mathbf{n}}) \hat{U}_{\mathbf{n}}^A \\ &= \pi_{\tau_{-\mathbf{m}}\varphi}^\rtimes(a). \end{aligned}$$

Now, we have finally all the pieces in place to construct a norm for the C^* -completion of the twisted crossed product algebra $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ to the C^* -algebra known as the non-commutative torus.

3.1.3. Non-commutative Torus Algebra

The non-commutative torus algebra is obtained as the C^* -completion of the (twisted) crossed product algebra. It is equivalent to the universal unital C^* -algebra of the unitaries which generate this algebra. In the following, we first define an ℓ^1 -norm on the (twisted) crossed product algebra to construct its B^* -algebra completion. Then, we construct a norm from all covariant representations to generate the so-called *full (twisted) crossed product C^* -algebra* as C^* -completion. To obtain a more tangible, explicit expression, we construct a second norm from just the family of integrated Schrödinger representations, which can be used to generate the *reduced (twisted) crossed product C^* -algebra*. Fortunately, in our case both notions coincide, such that we can use the explicit norm for the full (twisted) crossed product C^* -algebra, which is the non-commutative torus algebra describing the physical observables of our system. We end this section, by highlighting the relations of the unitary generators of the algebra. The non-commutative torus is precisely equivalent to the universal unital C^* -algebra of these unitaries.

The commutative algebra of complex-valued continuous functions on the r -torus $C(T^r)$ is a C^* -algebra with involution given by the complex conjugation and with the uniform norm ℓ^1 -norm

$$\|f\|_{T^r} = \sup_{\varphi \in T^r} |f(\varphi)|$$

being the unique norm fulfilling the C^* -condition from Def. 3.2. Using the uniform norm, we can construct a series of ℓ^n -norms on the (twisted) crossed product algebra $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ by

$$\|a\|_{\ell^n} = \left(\sum_{\mathbf{m} \in \mathbb{Z}^d} \|f_{\mathbf{m}}\|_{T^r}^n \right)^{\frac{1}{n}}$$

for any $a = \sum_{\mathbf{m} \in \mathbb{Z}^d} f_{\mathbf{m}} \otimes t^{\mathbf{m}}$. By $\ell^1(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ we denote the Banach $*$ -algebra which is obtained through the completion of $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ with respect to the ℓ^1 -norm. The (twisted) crossed product algebra is dense in $\ell^1(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ and a typical element is of the form $a = \sum_{\mathbf{m} \in \mathbb{Z}^d} f_{\mathbf{m}} \otimes t^{\mathbf{m}}$, where infinitely many $f_{\mathbf{m}}$ can be different from zero, if they satisfy $\sum_{\mathbf{m} \in \mathbb{Z}^d} \|f_{\mathbf{m}}\|_{T^r} < \infty$. Any integrated representation of $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$, as introduced in the last section, extends to a norm-decreasing representation on $\ell^1(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ [Ric14, Thm. 3.4.1, 5.2.5].

To arrive at a C^* -completion of $\ell^1(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ there are essentially two different constructions: The full (twisted) crossed product C^* -algebra $C(T^r) \rtimes_{\alpha}^{\gamma} \mathbb{Z}^d$ and the reduced (twisted) crossed product C^* -algebra $C(T^r) \rtimes_{\alpha, r}^{\gamma} \mathbb{Z}^d$. A brief, educational overview on this can be found in [Kha13, Example 2.2.7], while we refer to [Ped18, Ch. 7] or [Wil07, Chap.7.2] for a more detailed account. Both approaches have the following basic idea in common: Since every C^* -algebra is isomorphic to a C^* -subalgebra of the bounded C^* -norm

3. C^* -Algebra Theory of Multi-q Textures

operators $\mathcal{B}(\mathcal{H})$ on a Hilbert space $\mathcal{H}$, one can express the unique norm fulfilling the C^* -property in terms of the norm $\|\cdot\|_{\mathcal{B}(\mathcal{H})}$ and a suitable choice of Hilbert space representation.

For the construction of the full (twisted) crossed product C^* -algebra $C(T^r) \rtimes_{\alpha}^{\gamma} \mathbb{Z}^d$ we define the *universal norm* by

$$\|a\| = \sup_{(\mathcal{H}, \pi, \rho)} \|(\pi \rtimes \rho)(a)\|_{\mathcal{B}(\mathcal{H})},$$

where the supremum is over all covariant representations $(\mathcal{H}, \pi, \rho)$ of $(C(T^r), \mathbb{Z}^d, \alpha, \gamma)$. It is dominated by the ℓ^1 -norm, and the completion of $\ell^1(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ with respect to it is the full (twisted) crossed product C^* -algebra $C(T^r) \rtimes_{\alpha}^{\gamma} \mathbb{Z}^d$. Since the full C^* -algebra is defined in this abstract way it is useful to work with elements of the dense subalgebra $\ell^1(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ which typical elements are defined in an explicit form as discussed above.

Nevertheless, for physics it is relevant to have an explicit expression of the norm with respect to the operator norm on the physical Hilbert space $\ell^2(\mathbb{Z}^d)$, which can be constructed from the covariant Schrödinger representations $\{\ell^2(\mathbb{Z}^d), \pi_{\varphi}, \rho^A\}_{\varphi \in T^r}$ and provides an alternative C^* -completion, the reduced (twisted) crossed-product C^* -algebra $C(T^r) \rtimes_{\alpha, r}^{\gamma} \mathbb{Z}^d$. We define the corresponding *reduced norm* by

$$\|a\|_r = \sup_{\varphi \in T^r} \|(\pi_{\varphi}^{\rtimes})(a)\|_{\mathcal{B}(\ell^2(\mathbb{Z}^d))}. \quad (3.19)$$

The completion of $\ell^1(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ with respect to this norm is the reduced (twisted) crossed product C^* -algebra $C(T^r) \rtimes_{\alpha, r}^{\gamma} \mathbb{Z}^d$. Since $\mathbb{Z}^d$ is an amenable group, both completions give identical C^* -algebras [Wil07, Thm. 7.13]. Thus, we drop the distinction and denote the non-commutative torus from now on as $C(T^r) \rtimes_{\theta}^{\Phi} \mathbb{Z}^d$, where θ is the coefficient matrix which determines the action α and Φ is the magnetic flux matrix, which determines the magnetic 2-cocycle γ .

*Universal
 C^* -algebra*

By considering the Fourier series expansion of the continuous functions on the r -torus, we can interpret the C^* -algebra $C(T^r)$ as the universal C^* -algebra

$$C^*(\langle u_1, \dots, u_r | u_i u_j = u_j u_i \rangle)$$

with the unitary generators u_i as the continuous phase factors $u_j(\varphi) = e^{i\varphi_j}$. They obey the following commutation relations with the generators $t^{\mathbf{m}}$ of the translation group in $C(T^r) \rtimes_{\theta}^{\Phi} \mathbb{Z}^d$:

$$\begin{aligned} u_i t_j &:= (u_i \otimes t^{\mathbf{0}})(1 \otimes t_j) = u_i \otimes t_j = (1 \otimes t_j)(\alpha_{-\mathbf{e}_j}(u_i) \otimes t^{\mathbf{0}}) \\ &= e^{2\pi i \theta_{ij}} (1 \otimes t_j)(u_i \otimes t^{\mathbf{0}}) =: e^{2\pi i \theta_{ij}} t_j u_i \end{aligned} \quad (3.20)$$

and

$$\begin{aligned} t_i u_j &:= (1 \otimes t_i)(u_j \otimes t^{\mathbf{0}}) = \alpha_{\mathbf{e}_i}(u_j) \otimes t_i = e^{-2\pi i \theta_{ji}} u_j \otimes t_i \\ &= e^{-2\pi i \theta_{ji}} (u_j \otimes t^{\mathbf{0}})(1 \otimes t_i) =: e^{2\pi i (-\theta^T)_{ij}} u_j t_i, \end{aligned} \quad (3.21)$$

3.1. Non-commutative Torus

which follows from Eq. (3.6) with Eq. (3.2). Together with the commutation relation of the generators $t^{\mathbf{m}}$ as presented in Eq. (3.8)

$$t_i t_j = e^{2\pi i \Phi_{ij}} t_j t_i, \quad (3.22)$$

we have several commutation relations of unitaries of precisely the form $UV = \lambda VU$, with $\lambda = e^{2\pi i \Theta_{UV}}$, $\Theta_{UV} \in \mathbb{R}$. This means if we combine the generators u_i of the continuous torus functions and the translation generators t_j into a single notation

$$\mu = (\mu_1, \dots, \mu_{r+d}) = (u_1, \dots, u_r, t_1, \dots, t_d),$$

then we can give an equivalent description of the non-commutative torus algebra $\mathcal{A}_\Theta := C(T^r) \rtimes_\theta^\Phi \mathbb{Z}^d$ in terms of the universal C^* -algebra [Dav96, Chap. 6]

$$C^*(\langle \mu_1, \dots, \mu_{r+d} \mid \mu_a \mu_b = e^{2\pi i \Theta_{ab}} \mu_b \mu_a \rangle), \quad (3.23)$$

where Θ is the real antisymmetric $(r+d) \times (r+d)$ matrix

$$\Theta = \begin{pmatrix} 0 & \theta \\ -\theta^T & \Phi \end{pmatrix}. \quad (3.24)$$

The $(r \times d)$ matrix θ specifies the group action of the crossed product structure and the $(d \times d)$ matrix Φ determines the group cocycle for the twisted action. It is convenient to use the generators $(u_1, \dots, u_r, t_1, \dots, t_d)$ as labels for the elements of Θ , such that $\Theta_{u_i t_j} = \theta_{ij}$, $\Theta_{t_i u_j} = -\theta_{ji}$, and $\Theta_{t_i t_j} = \Phi_{ij}$.

Remark 3.4 (Convention: order of generators). The order of the generators and the subsequent form of the matrix Θ determine the label convention for the Chern numbers, which are antisymmetric under permutation of labels. In our publications [Lux+24] and [Pra+24] the order $(t_1, \dots, t_d, u_1, \dots, u_r)$ was chosen, which would imply $\Theta = \begin{pmatrix} \Phi & -\theta^T \\ \theta & 0 \end{pmatrix}$ in the presence of the magnetic field. When using the generators as labels for Θ the elements remain the same, which makes this subscription conveniently independent of this arbitrary choice of order.

In conclusion, the observable algebra of spin-1/2 electrons on the $\mathbb{Z}^d$ lattice permeated by a constant magnetic field and in contact with an ergodic multi- q spin texture is

Observable algebra

$$\mathcal{A} = M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta,$$

and we can extend $\pi_\varphi^\times$ to a faithful non-degenerate family of representations of $\mathcal{A}$ on $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$ by setting

$$\pi_\varphi^\times(m \otimes a) = m \otimes \pi_\varphi^\times(a),$$

for all $m \in M_2(\mathbb{C})$ and $a \in \mathcal{A}_\Theta$.

3.2. Differential Calculus

The C^* -algebra of physical observables, in conjunction with a differential calculus comprising a set of commuting $*$ -derivations and a faithful trace, constitutes a non-commutative manifold, known as the non-commutative Brillouin zone. Analogous to the commutative case, where differential geometry is employed to ascertain topological invariants, e.g. the Chern numbers as integrals over curvature forms, the tools of non-commutative geometry for a non-commutative manifold permit the determination of the topological invariants of the non-commutative algebra.

Fourier calculus

Since the commutation relations of the universal algebra in Eq. (3.23), and equally the twisted crossed product structure from Eq. (3.6)-(3.7), are invariant with respect to the multiplication with phase factors, we can define a $(r + d)$ -torus Lie group action on the non-commutative torus algebra $\mathcal{A}_\Theta$. With it, we can establish a Fourier calculus and expand any algebra element $a \in \mathcal{A}_\Theta$ into an infinite sum of translation generators with coefficients from $C(T^r)$ that decay with $\|\mathbf{m}\| \rightarrow \infty$, just as the typical elements from $\ell^1(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$. As we will see, we can even go further and decompose any $a \in \mathcal{A}_\Theta$ fully to

$$a = \sum_{\mathbf{m} \in \mathbb{Z}^d} f_{\mathbf{m}} \otimes t^{\mathbf{m}} = \sum_{\mathbf{l} \in \mathbb{Z}^r} \sum_{\mathbf{m} \in \mathbb{Z}^d} f_{\mathbf{l}\mathbf{m}} u^{\mathbf{l}} \otimes t^{\mathbf{m}}, \quad (3.25)$$

where $f_{\mathbf{l}\mathbf{m}} \in \mathbb{C}$ are the Fourier coefficients of the continuous r -torus functions $f_{\mathbf{m}} \in C(T^r)$, and where we use the multi-index notation $u^{\mathbf{l}} = u_1^{l_1} \dots u_r^{l_r}$. With the help of this decomposition, we can subsequently construct a continuous and faithful trace on the observable algebra, while the infinitesimal generators of the group action provide a set of commuting unbounded closed $*$ -derivations.

Torus action

Let us consider an action of the Lie group $T^{r+d} = U(1)^{(r+d)}$ on $\mathcal{A}_\Theta$. Let the action $\rho : T^{r+d} \rightarrow \text{Aut}(\mathcal{A}_\Theta)$, $\boldsymbol{\lambda} \mapsto \rho_{\boldsymbol{\lambda}}$ act on the translation generators and their coefficients the following way:

$$\rho_{\boldsymbol{\lambda}}(f)(\boldsymbol{\varphi}) = f(\boldsymbol{\varphi} + \boldsymbol{\xi}), \quad (3.26)$$

$$\rho_{\boldsymbol{\lambda}}(t_i) = e^{ik_i} t_i, \quad i = 1, \dots, d, \quad (3.27)$$

with $\boldsymbol{\lambda} = (\boldsymbol{\xi}, \mathbf{k}) \in [0, 2\pi]^r \times [0, 2\pi]^d$ and $f \in C(T^r)$. The prescription in Eq. (3.26) can be equally expressed on the unitary generators u_i by $\rho_{\boldsymbol{\lambda}}(u_i) = e^{i\xi_i} u_i$, $i = 1, \dots, r$. The definition on the generators can then be extended to a point-wise norm continuous group of $*$ -automorphisms on $\mathcal{A}_\Theta$, i.e. for each fixed $a \in \mathcal{A}_\Theta$ the map $\boldsymbol{\lambda} \rightarrow \rho_{\boldsymbol{\lambda}}(a)$ is norm continuous. The $*$ -automorphism property hereby stems from the aforementioned invariance of the algebraic structure under multiplication with phase factors [Pro17, Prop. 3.10.].

Remark 3.5 (Gauge transformations). The group of automorphisms can be interpreted as $U(1)$ -gauge transformations, which is the reason why the differential calculus discussed in this section can be used to describe electric charge transport phenomena [Pro17, Rem. 3.11.].

Using the established Fourier calculus, we can define Fourier coefficients for any element $a \in \mathcal{A}_\Theta$ by

*Fourier
coefficients*

$$\Phi_{\mathbf{m}}(a) = \left[\int_{T^d} \frac{d\mathbf{k}}{(2\pi)^d} e^{-i\mathbf{m} \cdot \mathbf{k}} \rho_{(0,\mathbf{k})}(a) \right] (t^{-\mathbf{m}}) \in C(T^r). \quad (3.28)$$

Going one step further, we can compute the Fourier coefficients of these coefficients

$$\Phi_{\mathbf{l}\mathbf{m}}(a) = \left[\int_{T^r} \frac{d\boldsymbol{\xi}}{(2\pi)^r} e^{-i\mathbf{l} \cdot \boldsymbol{\xi}} \rho_{(\boldsymbol{\xi},0)}(\Phi_{\mathbf{m}}(a)) \right] (u^{-1}) = \int_{T^r} \frac{d\boldsymbol{\varphi}}{(2\pi)^r} e^{-i\mathbf{l} \cdot \boldsymbol{\varphi}} \Phi_{\mathbf{m}}(a) \in \mathbb{C}. \quad (3.29)$$

The second equality holds, because the unitary generators are of the form $u_i = e^{i\varphi_i}$. If we have a typical element a of the form given in Eq. (3.25), then the Fourier coefficients are simply the coefficients of the infinite sum $\Phi_{\mathbf{m}}(a) = f_{\mathbf{m}}$ and $\Phi_{\mathbf{l}\mathbf{m}}(a) = f_{\mathbf{l}\mathbf{m}}$. This can even be generalised for a generic element $a \in \mathcal{A}_\Theta$, because the *Cesàro sums*

$$a^L = \sum_{\mathbf{m} \in V_L} \prod_{j=1}^d \left(1 - \frac{|m_j|}{L+1} \right) \Phi_{\mathbf{m}}(a) t^{\mathbf{m}},$$

with $V_L = \{-L, \dots, L\}^d$ converge in norm to a as $L \rightarrow \infty$ [Dav96, Thm. VIII.2.2] and, because the coefficients are continuous functions over T^r , which implies that their Fourier series converge uniformly as well. Consequently, any two elements in $\mathcal{A}_\Theta$ with identical Fourier coefficients are equal. This justifies the statement regarding the decomposition, which we made at the start of this section.

In the following, we will employ the Fourier decomposition to construct the canonical trace on the non-commutative torus, utilising the trace on $C(T^r)$ and the trace on the group algebra $\mathbb{C}\mathbb{Z}^d$. By invoking Birkhoff's ergodic theorem, it can be demonstrated that the canonical trace is equivalent to the physical trace per unit volume of the representation as bounded operator on the physical lattice Hilbert space $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$. Subsequently, we obtain $*$ -derivations on the algebra by derivatives with respect of the torus action and discuss the differential subalgebras and their properties. Lastly, we introduce the Itô derivatives, which are derivatives on the continuous field of (twisted) crossed product C^* -algebras $\{C(T^r) \rtimes_{\theta}^{\Phi} \mathbb{Z}^d\}_{\theta, \Phi}$ with respect to the components of θ and Φ . This section closely follows the approach outlined by Emil Prodan in [PS16, Chap. 3.3] and [Pro17, Chap. 3] while extending the differential calculus to the phase torus.

Section Content

3.2.1. The Canonical Trace and Birkhoff's Ergodic Theorem

In the context of differential calculus on an observable algebra, the trace assumes the role of integration from commutative geometry. Its relevance for the topological classification will become apparent in Sec. 3.3, as the trace property entails that homotopy equivalent projections are mapped to the same value, such that any bounded trace induces a unique group homomorphism from the algebras K_0 -group to $\mathbb{C}$. Using the covariant representations, we can express the canonical trace on the observable algebra also in terms of the trace for bounded Hilbert space operators.

3. C^* -Algebra Theory of Multi-q Textures

In the following, we introduce the canonical traces on the algebra of continuous functions over the torus and on the group algebra. From them, we can construct the canonical trace of the non-commutative torus, which is faithful and continuous. Subsequently, we introduce the physical trace per unit volume on the bounded operators and demonstrate that it converges to the trace on the non-commutative torus in the infinite volume limit.

In general, a (faithful) trace on a C^* -algebra is defined as follows:

Definition 3.6 (Trace). Let A be a C^* algebra. A *trace* on A is a linear map $\tau : A \rightarrow \mathbb{C}$ with the *trace property*:

$$\tau(ab) = \tau(ba) \quad \text{for } a, b \in A.$$

The trace is *faithful* if $\tau(aa^*) > 0$ for all $a \neq 0$.

Canonical trace

In Sec. 3.1, we constructed the non-commutative torus as a completion of the crossed product of the C^* -algebra $C(T^r)$ and the group $\mathbb{Z}^d$. Since the underlying vector space is the $\mathbb{C}$ -linear tensor product $C(T^r) \otimes \mathbb{C}\mathbb{Z}^d$, we can construct a faithful trace on the corresponding algebra from the faithful traces on $C(T^r)$ and $\mathbb{C}\mathbb{Z}^d$. In case of the commutative algebra $C(T^r)$ of continuous functions on the r -torus, the canonical trace is given by

$$\tau_{C(T^r)}(f) = \int_{T^r} \frac{d\varphi}{(2\pi)^r} f(\varphi),$$

with the useful property of being invariant under the $\mathbb{Z}^d$ -automorphisms α :

$$\tau_{C(T^r)}(\alpha_{\mathbf{m}} f) = \tau_{C(T^r)}(f), \quad \forall \mathbf{m} \in \mathbb{Z}^d.$$

This trace is clearly faithful and continuous and corresponds to the 0th Fourier coefficient of the torus function. On the group algebra $\mathbb{C}\mathbb{Z}^d$ a unique trace is given by the map from any generic element onto the coefficient of the identity element

$$\tau_{\mathbb{C}\mathbb{Z}^d} \left(\sum_{\mathbf{m} \in \mathbb{Z}^d} c_{\mathbf{m}} t^{\mathbf{m}} \right) = c_0.$$

It is faithful and continuous, and by defining a Fourier calculus on $\mathbb{C}\mathbb{Z}^d$ as in Eq. (3.27), this trace can be interpreted as a 0th Fourier coefficient in the sense of Eq. (3.28) as well. For any element $a \in A_{\Theta}$, we have the corresponding map $\Phi_0 : A_{\Theta} \rightarrow C(T^r)$. In composition with the trace on $C(T^r)$, we obtain the following continuous and faithful trace on the observable algebra $\mathcal{A} = M_2(\mathbb{C}) \otimes A_{\Theta}$:

$$\mathcal{T}(a) = \int_{T^r} \frac{d\varphi}{(2\pi)^r} \text{tr}(\Phi_0(a)) = \text{tr}(\Phi_{00}(a)), \quad (3.30)$$

where tr denotes the matrix trace on $M_2(\mathbb{C})$. The faithfulness of $\mathcal{T}$ follows from the faithfulness of Φ_0 , respectively Φ_{00} , as *expectations* (of a C^* -algebra) as demonstrated in

[Dav96, Thm. VI.1.1 and VIII.2.1] for the case $d = 1$, respectively $d = r = 1$. It can also be substantiated explicitly by computing aa^* for an arbitrary $a \neq 0$. We find

$$(aa^*)_0 = \sum_{\mathbf{m} \in \mathbb{Z}^d} a_{\mathbf{m}} \alpha_{\mathbf{m}}(a_{-\mathbf{m}}^*) = \sum_{\mathbf{m} \in \mathbb{Z}^d} a_{\mathbf{m}} a_{\mathbf{m}}^*$$

and, thus,

$$\mathcal{T}(aa^*) = \sum_{\mathbf{m} \in \mathbb{Z}^d} \int_{T^r} \frac{d\varphi}{(2\pi)^r} \text{tr}(a_{\mathbf{m}} a_{\mathbf{m}}^*).$$

Clearly, $\mathcal{T}(aa^*) = 0$ implies $a_{\mathbf{m}} = 0$ for all $\mathbf{m} \in \mathbb{Z}^d$, which is only satisfied by $a \equiv 0$, since the Fourier coefficients fully determine the elements $a \in \mathcal{A}_{\Theta}$. This is precisely the property of a faithful trace. Furthermore, the trace is normalised on $\mathcal{A}_{\Theta}$ with $\mathcal{T}(1 \otimes t^0) = 1$ and, by construction, invariant under the torus action automorphisms ρ_{λ} .

The physical relevance of the trace $\mathcal{T}$ is revealed through the ergodic properties of the translation action on T^r , which connects it to the trace per unit volume on the physical Hilbert space [Pro17, Prop. 2.5]. Let us consider a finite cube V of cardinality $|V|$ centred around the origin and let $\Pi_V = \mathbb{1}_{2 \times 2} \otimes \sum_{\mathbf{m} \in V} |\mathbf{m}\rangle \langle \mathbf{m}|$ be the partial isometry, which restricts bounded operators on $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$ to the finite-dimensional Hilbert space $\mathbb{C}^2 \otimes \ell^2(V)$. The trace per unit volume of an element $a \in \mathcal{A}$ is then defined as

$$\mathcal{T}_V(a) = \frac{1}{|V|} \text{Tr}_V(\Pi_V \pi_{\varphi}^{\times}(a) \Pi_V^*), \quad (3.31)$$

where Tr_V denotes the trace on $\mathbb{C}^2 \otimes \ell^2(V)$. Using the covariance property of the $*$ -representation $\pi_{\varphi}^{\times}$ given in Eq. (3.18), we can rewrite the trace per unit volume in terms of the summation

$$\begin{aligned} \mathcal{T}_V(a) &= \frac{1}{|V|} \sum_{\mathbf{m} \in V} \text{tr} \langle \mathbf{m} | \pi_{\varphi}^{\times}(a) | \mathbf{m} \rangle = \frac{1}{|V|} \sum_{\mathbf{m} \in V} \text{tr} \langle 0 | (\hat{V}_{\mathbf{m}}^A)^{-1} \pi_{\varphi}^{\times}(a) \hat{V}_{\mathbf{m}}^A | 0 \rangle \\ &= \frac{1}{|V|} \sum_{\mathbf{m} \in V} \text{tr} \langle 0 | \pi_{\tau_{\mathbf{m}}\varphi}(a) | 0 \rangle. \end{aligned}$$

With $\tau : T^r \rightarrow T^r$ ergodic, we have a measure-preserving ergodic system $(T^r, \mathcal{B}, \mu, \tau)$, where $\mathcal{B}$ is the Borel σ -algebra of T^r , τ are the irrational rotations acting on T^r and μ is the Lebesgue measure on T^r , invariant under τ . In fact, τ is *uniquely ergodic* in the sense that the Lebesgue measure is the only τ -invariant measure on T^r [KH95, Def. 4.1.7.]. Uniquely ergodic systems fulfil a stronger version of *Birkhoff's ergodic theorem* [KH95, Prop. 4.1.13.] such that

$$\lim_{|V| \rightarrow \infty} \frac{1}{|V|} \sum_{\mathbf{m} \in V} \text{tr} \langle 0 | \pi_{\tau_{\mathbf{m}}\varphi}(a) | 0 \rangle = \frac{1}{(2\pi)^r} \int_{T^r} d\varphi \text{tr} \langle 0 | \pi_{\varphi}^{\times}(a) | 0 \rangle = \mathcal{T}(a),$$

converges uniformly for all $\varphi \in T^r$ and is independent of φ . In summary, we thus have

$$\lim_{|V| \rightarrow \infty} \mathcal{T}_V(a) = \mathcal{T}(a). \quad (3.32)$$

*Birkhoff's
ergodic theorem*

3. C^* -Algebra Theory of Multi-q Textures

The trace per unit volume may be considered the more natural choice of trace, offering a straightforward physical interpretation within the relevant physical Hilbert space. The result in Eq. (3.32) demonstrates that this trace is identical to its purely algebraic counterpart in the thermodynamic limit, which is crucial to establish the physical significance of the algebraic formulation.

3.2.2. Derivations of the Torus Action

Derivations on an observable algebra introduce the concept of differentiability of elements and allow for the construction of geometric expressions. In the case of the non-commutative torus, we can define derivations associated with the real space and the momentum space by using the established Fourier calculus. This generates a system of $r + d$ unbounded closed $*$ -derivations. Here, we present the general concept of $*$ -derivation and construct explicitly the family of derivations generated by the Fourier calculus and their Hilbert space representations. This allows us to establish the smooth dense subalgebra, known as the smooth non-commutative torus, and to discuss its properties, in particular those regarding its K-Theory, such as the stability under holomorphic functional calculus.

Derivations A *derivation* on an algebra is a map which generalises the notion of a derivative, in particular, it satisfies the *Leibniz rule*. On a C^* -algebra, we define a $*$ -derivative in such a way that it preserves the involution [Bel92, Def. 1]:

Definition 3.7 ($*$ -derivation). A $*$ -derivation on a C^* -algebra A is a linear map ∂ defined on a dense subalgebra $\mathcal{D}(\partial) \subset A$, such that

- (i) $\partial(ab) = (\partial a)b + a(\partial b)$ (*Leibniz rule*),
- (ii) $\partial(a^*) = (\partial a)^*$ (*self-adjoint*),

for all $a, b \in \mathcal{D}(\partial)$.

In case the derivation is defined everywhere, i.e. $\mathcal{D}(\partial) = A$, ∂ is referred to as *bounded* and otherwise as *unbounded*. The following relation between $*$ -derivations and one-parameter groups of $*$ -automorphisms reveals how we can obtain a family of unbounded $*$ -derivations from the torus action of the Fourier calculus [Bel92, Def. 1]:

Lemma 3.3. A $*$ -derivation ∂ generates a one-parameter group of point-wise norm continuous $*$ -automorphisms $\{\alpha_t | t \in \mathbb{R}\}$, if and only if for $f \in \mathcal{D}(\partial)$, $\partial f = \left. \frac{d\alpha_t(f)}{dt} \right|_{t=0}$.

Such a derivation is always closed [BR75, Thm. 1] and is commonly known as *infinitesimal generator* of the one-parameter group.

Torus derivations For each parameter in $\lambda \in T^{r+d}$ a one-parameter group of point-wise norm continuous $*$ -automorphisms on $\mathcal{A}_\Theta$ is given through the torus Lie group action ρ . Therefore, we can evaluate the corresponding $*$ -derivations as the derivatives with respect to λ_i (if the corresponding limit exists). We obtain r phase derivations associated with real space

$$\partial_i^u a := \left. \frac{\partial \rho_\lambda(a)}{\partial \xi_i} \right|_{\lambda=0} = \left. \frac{\partial}{\partial \xi_i} \right|_{\xi=0} \left(\sum_{\mathbf{m} \in \mathbb{Z}^d} a_{\mathbf{m}}(\cdot + \xi) \otimes t^{\mathbf{m}} \right) = \sum_{\mathbf{m} \in \mathbb{Z}^d} \partial_{\varphi_i} a_{\mathbf{m}} \otimes t^{\mathbf{m}} \quad (3.33)$$

and d translation derivations associated with momentum space

$$\partial_i^t a := \left. \frac{\partial \rho_\lambda(a)}{\partial k_i} \right|_{\lambda=0} = \left. \frac{\partial}{\partial k_i} \right|_{\mathbf{k}=0} \left(\sum_{\mathbf{m} \in \mathbb{Z}^d} a_{\mathbf{m}} e^{i\mathbf{m} \cdot \mathbf{k}} \otimes t^{\mathbf{m}} \right) = i \sum_{\mathbf{m} \in \mathbb{Z}^d} m_i a_{\mathbf{m}} \otimes t^{\mathbf{m}}. \quad (3.34)$$

The linearity is an immediate consequence of the linearity of the partial derivatives, and in App. A6 we additionally verify conditions (i) and (ii) from Def. 3.7 with respect to the multiplication and involution defined in Eq. (3.6) and in Eq. (3.7). As the Lie group T^{r+d} is Abelian, the $(r+d)$ $*$ -derivations are mutually commuting by construction. Furthermore, since the canonical trace on the observable algebra is invariant under the torus action, which has the derivations as generators, it follows that for all $a \in \mathcal{A}_\Theta$ for which the derivative is defined, we have $\mathcal{T}(\partial a) = 0$, where ∂ is any of the $(r+d)$ derivations. This can be interpreted as the non-commutative Brillouin zone having no boundary.

The canonical representations on $\ell^2(\mathbb{Z}^d)$ are given by

*Canonical
Representation*

$$\pi_\varphi^\times(\partial_i^u a) = \sum_{\mathbf{n}, \mathbf{m} \in \mathbb{Z}^d} \partial_{\varphi_i}(\alpha_{-\mathbf{n}} a_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A = \partial_{\varphi_i} \pi_\varphi^\times(a) \quad (3.35)$$

and

$$\begin{aligned} \pi_\varphi^\times(\partial_i^t a) &= i \sum_{\mathbf{n}, \mathbf{m} \in \mathbb{Z}^d} m_i (\alpha_{-\mathbf{n}} a_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A = i(\hat{x}_i \pi_\varphi^\times(a) - \pi_\varphi^\times(a) \hat{x}_i) \\ &= i[\hat{x}_i, \pi_\varphi^\times(a)] \end{aligned} \quad (3.36)$$

where $\hat{x}_i = \sum_{\mathbf{x} \in \mathbb{Z}^d} x_i |\mathbf{x}\rangle \langle \mathbf{x}|$ denotes the position operator, and, thus, the commutator evaluates to $\hat{x}_i |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A - |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \hat{x}_i = (n_i - (n_i - m_i)) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A = m_i |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A$.

In general, the derivatives presented above are not well-defined on the entire algebra $\mathcal{A}_\Theta$. Elements $a \in \mathcal{A}_\Theta$ for which $\rho_\lambda(a)$ is n -times differentiable with respect to λ_i , $i = 0, \dots, r+d$, are called n -times differentiable themselves, and they form a dense linear subspace $C^n(\mathcal{A}_\Theta) \subset \mathcal{A}_\Theta$. The domain of the family of derivations is therefore the dense subalgebra $C^1(\mathcal{A}_\Theta)$, making the derivations unbounded, closed, and densely defined. The dense subalgebra

*Smooth
subalgebra*

$$\mathcal{A}_\Theta = C^\infty(\mathcal{A}_\Theta) = \bigcap_{n \geq 1} C^n(\mathcal{A}_\Theta)$$

of smooth, i.e., infinitely differentiable, elements endowed with the topology induced by the semi-norms

$$\|a\|_\nu = \|\partial^\nu a\|_r, \quad \partial^\nu = (\partial_1^u)^{\nu_1} \dots (\partial_r^u)^{\nu_r} (\partial_1^t)^{\nu_{r+1}} \dots (\partial_d^t)^{\nu_{r+d}}, \quad \nu \in \mathbb{N}_0^{r+d},$$

with $\|\cdot\|_r$ denoting the reduced C^* -algebra norm as defined in Eq. (3.19), is a Fréchet pre- C^* -algebra [GVF00, Prop. 3.45]. The significance of this property for the topological classifications arises from the following implication: Since the C^* -completion of the Fréchet

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pre- C^* -algebra $\mathcal{A}_\Theta$ is the full non-commutative torus $\mathcal{A}_\Theta$, the inclusion $i : \mathcal{A}_\Theta \rightarrow \mathcal{A}_\Theta$ induces an isomorphism of K_0 -groups $K_0(i) : K_0(\mathcal{A}_\Theta) \rightarrow K_0(\mathcal{A}_\Theta)$ [GVF00, Thm. 3.44]. This entails that the smooth non-commutative torus $\mathcal{A}_\Theta$ has the same K_0 group as the full non-commutative torus C^* -algebra $\mathcal{A}_\Theta$ itself.

Functional calculus

Moreover, the pre- C^* -property ensures that the algebra is *stable under holomorphic functional calculus*, which is crucial for our objective. The *holomorphic functional calculus* enables us to define the algebra element $f(a)$ for any a in an unital Banach algebra B and holomorphic function f defined in a neighbourhood of $\sigma(a)$ by

$$f(a) := \frac{1}{2\pi i} \oint_{\Gamma} dz f(z)(z - a)^{-1},$$

where Γ is a contour around $\sigma(a)$, e.g. a closed curve of finite length without self-intersection in the neighbourhood encircling $\sigma(a)$ only once and counterclockwise [GVF00, Chap. 1A]. An unital and dense subalgebra $\mathcal{B}$ is then called *stable under holomorphic calculus* if $f(a) \in \mathcal{B}$ for any $a \in \mathcal{B}$ and f holomorphic in a neighbourhood of $\sigma(a)$. It has been shown, that the smooth non-commutative torus $\mathcal{A}_\Theta$ is furthermore stable under the *smooth functional calculus with self-adjoint elements* [Pro17, Prop. 3.25.]. This property is derived from the stability under the holomorphic calculus and implies that $f(a) \in \mathcal{A}_\Theta$ for any $a \in \mathcal{A}_\Theta$ self-adjoint and f smooth.

This guarantees, in particular, that any Fermi projection p_F of a Hamiltonian $h \in \mathcal{A}_\Theta$ belongs to the smooth non-commutative torus, provided that the Fermi energy E_F lies within a gap of the Hamiltonian's spectrum $\sigma(h)$. For that we define $p_F := \chi(h \leq E_F)$ where χ denotes the indicator function. Although χ is discontinuous, with E_F inside a spectral gap of h we can deform it to a smooth function making it eligible for the smooth calculus. An alternative form of the Fermi projection p_F may be defined by the Riesz projector. Let $E_F \notin \sigma(h)$ and Γ_F be the contour in $\mathbb{C}$ which encircles $\sigma(h) \cap (-\infty, E_F)$ and does not intersect $\sigma(h)$, then it is

$$p_F = \frac{1}{2\pi i} \oint_{\Gamma_F} dz (z - h)^{-1}. \quad (3.37)$$

Fast decay property

The smoothness of an element $a \in \mathcal{A}_\Theta$ can be quantified explicitly by considering the decay of its Fourier coefficients [PS16, Prop. 3.3.4.]: Let $a \in \mathcal{A}_\Theta$, then we have for the coefficient with $\mathbf{l} \in \mathbb{Z}^r$ and $\mathbf{m} \in \mathbb{Z}^d$, and for any multi-index $\boldsymbol{\nu} = (\boldsymbol{\nu}_1, \boldsymbol{\nu}_2) \in \mathbb{N}_0^{r+d}$

$$|(\mathbf{l}, \mathbf{m})^\nu \Phi_{\mathbf{l}\mathbf{m}}(a)| \leq \|\partial^\nu a\|_r < \infty, \quad (\mathbf{l}, \mathbf{m})^\nu = l_1^{\nu_1} \dots l_r^{\nu_r} m_1^{\nu_{r+1}} \dots m_d^{\nu_{r+d}}. \quad (3.38)$$

In particular, the cases with $\boldsymbol{\nu}_2 = 0$ imply $|\mathbf{l}^{\nu_1} \Phi_{\mathbf{l}\mathbf{m}}(a)| \leq \|\partial_{\boldsymbol{\varphi}}^{\nu_1} \Phi_{\mathbf{m}}(a)\|_{Tr} < \infty$, and thus $\Phi_{\mathbf{m}}(a) \in C^\infty(T^r)$. Conversely, if for every multi-index $\boldsymbol{\nu} = (\boldsymbol{\nu}_1, \boldsymbol{\nu}_2) \in \mathbb{N}_0^{r+d}$, we have

$$|(\mathbf{l}, \mathbf{m})^\nu \Phi_{\mathbf{l}\mathbf{m}}(a)| < \infty$$

uniformly in $(\mathbf{l}, \mathbf{m}) \in \mathbb{Z}^{r+d}$, then a belongs to $\mathcal{A}_\Theta$. The useful Fourier coefficient inequality $|(\mathbf{l}, \mathbf{m})^\nu \Phi_{\mathbf{l}\mathbf{m}}(a)| \leq \|\partial^\nu a\|_r$ is verified in App. A7.

3.2.3. Itô Derivatives

For many physics formulas, such as orbital magnetisation, it is of interest to compute the derivative of physical quantities with respect to the strength of the magnetic field. As the observable algebra is constructed for a fixed magnetic flux, it is necessary to consider continuous fields of observable algebras. Magnetic derivatives of observables can then be expressed in terms of Itô-like derivatives as introduced by Jean Bellissard [RB90] (named after Kiyosi Itô due to the similarity of the product rule in Ito's lemma in stochastic calculus). Beyond the magnetic field components, Itô derivatives can be defined in terms of all the $\frac{1}{2}(r+d)(r+d-1)$ parameters in the Θ matrix, which determine the structure of a non-commutative torus. In the context of our construction, the eligible parameters are limited to the rd pitch parameters of the r spin waves and the aforementioned $\frac{1}{2}d(d-1)$ flux parameters of the magnetic field.

We start by defining continuous fields of C^* -algebras in order to set up the field of the non-commutative torus algebras. Next, we consider the natural torus Lie group action on this field and construct the derivatives as the infinitesimal generators of the group of automorphisms. In this framework, we can then present the corresponding rules of calculus and the behaviour of the Itô derivatives with respect to the $*$ -derivations and the trace on the non-commutative torus algebra.

First, let us briefly introduce the definitions of continuous fields of Banach spaces and C^* -algebras as given by [Pro17, Chap. 3.7] based on [Dix82, Chap. 10].

*Field of
 C^* -algebras*

Definition 3.8 (Continuous field of Banach spaces). Let Σ be a topological space. A *continuous field* $\mathcal{E} = (\{E(t)\}_{t \in \Sigma}, \Sigma)$ of Banach spaces over Σ is a family $\{E(t)\}_{t \in \Sigma}$ of Banach spaces, with a set $\Gamma \subset \prod_{t \in \Sigma} E(t)$ of sections, such that:

- (i) Γ is a complex linear subspace of $\prod_{t \in \Sigma} E(t)$.
- (ii) For every $t \in \Sigma$, the set of $s(t)$ for $s \in \Gamma$ is dense in $E(t)$.
- (iii) For every $s \in \Gamma$ the function $t \mapsto \|s(t)\|$ is continuous.
- (iv) Let $s \in \prod_{t \in \Sigma} E(t)$ be a section. If for every $t \in \Sigma$ and every $\epsilon > 0$ there exists an $s' \in \Gamma$ such that $\|s(t) - s'(t)\| \leq \epsilon$ throughout some neighbourhood of t , then $s \in \Gamma$.

Definition 3.9 (Continuous field of C^* -algebras). Let Σ be a compact topological space. A *continuous field* of C^* -algebras over Σ is a continuous field $(\{A(t)\}_{t \in \Sigma}, \Gamma)$ of Banach spaces, such that each $A(t)$ is endowed with a multiplication and an involution with which it is a C^* -algebra and the space of sections Γ is closed under multiplication and involution.

3. C^* -Algebra Theory of Multi-q Textures

Field of non-commutative tori

The family of non-commutative tori $\mathcal{A}_\Theta$, with Θ of the form given in Eq. (3.24), depends on $n_{r+d} = rd + \frac{1}{2}d(d-1)$ real parameters in S^1 . Thus, the underlying compact topological space is the n_{r+d} -torus $T^{n_{r+d}}$ and the set of sections Γ can be expressed the following way:

$$\Gamma = \left\{ s \in \prod_{\Theta \in T^{n_{r+d}}} \mathcal{A}_\Theta, s(\Theta) = \sum_{\mathbf{m} \in \mathbb{Z}^d} a_{\mathbf{m}}(\Theta) \otimes t^{\mathbf{m}}(\Theta) \mid a_{\mathbf{m}} \in C(T^{n_{r+d}}, C(T^r)) \right\}.$$

The continuous field of C^* -algebras is then given by $(\{A_\Theta\}_{\Theta \in T^{n_{r+d}}}, \Gamma)$ and Γ becomes a C^* -algebra when endowed with the natural algebraic operations for functions and the C^* -norm

$$\|s\|_\Gamma = \sup_{\Theta \in T^{n_{r+d}}} \|s(\Theta)\|_r,$$

Torus action

where $\|\cdot\|_r$ the reduced C^* -algebra norm on $\mathcal{A}_\Theta$ as defined in Eq. (3.19). To construct the derivatives with respect to the parameters, we consider an action of the Lie group $T^{n_{r+d}}$ on Γ [Pro17, Prop. 3.36.]. Let the action $\sigma : T^{n_{r+d}} \rightarrow \text{Aut}(\Gamma)$, $\Xi \mapsto \sigma_\Xi$ act on $C(T^{n_{r+d}}, C(T^r))$ as the natural action

$$\sigma_\Xi(f)(\Theta) = f(\Theta + \Xi),$$

which can be lifted to a continuous group of automorphisms on Γ given by

$$\sigma_\Xi(s) = \sum_{\mathbf{m}} \sigma_\Xi(a_{\mathbf{m}}) \otimes t^{\mathbf{m}}.$$

The Itô derivatives are the infinitesimal generators in terms of derivatives with respect to the parameters:

$$\delta_{\Theta_{ab}} s = \sum_{\mathbf{m}} \partial_{\Theta_{ab}} a_{\mathbf{m}} \otimes t^{\mathbf{m}}. \quad (3.39)$$

They are defined on the subspace of Γ on which $\sigma_\Xi(s)$ is differentiable, denoted by $C^1(\Gamma)$, which is a Banach space when endowed with the norm

$$\|s\|_1 = \|s\|_\Gamma + \sum_{a=1}^{r+d} \|\partial_a s\|_\Gamma + \sum_{a < b} \|\delta_{\Theta_{ab}} s\|_\Gamma.$$

Rules of calculus

The Itô derivatives obey the following relations with the differential calculus on the non-commutative Brillouin zone [Pro17, Prop. 3.37] for $s, s' \in C^1(\Gamma)$.

- (i) Compatibility with the trace: $\partial_{\Theta_{ab}} \mathcal{T}(s(\Theta)) = \mathcal{T}((\delta_{\Theta_{ab}} s)(\Theta))$ for $1 \leq a, b \leq r+d$.
- (ii) Commutation with $*$ -derivations: $\delta_{\Theta_{ab}} \partial_c = \partial_c \delta_{\Theta_{ab}}$ for $1 \leq a, b, c \leq r+d$.
- (iii) Self-adjointness: $(\delta_{\Theta_{ab}} s)^* = \delta_{\Theta_{ab}} s^*$ for $1 \leq a, b \leq r+d$.

(iv) Ito-like product rules: For $\delta_{\Theta_{(r+i)(r+j)}} = \delta_{\Theta_{t_i t_j}} =: \delta_{\Phi_{ij}}$ with $1 \leq i, j \leq d$ it is

$$\delta_{\Phi_{ij}}(ss') = (\delta_{\Phi_{ij}}s)s' + s(\delta_{\Phi_{ij}}s') - \frac{2\pi i}{2}(\partial_i^t s \partial_j^t s' - \partial_j^t s \partial_i^t s') \quad (3.40)$$

and for $\delta_{\Theta_{(i)(r+j)}} = \delta_{\Theta_{u_i t_j}} =: \delta_{\theta_{ij}}$ with $1 \leq i \leq r$ and $1 \leq j \leq d$ one has

$$\delta_{\theta_{ij}}(ss') = (\delta_{\theta_{ij}}s)s' + s(\delta_{\theta_{ij}}s') + 2\pi i \partial_j^t s \partial_i^u s'. \quad (3.41)$$

Hereby, relation (i) is obtained directly from the definition in Eq. (3.39), as the trace on $\mathcal{A}_\Theta$ reduces to the trace on $C(T^r)$ of the 0th-Fourier coefficient, relation (ii) is a consequence of the corresponding automorphisms commuting, and relation (iii) follows from the same calculation as for Eq. (3.33) as presented in App. A6.

The relations in (iv) are the Itô-like product rules, which grant the derivative its name. They are not of the same form, since the multiplication of the translation generators is presented symmetrically $(1 \otimes t^{\mathbf{m}})(1 \otimes t^{\mathbf{n}}) = e^{2\pi i(\mathbf{m} \wedge \Phi \mathbf{n})}(1 \otimes t^{\mathbf{m}+\mathbf{n}})$, whereas the multiplication of phase torus function and translation generators is presented asymmetrically with $(1 \otimes t^{\mathbf{m}})(u^{\mathbf{n}} \otimes t^{\mathbf{0}}) = \alpha_{\mathbf{m}}(u^{\mathbf{n}}) \otimes t^{\mathbf{m}}$ and $(u^{\mathbf{n}} \otimes t^{\mathbf{0}})(1 \otimes t^{\mathbf{m}}) = u^{\mathbf{n}} \otimes t^{\mathbf{m}}$. We verify the relations in App. A8 for the Itô derivative as defined in Eq. (3.39) of the product defined in Eq. (3.6).

By definition of the Itô derivative in Eq. (3.39), an algebra element is precisely k -times Itô-differentiable if its Fourier coefficients are k -times differentiable with respect to Θ . Moreover, by the functional calculus introduced in Sec. 3.2.2, any algebra element obtained by a smooth function of an Itô-differentiable element is Itô-differentiable itself [PS16, Prop. 3.40.]. In particular, the Fermi projections for an Itô-differentiable Hamiltonian from the smooth non-commutative torus are Itô-differentiable.

Itô-differentiability

3.3. Non-commutative Geometry

Non-commutative geometry is the study of non-commutative C^* -algebras using methods generalised from differential geometry and topology. This mathematical branch was developed by Alain Connes [Con94] in his pursuit to extend the duality between locally compact Hausdorff spaces and commutative C^* -algebras as given by Thm. 3.2 to the non-commutative case.

Homotopy invariants associated with topological spaces can be obtained by a variety of algebraic methods, such as the *topological K-theory* of Atiyah and Hirzebruch for the classification of complex vector bundles over compact Hausdorff spaces, or the *Atiyah-Singer index theorem* for elliptic operators on compact manifolds.

Commutative geometry

The topological K -theory of a space can be related to its rational cohomology by a *Chern character*. In the *Chern-Weil theory* definition of the Chern characters for smooth manifolds one obtains classes in the *de Rham cohomology* constructed from a connection on the vector bundle, which is independent of the choice of connection. On

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even dimensional closed oriented manifolds, the top Chern character can be paired with the de Rham current of the manifold to obtain an invariant number, comprised of the integer *Chern numbers* of the vector bundle.

The Chern character also occurs in the definition of the topological index of an elliptic differential operator, which is equal to its Fredholm index by the Atiyah-Singer index theorem [Nak18, Chap. 12.2]. For the exterior derivative of the de Rham complex this index is precisely the Euler characteristic, which coincides with the top Chern number of the complexified tangent bundle. This application of the index theorem is the Chern-Gauß-Bonnet theorem for which we presented an example in Chap. 1.3.2.

*Non-
commutative
geometry*

Both concepts, topological K -theory and Chern characters, can be naturally extended to the non-commutative case. Topological K -theory is generalised by *operator K -theory*, also known as K -theory for C^* -algebras, which considers Abelian groups of equivalence classes of projections and unitary elements, respectively, in matrix algebras over arbitrary C^* -algebras. In the case of commutative C^* -algebras, which can be expressed as the algebras of continuous functions over compact Hausdorff spaces, the projections are associated to the complex vector bundles of topological K -theory. By the non-commutative Chern character, K -theory classes can be paired with classes of cyclic cocycles to obtain the non-commutative Chern numbers.

There is also a non-commutative generalisation of the index theorem. Under the right conditions the pairing of K -theory and cyclic cohomology can be expressed as the index of a Fredholm operator. This property extends to more general algebras than considered in this work and is useful for physical observables not contained in C^* -algebras, e.g. the Fermi projector in the case of strong disorder.

Section content

In this section, we first present a short introduction to the K -theory of C^* -algebras. This includes the definition of the equivalence classes, the construction and properties of the K -groups, and the case of the non-commutative torus. Next, we introduce the concept of cyclic cohomology and use the differential calculus established in the last section to construct cyclic cocycles, which can be paired with the K_0 -group to obtain the invariant Chern numbers. Finally, we use the Itô derivatives from last section to derive generalised Středa formulas, that allow us to decompose the Chern numbers into invariant integer labels.

3.3.1. Operator K -Theory

Operator K -theory is the non-commutative analogue of topological K -theory developed by Michael Atiyah and Friedrich Hirzebruch for the classification of vector bundles over topological spaces. The name originates from the German word 'Klasse' for 'class' and was introduced by Alexander Grothendieck as topological K -theory studies the stable isomorphism classes of complex vector bundles over compact Hausdorff spaces. By theorems of Serre [Ser55] and Swan [Swa62] these stand in a one-to-one correspondence with the stable isomorphism classes of finitely generated projective modules over the ring of continuous, real-valued functions on these spaces. Thus, we can classify projections of the C^* -algebra of continuous complex-valued function and the algebra generated by finite ranked matrices over it.

3.3. Non-commutative Geometry

Operator K -theory can also be applied to classify projections in more difficult, non-commutative C^* -algebras, such as the non-commutative torus. The corresponding functors K_i , $i = 0, 1$ associate Abelian groups to these algebras.

The relevance to physical properties follows directly from this: The observable C^* -algebra describing a physical system contains all spectral (Fermi) projections, which can thus be labelled by topologically invariant numbers, the so-called Chern numbers. They are closely related to further physical quantities, e.g., electronic transport behaviour.

The following short introduction to the K -theory of C^* -algebras is based on the textbook account of [RLL00] and focusses on the concepts relevant in the context of this work. These are in particular the different notions of equivalence which are met by the equivalence classes of projections, the K_0 -group of C^* -algebras, and the universal property of the functor K_0 . We will only touch slightly on the definition of the K_0 -group in the non-unital case, the equivalence of unitaries, the K_1 -group, and the functoriality of K_1 . These concepts are only used to define the six-term exact sequence from which we can then infer the K_0 group of the observable algebra.

Projections and unitaries are the key elements for which operator K -theory establishes equivalence classes and an Abelian group structure. As introduced right after Def. 3.2 of a C^* -algebra, we characterise a projection in a C^* -algebra A as a self-adjoint, idempotent element $p \in \mathcal{P}(A)$, such that $p = p^* = p^2$, and a unitary in an unital C^* -algebra A as an element $u \in \mathcal{U}(A)$, that satisfies $uu^* = \mathbb{1}_A = u^*u$. To be able to make sense of this notion for any C^* -algebra A , unital or not, we can always associate a unique *unitisation* $A^+ = \{a + \alpha\mathbb{1}_+ | a \in A, \alpha \in \mathbb{C}\}$, which contains A as an ideal, such that $A^+/A \cong \mathbb{C}$ and that the short exact sequence

Projections and Unitaries

$$0 \longrightarrow A \xhookrightarrow{i} A^+ \xrightleftharpoons[\lambda]{\pi} \mathbb{C} \longrightarrow 0 \quad (3.42)$$

is split exact with $i(a) = a$, $\pi(a + \alpha\mathbb{1}_+) = \alpha$, and $\lambda(\alpha) = \alpha\mathbb{1}_+$ for any $a \in A$, $\alpha \in \mathbb{C}$ [RLL00, Chap. 1.1.6].

There are several ways to establish equivalence between C^* -algebra elements. From topology, we are familiar with the concept of *homotopy* for continuous functions as given in Def. 1.1. Analogously, we define two elements a, b of a topological space X to be *homotopic* $a \sim_h b$ in X , if there exists a continuous map $v : [0, 1] \rightarrow X, t \mapsto v(t)$ with $v(0) = a$ and $v(1) = b$. Since every C^* -algebra A is in particular a vector space, all its elements are homotopic in A , and, thus, for the homotopy of projections or unitaries, we demand additionally that the image of v is fully restricted to $\mathcal{P}(A)$ or $\mathcal{U}(A)$.

Equivalence classes

For projections, there are two additional useful concepts for equivalence given by the *Murray-von Neumann equivalence* $p \sim q$, if there exist a so-called *partial isometry* $v \in A$ with *support projection* $p = v^*v$ and *range projection* $q = vv^*$, and by the *unitary equivalence* $p \sim_u q$, if there exists a unitary u in A^+ with $q = upu^*$ [RLL00, Def. 2.2.1].

3. C^* -Algebra Theory of Multi- q Textures

The three concepts of equivalence have a clear hierarchy [RLL00, Prop. 2.2.7]: For $p, q \in \mathcal{P}(\mathcal{A})$, it is

$$p \sim_h q \Rightarrow p \sim_u q \Rightarrow p \sim q.$$

However, passing to matrix algebras $M_n(A) := M_n(\mathbb{C}) \otimes A$ with arbitrary but finite dimension $n \in \mathbb{N}$ they become interchangeable [RLL00, Prop. 2.2.8]. Therefore, we consider projections in $\mathcal{P}_\infty(A) := \bigcup_{n=1}^\infty \mathcal{P}(M_n(A))$, interpreted as the limit of the union over pairwise disjoint sets of projections in all finite-dimensional matrix algebras.

On this set, one can now extend the Murray-von Neumann equivalence relation to different matrix algebras: $p \sim_0 q$ for projections $p \in \mathcal{P}(M_n(A))$ and $q \in \mathcal{P}(M_m(A))$ if there exists $v \in M_{m,n}(\mathbb{C}) \otimes A$ such that $p = v^*v$ and $q = vv^*$. The set of equivalence classes $\mathcal{P}_\infty(A)/\sim_0$ is an Abelian semigroup with addition induced by the direct sum on $\mathcal{P}_\infty(A)$

$$p \oplus q = \text{diag}(p, q) = \begin{pmatrix} p & 0 \\ 0 & q \end{pmatrix}. \quad (3.43)$$

If we denote the equivalence classes of $p \in \mathcal{P}_\infty(A)$ by $[p]_0$, we get the following summation law for them: $[p]_0 + [q]_0 = [p \oplus q]_0$. The notion of an inverse element which is crucial in the definition of a group is missing as of now.

K_0 -group

We define the group $K_{00}(A)$ as the enveloping Abelian Grothendieck group of $\mathcal{P}_\infty(A)/\sim_0$. One can view this process as similar to the way the integers are constructed out of natural numbers by “inventing” negative numbers. For details on this construction, we refer to [RLL00, Chap. 3.1.1]. If the C^* -algebra A is unital, $K_{00}(A)$ coincides with $K_0(A)$, however, we choose to define $K_0(A)$ for general C^* -algebras differently. The reason for this is, that while K_{00} is a half-exact functor on the category of unital algebras, this is not the case on the category of non-unital C^* -algebras. To fix this, we apply it to the short exact sequence Eq. (3.42) and enforce the half-exactness of K_0 by defining

Definition 3.10 (K_0 -group). Let A be a C^* -algebra and let $K_{00}(A)$ be the Abelian Grothendieck group of the semigroup $\mathcal{P}_\infty(A)/\sim_0$. The Abelian group $K_0(A)$ is defined by

$$K_0(A) := \ker \{K_{00}(\pi) : K_{00}(A^+) \rightarrow K_{00}(\mathbb{C})\}.$$

If A is already unital, we have $K_0(A) \cong K_{00}(A)$, and the structure of the K_0 -group is unique up to isomorphisms, as given by universal property of K_{00} [RLL00, Prop. 3.1.8]. Thus, we can use this definition uniformly and construct a standard presentation of the K_0 -group from it [PS16, Prop. 4.1.3] [RLL00, Prop. 4.2.2]. Let $s := \lambda \circ \pi : A^+ \rightarrow A^+$ be the scalar mapping with $a + \alpha \mathbb{1}_+ \mapsto \alpha \mathbb{1}_+$ for $a \in A$, $\alpha \in \mathbb{C}$. Let us also extend it to $M_n(A^+)$ with the same notation, and denote the unit element of $M_n(A^+)$ with $\mathbb{1}_n$. For any element a in A^+ or $M_n(A^+)$ it is $a - s(a) \in \ker \pi$, and it is called scalar if $s(a) = a$.

Lemma 3.4 (Standard picture of K_0). *Let A be a C^* -algebra. Then, the K_0 -group can be presented as*

$$K_0(\mathcal{A}) = \{[p]_0 - [s(p)]_0 \mid p \in \mathcal{P}_\infty(A^+)\}.$$

Moreover, the following hold:

- (i) It is $[p \oplus q]_0 - [s(p) \oplus s(q)]_0 = ([p]_0 - [s(p)]_0) + ([q]_0 - [s(q)]_0)$.
- (ii) The inverse of $[p]_0 - [s(p)]_0$ with $p \in \mathcal{P}(M_n(A^+))$ is $-([p]_0 - [s(p)]_0) = [\mathbb{1}_n - p]_0 - [\mathbb{1}_n - s(p)]_0$.
- (iii) If p, q are mutually orthogonal projections in $\mathcal{P}(M_n(A^+))$, i.e. $pq = 0$, then it is $[p \oplus q]_0 = [p + q]_0$ and $[s(p) \oplus s(q)]_0 = [s(p + q)]_0$.
- (iv) For any $p, q \in \mathcal{P}_\infty(A^+)$, the following conditions are equivalent:
 - (a) $[p]_0 - [s(p)]_0 = [q]_0 - [s(q)]_0$
 - (b) $\exists k, l \in \mathbb{N}^*$ such that $p \oplus \mathbb{1}_k \sim_0 q \oplus \mathbb{1}_l$ in $\mathcal{P}_\infty(A^+)$
 - (c) there exist scalar projections r_1, r_2 such that $p \oplus r_1 \sim_0 q \oplus r_2$
 In particular, if $p \in \mathcal{P}_\infty(A^+)$ satisfies $[p]_0 - [s(p)]_0 = 0$, then there is $m \in \mathbb{N}^*$ with $p \oplus \mathbb{1}_m \sim_0 s(p) \oplus \mathbb{1}_m$.
- (v) If $\psi : A \rightarrow B$ is a $*$ -homomorphism between C^* -algebras A and B , then it induces a unique group homomorphism

$$K_0(\psi)([p]_0 - [s(p)]_0) = [\psi^+(p)]_0 - [s(\psi^+(p))]_0,$$

for each $p \in \mathcal{P}_\infty(A^+)$, with $\psi^+(a + \alpha \mathbb{1}_+) = \psi(a) + \alpha \mathbb{1}_+$, $a \in A$, $\alpha \in \mathbb{C}$.

- (vi) If $p \in \mathcal{P}_\infty(A)$, then it is also $p \in \mathcal{P}_\infty(A^+)$ and $s(p) = 0$. As such, $[p]_0$ is an element of $K_0(A)$.

The K_1 -group of a C^* -algebra is the Abelian group of homotopy equivalence classes of unitary elements in the matrix algebra of the C^* -algebra's unitisation, and can thus be defined without the Grothendieck construction or special construction for the non-unital case. We start by considering the set $\mathcal{U}_\infty(A^+) := \bigcup_{n=1}^\infty \mathcal{U}(M_n(A^+))$ of all unitary elements of matrix algebras over the unitisation of a C^* -algebra A . Here, we introduce the equivalence relation $\sim_1$ on $\mathcal{U}_\infty(A^+)$, such that $u \sim_1 v$ for $u \in \mathcal{U}(M_n(A^+))$ and $v \in \mathcal{U}(M_m(A^+))$ if and only if there exists an integer $\mathbb{N}^* \ni k \geq \max\{m, n\}$ such that $u \oplus \mathbb{1}_{k-n} \sim_h v \oplus \mathbb{1}_{k-m}$ in $\mathcal{U}(M_k(A^+))$.

The direct sum on $\mathcal{U}_\infty(A^+)$, as defined in Eq. (3.43), introduces an addition on $\mathcal{U}_\infty(A^+)/\sim_1$. By Whitehead's Lemma [RLL00, Lem. 2.1.5] it is $u \oplus u^* \sim_1 1$ for any element $u \in \mathcal{U}_\infty(A^+)$, which implies that the inverse of the equivalence class of any unitary u is given by the equivalence class of u^* . Consequently, the set of equivalence classes $\mathcal{U}_\infty(A^+)/\sim_1$ has a group structure, and we define [RLL00, Def. 8.1.3]:

K_1 -group

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Definition 3.11 (K_1 -group). For each C^* -algebra A define

$$K_1(A) := \mathcal{U}_\infty(A^+)/\sim_1.$$

Let $[u]_1 \in K_1(A)$ denote the equivalence class containing u in $\mathcal{U}_\infty(A^+)$. Define a binary operation on $K_1(A)$ by $[u]_1 + [v]_1 = [u \oplus v]_1$, where $u, v \in \mathcal{U}_\infty(A^+)$.

The group structure of the K_1 -group is unique up to isomorphisms, as given by the universal property of K_1 [RLL00, Prop. 8.1.5], and we can present it in a standard form [PS16, Prop. 4.1.5] [RLL00, Prop. 8.1.4].

Lemma 3.5 (Standard picture of K_1). *Let A be a C^* -algebra. Then*

$$K_1(A) = \{[u]_1 \mid u \in \mathcal{U}_\infty(A^+)\}$$

and the map $[\cdot]_1 : \mathcal{U}_\infty(A^+) \rightarrow K_1(A)$ has the following properties:

- (i) It is $[u \oplus v]_1 = [u]_1 + [v]_1$.
- (ii) The inverse of $u \in \mathcal{U}_n(A^+)$ is $-[u]_0 = [u^{-1}]_0 = [u^*]_0$.
- (iii) If $u, v \in \mathcal{U}_n(A^+)$, $n \in \mathbb{N}^*$, then $[uv]_1 = [vu]_1 = [u]_1 + [v]_1$.
- (iv) For all $u \in \mathcal{U}_\infty(A^+)$ it is $u \otimes \mathbb{1}_n \sim_1 u$ for all $n \in \mathbb{N}^*$. In particular, it is $\mathbb{1}_n \sim_1 \mathbb{1}_m$ for all $n, m \in \mathbb{N}^*$ with the common equivalence class $[1]_1 = 0$.
- (v) If $u, v \in \mathcal{U}_n(A^+)$, $n \in \mathbb{N}^*$, $u \sim_h v$ in $\mathcal{U}_n(A^+)$, then $[u]_1 = [v]_1$.
- (vi) If $\psi : A \rightarrow B$ is a $*$ -homomorphism between C^* -algebras A and B , then it induces a unique group homomorphism

$$K_0(\psi)([u]_1) = [\psi^+(u)]_1,$$

for each $u \in \mathcal{U}_\infty(A^+)$.

- (vii) If A is unital and $u \in A$ is a unitary, then u can be promoted to a unitary in A^+ by $u^+ = u + (\mathbb{1}^+ - \mathbb{1})$. This group homomorphism can be extended to $\mathcal{U}_\infty(A)$ and $\mathcal{U}_\infty(A^+)$, and it follows $\mathcal{U}_\infty(A)/\sim_1 = \mathcal{U}_\infty(A^+)/\sim_1$.

Functoriality of K_i

Both K_i , $i = 0, 1$, are functors from the category of C^* -algebras into the category of Abelian groups [RLL00, Prop. 4.1.3, Prop. 8.2.2]. In Lem. 3.4 (v) and Lem. 3.5 (vi) we have already seen, that $*$ -homomorphisms induce unique group homomorphisms. Moreover, K_i are *homotopy invariant* [RLL00, Prop. 4.1.4, Prop. 8.2.2], *half-exact* [RLL00, Prop. 4.3.2, Prop. 8.2.4], and *split exact* [RLL00, Prop. 4.3.3, Prop. 8.2.5] functors. This means, that two homotopic $*$ -homomorphisms $\psi, \psi' : A \rightarrow B$ induce the same group homomorphism $K_i(\psi) = K_i(\psi')$, a short exact sequence of C^* -algebras is mapped onto an exact sequence of Abelian groups, and a split exact sequence of C^* -algebras is mapped onto a split exact sequence of Abelian groups.

We can define higher functors K_i , $i \geq 2$, by iteratively composing the so-called *suspension* functor. The suspension of a C^* -algebra A is defined as $SA = C_0((0, 2\pi); A)$, the continuous functions f from the interval $[0, 2\pi]$ to A that vanish at the border, such that $f(0) = 0 = f(2\pi)$. With the supremum norm $\|f\|_{SA} = \sup_{x \in [0, 2\pi]} \|f(t)\|_A$ and the involution from A acting point-wise, it is a non-unital C^* -algebra.

Bott periodicity

It can then be shown, that the K_1 -group of A and the K_0 -group of SA are isomorphic [RLL00, Thm. 10.1.3], and this motivates the following construction: With the suspension S being an exact functor from the category of C^* -algebras onto itself [RLL00, Prop. 10.1.2], a higher functor $K_i := K_{i-1} \circ S$ from the category of C^* -algebras to the category of Abelian groups is given inductively for each integer $i \geq 2$ [RLL00, Def. 10.2.1]. This construction collapses again by the Bott periodicity theorem [RLL00, Thm. 11.1.2], which states that for any C^* -algebra A there exists an isomorphism such that $K_0(A) \cong K_1(SA)$. Consequently, for any integer $i \in \mathbb{N}_0$ we have

$$K_{i+2}(A) = K_i(A).$$

Applying the higher functors to a short exact sequence of C^* -algebras induces a long exact sequence of K -groups, which collapses to the *six-term exact sequence* with the *index map* Ind and the *exponential map* Exp [RLL00, Thm. 12.1.2]:

Six-term exact sequence

Theorem 3.6 (The six-term exact sequence). *Every short sequence of C^* -algebras*

$$0 \longrightarrow A \xrightarrow{\varphi} B \xrightarrow{\psi} C \longrightarrow 0$$

gives rise to the six-term exact sequence

$$\begin{array}{ccccc} K_1(A) & \xrightarrow{K_1(\varphi)} & K_1(B) & \xrightarrow{K_1(\psi)} & K_1(C) \\ \text{Exp} \uparrow & & & & \downarrow \text{Ind} \\ K_0(C) & \xleftarrow{K_0(\psi)} & K_0(B) & \xleftarrow{K_0(\varphi)} & K_0(A). \end{array}$$

For an explicit discussion of the connecting homomorphisms Ind and Exp , we refer to [RLL00, Chap. 9] and [RLL00, Chap. 12]. Their mere existence already allows for the computation of K -groups, as we will exploit in the following, and their explicit form can be used for the construction of the corresponding generators. For our purposes, we limit ourselves to some brief motivational remarks:

Clearly, the index map $\text{Ind} : K_1(C) \rightarrow K_0(A)$ measures how much an element $[u]_1 \in K_1(C)$ fails to be the image of an element of $K_1(B)$. This can be made explicit if A is an ideal in B : Let u be a unitary in $M_n(C^+)$. By surjectivity of ψ , u can be lifted to a partial isometry $v \in M_n(B^+)$ with $\psi^+(v) = u$. Since A is an ideal in B , it is measured by the difference of the projections $\mathbb{1}_n - v^*v$ and $\mathbb{1}_n - vv^*$ in $M_n(A)$ how much v fails to be invertible: $\text{Ind}([u]_1) = [\mathbb{1}_n - v^*v]_0 - [\mathbb{1}_n - vv^*]_0$ [RLL00, Prop. 9.2.4].

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Remark 3.6 (Fredholm index). In this sense, the index map generalises the notion of the classical *Fredholm index* of a *Fredholm operator* on a Hilbert space, which fails to be invertible in the C^* -algebra of bounded operators by a compact contribution. This correspondence is elaborated in [RLL00, Chap. 9.4].

The exponential map $\text{Exp} : K_0(C) \rightarrow K_1(A)$ owes its name to the following correspondence: Let $[p]_0 - [s(p)]_0 \in K_0(C)$ be the equivalence class of some $p \in \mathcal{P}(M_n(C^+))$, $n \in \mathbb{N}$. Since ψ is surjective, there is a self-adjoint $a \in M_n(B^+)$ with $\psi^+(a) = p$, and, since φ is injective and $e^{2\pi ia} \in \ker \psi$, there exists precisely one unitary $u \in \mathcal{U}(M_n(A^+))$ which maps to the unitary $\varphi^+(u) = e^{2\pi ia}$. The inverse of the equivalence class of this unitary is precisely the image of the K_0 -group element under the exponential map, i.e. $\text{Exp}([p]_0 - [s(p)]_0) = -[u]_1$ [RLL00, Prop. 12.2.2].

Crossed product algebra

As mentioned above, the six-term exact sequence can be used to compute the K -groups of several C^* -algebras. We are particularly interested in those constructed as the crossed product of a separable C^* -algebra A and the group $\mathbb{Z}$ as studied by Michael Pimsner and Dan Voiculescu [PV80a]. A useful formulation of their result is given by Jean Bellissard [Bel92, Thm. 13]:

Theorem 3.7 (Pimsner-Voiculescu). *Let A be a separable C^* -algebra, and α be a $*$ -isomorphism of A generated by a unitary u such that $uau^{-1} = \alpha(a)$ for all $a \in A$. Let j be the canonical injection of A onto the crossed product $A \rtimes_{\alpha} \mathbb{Z}$. Then there exists a six-term exact sequence of the form:*

$$\begin{array}{ccccccc}
 K_1(A) & \xrightarrow{\mathbb{1}_{K_1(A)} - K_1(\alpha)} & K_1(A) & \xrightarrow{K_1(j)} & K_1(A \rtimes_{\alpha} \mathbb{Z}) \\
 \uparrow \text{Exp} & & & & \downarrow \text{Ind} \\
 K_0(A \rtimes_{\alpha} \mathbb{Z}) & \xleftarrow{K_0(j)} & K_0(A) & \xleftarrow{\mathbb{1}_{K_0(A)} - K_0(\alpha)} & K_0(A).
 \end{array}$$

It states, that the K -groups of crossed product C^* -algebras with $\mathbb{Z}$ depend on the homomorphism induced by the group action α . In particular, if α is homotopic to the trivial action, $\mathbb{1}_{K_i(A)} - K_i(\alpha)$ is equal to the zero morphism, and the Pimsner-Voiculescu six-term exact sequence decouples into two short exact sequences:

$$0 \longrightarrow K_0(A) \xrightarrow{K_0(j)} K_0(A \rtimes_{\alpha} \mathbb{Z}) \xrightarrow{\text{Exp}} K_1(A) \longrightarrow 0 \quad (3.44)$$

$$\text{and } 0 \longrightarrow K_1(A) \xrightarrow{K_1(j)} K_1(A \rtimes_{\alpha} \mathbb{Z}) \xrightarrow{\text{Ind}} K_0(A) \longrightarrow 0. \quad (3.45)$$

With the K -groups being Abelian, it follows that if these sequences split, then the K -groups of the crossed product can be computed as the direct sum of the individual K -groups of the C^* -algebra A

$$K_i(A \rtimes_{\alpha} \mathbb{Z}) \cong K_0(A) \oplus K_1(A). \quad (3.46)$$

K-theory of the Non-commutative Torus

By the above construction, the K -groups of the observable algebra of spin-1/2 electrons $\mathcal{A} = M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta$ are equal to the ones of the non-commutative torus $\mathcal{A}_\Theta = C(T^r) \rtimes_\theta^\Phi \mathbb{Z}^d$ of dimension $r + d$. The twisted crossed product C^* -algebra can be expressed as d iterated crossed products of $C(T^r)$ with $\mathbb{Z}$

Non-commutative torus

$$\mathcal{A}_\Theta = C(T^r) \rtimes_{\alpha_1} \mathbb{Z} \rtimes_{\alpha_2} \mathbb{Z} \cdots \rtimes_{\alpha_d} \mathbb{Z},$$

where the individual actions α_i , $i = 1 \dots, d$, are given by

$$\alpha_i(f \otimes t^{\mathbf{m}}) = (1 \otimes t_i)(f \otimes t^{\mathbf{m}})(1 \otimes t_i)^* = e^{4\pi i(\hat{\mathbf{e}}_i \wedge_\Phi \mathbf{m})} \alpha_{\hat{\mathbf{e}}_i}(f) \otimes t^{\mathbf{m}},$$

with α as defined in Eq. (3.1) and for all $f \in C(T^r)$ and $\mathbf{m} \in \mathbb{Z}^{i-1}$. These actions are all homotopic to the trivial action by homotopies α_i^s of the form

$$\alpha_i^s(f \otimes t^{\mathbf{m}}) = e^{4\pi i(\hat{\mathbf{e}}_i \wedge_{s\Phi} \mathbf{m})} \alpha_{\hat{\mathbf{e}}_i}^s(f) \otimes t^{\mathbf{m}} \quad \text{with} \quad \alpha_{\hat{\mathbf{e}}_i}^s(f)(\varphi) = f(\varphi - 2\pi s\theta \hat{\mathbf{e}}_i)$$

for $s \in [0, 1]$. This allows us to split the six-term exact sequence as in Eq. (3.44) and Eq. (3.45). We further know, that the operator K -groups of the commutative algebra $C(T^r)$ of continuous complex-valued functions on the r -torus are equal to the topological K -groups of the r -torus T^r , i.e. $K_i(C(T^r)) = K^i(T^r) = \mathbb{Z}^{2^{r-1}}$. Since every short exact sequence that projects onto finitely generated Abelian groups such as $\mathbb{Z}^n$, $n \in \mathbb{N}$, is split exact [Miy67], this implies $K_i(C(T^r) \rtimes_{\alpha_1} \mathbb{Z}) \cong \mathbb{Z}^{2^{r-1}} \oplus \mathbb{Z}^{2^{r-1}}$, and then inductively

$$K_i(\mathcal{A}_\Theta) \cong \mathbb{Z}^{2^{r+d-1}}, \quad i = 0, 1.$$

It is important to remark that the K -groups do not at all depend on the parameter values in the matrix Θ . For more on the K -groups of higher dimensional non-commutative tori, we refer to [Rie88].

For the K_0 -group, this result implies that there are 2^{r+d-1} projection generators $[e_J]_0$. These can be uniquely labelled by the subsets of indices $J \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\}$ of even cardinality and the equivalence class of any projection from $\mathcal{P}_\infty(\mathcal{A}_\Theta)$ can be uniquely decomposed into these generators with integer coefficients n_J :

$$[p]_0 = \sum_{\substack{J \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\} \\ |J| \text{ even}}} n_J [e_J]_0. \quad (3.47)$$

When p is homotopically deformed, its K_0 class remains unchanged, and, thus, the integer labels n_J also do not change. They are the complete set of topological invariants associated with the projection p . For a Fermi projection of a physical observable algebra, they label the energy gap of the spectrum in which the Fermi energy is located. The aim of the remainder of this section is to develop the tools to obtain access to these integer labels. We find them encoded in a set of Θ -dependent gap invariants known as the non-commutative Chern numbers.

3.3.2. Cyclic Cocycles and the Non-commutative Chern Numbers

The non-commutative Chern numbers of a projection are obtained by pairing the cohomology classes of cyclic cocycles with the K_0 -equivalence class of the projection. The pairing with cyclic cocycles can be regarded as a generalisation of the concept of a bounded trace, giving access to topological invariants.

Before we properly introduce and define the required concepts, let us start with a brief synopsis: In general, cyclic cocycles are multilinear maps from an algebra to $\mathbb{C}$, which are cyclic and have no coboundary. They can be constructed from a closed trace and a differential algebra, as provided by the differential calculus established in Sec. 3.2. The cohomology class of an even cyclic cocycle is invariant under composition with inner automorphisms. This property renders the pairing with the K_0 equivalence classes of projections well-defined. The value of the pairing is thus a homotopy invariant of the projection and represents a generalisation of the concept of Chern numbers of vector bundles in topological K -theory. Through normalisation, the top Chern number can be chosen to be an integer. Indeed, its stability can be extended by an index theorem that guarantees its integrality, even in the presence of disorder, for which the gap projections do not belong to the smooth subalgebra of the observable algebra. The index theorem was the original impetus for the development of cyclic cocycles, which Alain Connes designed as the natural receptacle for the Chern character in K -homology obtained from Fredholm modules [Con94, Chap.IV].

In the following, the concept of cyclic cocycles is introduced, and their description in terms of characters of cycles that can be constructed from a differential calculus is presented. The subsequent introduction of the cup product serves to extend the cyclic cocycles to the finite-dimensional matrix algebras as they arise in the definition of K -theory, and thereby to define the pairing with the K_0 -group. This ultimately leads to the definition of the Chern numbers employed in this work to access the K_0 labels of spectral gaps. For a textbook account, we refer to the third chapter of Masoud Khalkhali's book [Kha13, Chap. 3] and of Alain Connes' book [Con94, Chap. III]. We only briefly address the connection to the index theorems and stability under disorder.

Cyclic cohomology Let us consider the sets of $(n + 1)$ -linear functionals $C^n(A) := \text{Hom}_{\mathbb{C}}(A^{\otimes(n+1)}, \mathbb{C})$, $n \in \mathbb{N}_0$, on a complex, associative algebra A , and refer to their elements as *n-cochains* [Kha13, Chap. 3.6]. On these sets, we define the cyclic and boundary operators $\lambda : C^n(A) \rightarrow C^n(A)$ and $b : C^n(A) \rightarrow C^{n+1}(A)$ by

$$(\lambda\eta)(a_0, \dots, a_n) := (-1)^n \eta(a_n, a_0, \dots, a_{n-1}), \quad (3.48)$$

$$\begin{aligned} (b\eta)(a_0, \dots, a_{n+1}) &:= \sum_{j=0}^n (-1)^j \eta(a_0, \dots, a_j a_{j+1}, \dots, a_n) \\ &\quad + (-1)^{n+1} \eta(a_{n+1} a_0, \dots, a_n), \end{aligned} \quad (3.49)$$

for any $\eta \in C^n(A)$ and $a_0, \dots, a_{n+1} \in A$. Elements $\eta \in C^n(A)$ satisfying $\lambda\eta = \eta$ are called *cyclic*, and we denote by $C_\lambda^n(A) := \ker(1 - \lambda)$ the set of these *cyclic n-cochains*.

The operator b is known as the *Hochschild coboundary map* from Hochschild cohomology, and possesses the properties $bC_\lambda^n(A) \subset C_\lambda^{n+1}(A)$ and $b^2 = 0$. From it, we define the *cyclic complex* of A by

$$C_\lambda^0(\mathcal{A}) \xrightarrow{b} C_\lambda^1(\mathcal{A}) \xrightarrow{b} C_\lambda^2(\mathcal{A}) \xrightarrow{b} \dots$$

We define *cyclic cohomology* as the cohomology of the cyclic complex:

A *cyclic n -cocycle* is a cyclic n -cochain $\eta \in C_\lambda^n(A)$ satisfying $b\eta = 0$. For the set of all such cocycles we write $Z_\lambda^n(A) := \ker(b : C_\lambda^n(A) \rightarrow C_\lambda^{n+1}(A))$.

A cyclic n -cocycle $\eta \in Z_\lambda^n(A)$ which is the boundary $\eta = b\nu$ of a cyclic $(n-1)$ -cochain $\nu \in C_\lambda^{n-1}(A)$ is referred to as *cyclic n -coboundary*. The set of all such coboundaries is defined as $B_\lambda^n(A) := b(C_\lambda^{n-1}(A))$.

The cohomology of the cyclic complex is known as *cyclic cohomology* $HC(A)$ of A with $HC^n(A) := Z_\lambda^n(A)/B_\lambda^n(A)$ for $n \in \mathbb{N}_0$. Its elements are called *cyclic cohomology classes*.

Cyclic cocycles can be conveniently described by duality as the characters of so-called *n -cycles*. They are given by triples $(\Omega, d, \int)$ consisting of a *differential graded algebra* (Ω, d) and a closed graded trace $\int$ of dimension n :

The differential graded algebra (Ω, d) consists of a graded algebra $\Omega = \bigoplus_{j=0}^n \Omega^j$ over $\mathbb{C}$, where every individual Ω^j is a vector space over $\mathbb{C}$ such that $\omega_j \omega_k \in \Omega^{j+k}$, and a graded derivation d of grade 1. The latter indicates that d satisfies the *graded Leibniz rule* $d(\omega_j \omega_k) = (d\omega_j)\omega_k + (-1)^j \omega_j(d\omega_k)$ for all $\omega_j \in \Omega^j$ and $\omega_k \in \Omega^k$.

The closed graded trace of dimension n on the other hand is a linear functional $\int : \Omega^n \rightarrow \mathbb{C}$ such that $\int d\omega = 0$ for any $\omega \in \Omega^{n-1}$ and $\int \omega_j \omega_k = (-1)^{j+k} \int \omega_k \omega_j$ for all $\omega_j \in \Omega^j$, $\omega_k \in \Omega^k$ with $j+k=n$.

An *n -cycle over the algebra A* is additionally equipped with an algebra homomorphism $\rho : A \rightarrow \Omega^0$. The character η of any n -cycle over the algebra A can then be defined as [Con94, III.1.α. Prop. 4]

Characters of cycles

$$\eta(a_0, \dots, a_n) = \int \rho(a_0) d\rho(a_1) \dots d\rho(a_n).$$

It satisfies all conditions to be a cyclic n -cocycle.

The domains of the cyclic cocycles are not in general the entire algebra A . In case A is a C^* -algebra, and we want to construct the differential algebra structure from a family of $*$ -derivations, then the cyclic cocycle may be defined on a dense smooth subalgebra $\mathcal{A}$. If we consider, for instance, a family of n mutually commuting derivations $\partial_1, \dots, \partial_n$ on an unital C^* -algebra A with smooth subalgebra $\mathcal{A}$, and a continuous trace $\mathcal{T}$ such that $\mathcal{T}(\partial_j(a)) = 0$ for any $a \in \mathcal{A}$ and $j = 1, \dots, n$, then a cyclic n -cocycle is given by the character [PS16, Example 5.1.1]

Standard cocycles

$$\eta(a_0, \dots, a_n) = \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}(a_0 \partial_{\sigma_1} a_1 \dots \partial_{\sigma_n} a_n). \quad (3.50)$$

Here, S_n denotes the permutation group of n elements and $(-1)^\sigma$ denotes the signature of the permutation $\sigma \in S_n$.

3. C^* -Algebra Theory of Multi-q Textures

Cup product

The K -groups of a C^* -algebra A are constructed from the union of matrix algebras $M_n(A) = A \otimes M_n(\mathbb{C})$ over all finite $n \in \mathbb{N}$. Therefore, a character of a cycle over A needs to be extended to this tensor product algebra to facilitate a pairing with representatives of K -groups. In general, the character of a tensor product of two cycles can be given in terms of the *cup product* of their individual characters.

Here, the cup product $\eta \otimes \eta' \mapsto \eta \# \eta'$ for arbitrary cochains $\eta \in C^n(A)$, $\eta' \in C^{n'}(A')$ defines a homomorphism $\# : HC^n(A) \otimes HC^{n'}(A') \rightarrow HC^{n+n'}(A \otimes A')$ [Con94, III.1.α. Thm. 12]. Its explicit form is particularly simple in the case where $\eta' \in HC^0(A')$ is a trace on A' :

$$(\eta \# \eta')(a_0 \otimes a'_0, \dots, a_n \otimes a'_n) = \eta(a_0, \dots, a_n) \eta'(a'_0 a'_1 \dots a'_n).$$

Pairing with K -Theory

For n even, the pairing of the cohomology class of a cyclic n -cocycle $[\eta] \in HC^n(A)$ with a K_0 -group element $[p]_0 \in K_0(A)$ over a C^* -algebra A refers to applying the cup product $\eta \# \text{tr}_l \in Z_\lambda^n(M_l(A))$ of a representative cyclic n -cocycle $\eta \in Z_\lambda^n(A)$ with an appropriate matrix trace $\text{tr}_l \in Z_\lambda^0(M_l(\mathbb{C}))$ to $(n+1)$ copies of a representative projection $p \in \mathcal{P}(M_l(\mathcal{A}))$ for some arbitrary matrix dimension $l \in \mathbb{N}$:

$$\langle \cdot | \cdot \rangle : HC^n(A) \otimes K_0(A) \rightarrow \mathbb{C}, \quad \langle [\eta] | [p]_0 \rangle = (\eta \# \text{tr})(\underbrace{p, \dots, p}_{n+1 \text{ times}}).$$

The pairing of any cyclic cocycle η and projection p only depends on their cyclic cohomology class and K_0 -class:

The invariance with respect to coboundaries is an immediate consequence of the definition of the boundary operator Eq. (3.49). With the idempotent property $p = p^2$ follows that every pairing of a projection $p \in A$ with a cyclic n -coboundary $b\nu$ of a cyclic $(n-1)$ -cochain $\nu \in C_\lambda^{n-1}(A)$ consists of $(n+1)$ individually vanishing terms

$$b\nu(p, \dots, p) = \sum_{j=0}^{n-1} (-1)^j \nu(p, \dots, p) + \nu(p, \dots, p) = 0,$$

since $\nu(p, \dots, p) = -\nu(p, \dots, p) = 0$ due to cyclicity with $(n-1)$ odd.

The invariance on the K_0 -equivalence classes follows from the fact, that the composition of any cyclic cocycle with a map changing the representative of the K_0 -class only differs by a coboundary from the initial cocycle [Con94, Chap.III.3 Lem. 1]. Such a map can always be expressed as a conjugation with an invertible element in the matrix algebra over A . In general, every algebra homomorphism induces a morphism of cocycles by composition, and for all inner automorphism, i.e. given by conjugation, the induced map on the cohomology groups is the identity [Con94, Chap. III.1α Prop. 8]. As a central consequence, the map from the K_0 -group to $\mathbb{C}$ given by pairing with a cyclic cohomology class is a homomorphism of Abelian groups. For $K_0(A)$ countable its image is therefore a countable subgroup of $\mathbb{C}$.

In Sec. 1.3.3, we already considered an example of such a pairing over a commutative algebra using classical de Rham theory to demonstrate the smooth deformation invariance of the winding number. In the example, the unit normal field $\mathbf{s}$ on the compact manifold Σ determines a projection $e = \frac{1}{2}(\mathbb{1}_2 - \mathbf{s} \cdot \boldsymbol{\sigma})$ in $M_2(C^\infty(\Sigma))$ whose homotopy class is precisely its K_0 -class $[e]_0$. The functional τ satisfies the conditions of a cyclic 2-cocycle as verified in Lem. 1.3 and by pairing its cup product with the (2×2) -matrix trace $\tau_2 \equiv \tau \# \text{tr}_2$ with an idempotent, we obtain an expression proportional to the winding number $\deg \mathbf{s}$ and the Euler characteristic $\chi(\Sigma)$ as concluded in Lem. 1.4. Subsequently, in Lem. 1.2, we demonstrated, that any such pairing is invariant under smooth deformations, which is a special case of its homotopy and K_0 -invariance discussed above.

The cyclic 2-cocycle τ can now be recognised as the character of the 2-cycle over $C^\infty(\Sigma)$ with the differential algebra given by the de Rham complex $(\Omega^\bullet(\Sigma), d)$ of differential forms on Σ and the trace $\int$ given by the integral over Σ . In general, the theory of cyclic cohomology for C^* -algebras can be seen as the natural extension of the classical de Rham theory. It has been shown by Alain Connes, that there exists a natural isomorphism between the space of de Rham currents on a smooth manifold and the continuous Hochschild cohomology on the algebra of smooth functions over it [Con85, Chap. II, Lem. 45], and the cyclic complex is a subcomplex of the Hochschild complex.

With the concepts established above, we can eventually construct cyclic n -cocycles on the non-commutative observable algebra $\mathcal{A} = M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta$ and pair them for any even n with the elements of the K_0 -group $K_0(\mathcal{A})$. From the differential calculus introduced in Sec. 3.2, we can construct a cyclic cocycle along the lines of Eq. (3.50) using the faithful continuous trace $\mathcal{T}$ on the observable algebra defined in Eq. (3.30) and the $(r + d)$ commuting $*$ -derivations defined in Eq. (3.33) and Eq. (3.34).

Let $I \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\}$ be a subset of indices for the generators of the non-commutative torus algebra. Then, for each even $|I| \leq r + d$ with $n = |I|/2$, we define the n th Chern number of a K_0 -group element $[p]_0 \in K_0(\mathcal{A})$ as the pairing of this cyclic $2n$ -cocycle with a smooth representative $p \in \mathcal{P}(\mathcal{A})$:

$$Ch_I([p]_0) = \frac{(2\pi i)^n}{n!} \sum_{\sigma \in S_{2n}} (-1)^\sigma \mathcal{T}(p \partial_{\sigma_1} p \dots \partial_{\sigma_{2n}} p). \quad (3.51)$$

For any projection there exists a K_0 -equivalent smooth projection [BES94, Lem. 9]. This follows from the norm density of the smooth subalgebra and the homotopy equivalence of projections whose difference is of norm smaller 1 [RLL00, Prop. 2.2.4.]. In the context of Eq. (3.51), the permutation $\sigma \in S_{2n}$ is viewed as a bijective map between $\{1, \dots, 2n\}$ and I with signature $\text{sgn}(\sigma) = (-1)^\sigma$. For the particular case of $I = \emptyset$, one has $n = 0$ and $Ch_\emptyset([p]_0) = \mathcal{T}(p)$. We refer to the cyclic $|I|$ -cocycles Ch_I as *Chern cocycles*.

For the normalisation of the Chern numbers, the prefactor $\Lambda_n = \frac{(2\pi i)^n}{n!}$ is chosen to ensure that the top Chern number ($|I| = r + d$) is an integer [PS16, Sec. 5.2]. In that case, the Chern cocycle Ch_I is a representative of the so-called *Connes-Chern character* [PS16, Sec. 6.3], which generates the entire (periodic) cyclic cohomology class (cf. Rem. 3.7) of the smooth non-commutative torus. The integrality of its pairings can also be expressed in terms of an index theorem which maintains its validity in cases where the projection is not

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element of a C^* -algebra any more. This is the case for Fermi projections of an electronic system in the presence of disorder, where the spectral gaps are no longer empty but filled with localised states. We refer thus to the top Chern numbers as *strong invariants* and to the lower Chern numbers as *weak invariants*.

*Connes-Chern
character*

Remark 3.7 (Connes-Chern character in K -homology and Fredholm index theorem). Cyclic cohomology was originally designed in 1981 by Alain Connes as the natural receptacle of the Chern character in K -homology, now known as the Connes-Chern character. K -homology is associated to K -theory by duality and consists of classes of cyclic cocycles constructed from algebra representations on auxiliary Hilbert spaces with an additional quantised differential calculus structure, so-called Fredholm modules. If a Fredholm module fulfils a certain finite summability condition, which makes some products of derivatives in the differential algebra trace class, then the cyclic n -cocycles with sufficiently large n to meet this condition pair integrally with K -theory. Up to an n -dependent prefactor, this can be expressed as the n -independent Fredholm index of a Fredholm operator constructed from the K -group element. The Connes-Chern character can be represented by any of these cyclic n -cycles. By introducing a periodicity operator with degree 2 mapping the cohomology group of n -cocycles to the cohomology group of $(n+2)$ -cocycles, one defines the *periodic cyclic cohomology* of the algebra as the direct limit under the periodicity operator of the cyclic cohomology groups [Con94, Chap. IV.1 β]. The Connes-Chern character then generates the periodic cyclic cohomology class of these cocycles.

In case of our $(r+d)$ -dimensional non-commutative torus algebra, one can construct a suitable Fredholm module as demonstrated in [PS16, Sec. 6.2]. For them, the summability condition is only satisfied for cyclic n -cocycles with $n \geq r+d$ [PS16, Lem. 6.2.2.]. Therefore, only the top Chern cocycle corresponds to the Connes-Chern character [PS16, Thm. 6.3.1.] and pairs integrally with K -theory via the Fredholm index. Since the index theorem can be extended to larger classes of projections in non-commutative Sobolev spaces, the stability of the strong invariants is also valid in the presence of strong disorder in the electronic system [PS16, Sec. 6.5]. However, this does not generally extend to the weak invariants.

*Image of the
Chern cocycles*

Since all Chern cocycles on an algebra induce group homomorphisms from its K_0 -group to $\mathbb{C}$, their image is a countable subset of $\mathbb{C}$ which can be calculated from the image of the K_0 -group generators. For the K_0 equivalence class $[p]_0$ of a projection $p \in \mathcal{P}_\infty(\mathcal{A}_\Theta)$ with linear decomposition

$$[p]_0 = \sum_{\substack{J \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\} \\ |J| \text{ even}}} n_J [e_J]_0,$$

into the K_0 -group generators $[e_J]_0$, $J \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\}$ and $|J|$ even, with integer coefficients $n_J \in \mathbb{Z}$, we obtain for instance the Chern numbers

$$Ch_I([p]_0) = \sum_{\substack{J \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\} \\ |J| \text{ even}}} n_J Ch_I([e_J]_0).$$

In the next part, we evaluate the Chern numbers of the generators, which finally gives us access to the gap labels.

3.3.3. Generalised Středa Formulas and Higher Gap Labelling

The generalised Středa formulas establish a connection between lower and higher Chern numbers. In the context of the quantum Hall effect in two spatial dimensions, the original Středa formula describes that the derivative of the electron density with respect to the magnetic field strength is equal to the Hall conductance [Str82]. This can be rephrased as a linear relationship between the 0th Chern number, which coincides with the integrated density of states, and the magnetic flux, with the slope proportional to the 1st momentum space Chern number. Rammal and Bellissard [RB90] proved this identity within the framework of non-commutative tori expressing the derivative in the magnetic flux as Itô derivatives as introduced in Sec. 3.2.3.

In the book of Prodan and Schulz-Baldes [PS16] the relation was generalised to higher dimensions and, thereby, a higher number of (magnetic flux) parameters. It is straightforward to expect that this further extends to the pitch parameters of the spin waves as used in [Lux+24]. This is indeed the case, although the derivation must be modified to accommodate the different expressions of the Itô derivatives that we introduced in Eq. (3.40) and Eq. (3.41). As a consequence of the generalised Středa formulas, one can decompose the image of the pairings of K -theory with the cyclic cocycles and derive a formula for higher gap labelling. The image of the pairing with the trace was first computed in [Ell83], and we refer to [BM18] for extensions and the notation adopted in this work.

In the following, we present the generalised Středa formulas for the magnetic flux and pitch parameters. For the proof of the former, we refer to [PS16, Chap. 5.6]. For the latter, we provide calculations in App. A10 to highlight the necessary modifications. We can then also present the higher gap labelling formula for our systems, and refer the reader to [PS16, Chap. 5.7] for the details of the proof.

The original Středa formula $\partial_B n = \sigma_{xy}$ [Str82], with the electron density $n = \mathcal{T}(p)$ and Hall conductivity σ_{xy} , can be expressed in our framework as *Středa formulas*

$$\partial_{\Phi_{ij}} \text{Ch}_0([p]_0) = \text{Ch}_{\{t_i, t_j\}}([p]_0), \quad (3.52)$$

for $p \in \mathcal{P}(\mathcal{A}_\Theta)$ Itô-differentiable and any $i, j = 1, \dots, d$ with $i < j$. The formula can be derived from the Itô-like product rule Eq. (3.40) as shown in [PS16, Prop. 5.6.1] and replicated in App. A9. In our context, we can derive an analogous identity for the pitch parameters

$$\partial_{\theta_{ij}} \text{Ch}_0([p]_0) = \text{Ch}_{\{u_i, t_j\}}([p]_0), \quad (3.53)$$

again for $p \in \mathcal{P}(\mathcal{A}_\Theta)$ Itô-differentiable and any $i = 1, \dots, r$ and $j = 1, \dots, d$. This follows from the Itô-like product rule Eq. (3.41) and its derivation requires some modification as shown in App. A9. Both formulas can be reformulated in a unified way in terms of the generators μ_a , $a = 1, \dots, r + d$, of the universal C^* -algebra and its parameter matrix Θ by

$$\partial_{\Theta_{ab}} \text{Ch}_0([p]_0) = \text{Ch}_{\{\mu_a, \mu_b\}}([p]_0). \quad (3.54)$$

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*Generalised
Středa formulas*

Here, we exclude the case $a, b = 1, \dots, r$ and $a = b$ for which Θ_{ab} is 0. Evidently, the classical Středa formulas connect the derivatives of the 0th Chern numbers with 1st Chern numbers. This relationship can be generalised to higher Chern numbers in the following way:

Theorem 3.8 (The generalised Středa formulas). *Let $I \subset \{\mu_1, \dots, \mu_{r+d}\}$ be an ordered set and $a, b = 1, \dots, r + d$ (but not $a, b = 1, \dots, r$) with $\mu_a, \mu_b \notin I$. If $|I|$ is even and $p \in \mathcal{P}(\mathcal{A}_\Theta)$ Itô-differentiable, then it is*

$$\partial_{\Theta_{ab}} \text{Ch}_I([p]_0) = \text{Ch}_{\{\mu_a, \mu_b\} \cup I}([p]_0). \quad (3.55)$$

The derivation for the magnetic flux parameters Φ_{ij} , $i, j = 1, \dots, d$ can be found in the proof of [PS16, Thm. 5.6.3 (i)]. For the pitch parameters θ_{ij} , $i = 1, \dots, r$ and $j = 1, \dots, d$ and vice versa, the different form of the Itô derivative product formula again necessitates some modifications. A detailed derivation along the lines of [PS16, Thm. 5.6.3 (i)] is conducted in App. A10.

*Image of the
generators*

In [PS16, Sec. 4.2.3] Emil Prodan presented the generators of the K_0 -group $K_0(A_d)$ of a non-commutative torus C^* -algebra A_d in d dimensions. Subsequently, he used the generalised Středa formulas to derive the explicit image of their pairing with the Chern cocycles in the proof of [PS16, Thm. 5.7.1.]. Since the generalised Středa formulas are valid for our case as demonstrated above, we can infer the same implications.

Let $I, J \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\}$ be increasingly ordered sets of even cardinality and e_J the generators of $K_0(\mathcal{A}_\Theta)$ (as presented in [PS16, Sec. 4.2.3]). Then, the Chern cocycles pair with the generators as follows:

$$\text{Ch}_I([e_J]_0) = \begin{cases} 0 & I \setminus J \neq \emptyset, \\ 1 & I = J, \\ \eta_{(J \setminus I) \cup I} \text{Pf}(\Theta_{J \setminus I}) & I \subsetneq J. \end{cases} \quad (3.56)$$

The operation Pf denotes the Pfaffian, $\Theta_{J \setminus I} = (\Theta_{ab})$ with $a, b \in J \setminus I$ is the submatrix of Θ in the reduced index set, and $\eta_{(J \setminus I) \cup I}$ is the signum of the permutation for reordering $(J \setminus I) \cup I$ to J^1 .

In the following, we give a brief explanation for these values and refer to the proof of [PS16, Thm. 5.7.1.] for an in-depth derivation:

For $\mu_i \in I \setminus J$, the Chern cocycle contains derivations ∂_{μ_i} while the representative e_J of the projection generator $[e_J]_0$ only lies in the subalgebra generated by $\mu_j \in J$. Therefore, the image is zero for $I \setminus J \neq \emptyset$.

Next up, for $I = J$, the image being 1 follows for $J = \emptyset$ from the normalisation of the trace and for $J \neq \emptyset$ from an iterative approach using the bulk-boundary correspondence which we did not introduce in our work.

¹This sign of the Pfaffian is missing in the original source. We find it occurring in Eq. (3.57).

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Finally, the cases with $I \subsetneq J$ make use of the generalised Středa formulas Eq.(3.55). For any pair partition $(p_1, \dots, p_k)$ of $J \setminus I$ we have

$$\partial_{\Theta_{p_1}} \dots \partial_{\Theta_{p_k}} \text{Ch}_I([e_J]_0) = \text{Ch}_{\{p_1, \dots, p_k\} \cup I}([e_J]_0) = \eta_{(J \setminus I) \cup I} \eta_{p_1, \dots, p_k} \text{Ch}_J([e_J]_0). \quad (3.57)$$

Reordering the indices $\{p_1, \dots, p_k\} \cup I$ into the increasing order of J yields the signs $\eta_{(J \setminus I) \cup I}$ for reordering $(J \setminus I) \cup I$ to J and $\eta_{p_1, \dots, p_k}$ for reordering $\{p_1, \dots, p_k\}$ to $J \setminus I$. The reordered pairing is $\text{Ch}_J([e_J]_0) = 1$.

This implies, that $\text{Ch}_I([e_J]_0)$ is a polynomial in $\Theta_{p_1} \dots \Theta_{p_k}$ running over all pair partitions of even cardinality subsets of $I \setminus J$. In fact, one finds that the coefficients for pair partitions of true subsets vanish. Therefore, only the $(2k-1)!!$ terms with pair partitions of $I \setminus J$ remain. Let $p_l = (i_l, j_l)$, $l = 1, \dots, k$, be ordered with $i_l < j_l$ and $i_l < i_{l+1}$. Then, this is, up to $\eta_{(J \setminus I) \cup I}$, precisely the definition of the Pfaffian determinant of $\Theta_{J \setminus I}$

$$\text{Ch}_I([e_J]_0) = \text{Ch}_J([e_J]_0) \eta_{(J \setminus I) \cup I} \sum_{(p_1, \dots, p_k)} \eta_{p_1, \dots, p_k} \Theta_{p_1} \dots \Theta_{p_k} = \eta_{(J \setminus I) \cup I} \text{Pf}(\Theta_{J \setminus I}). \quad (3.58)$$

For the quantum Hall effect in two dimensions the K_0 -group is $\mathbb{Z}^2$ and there are precisely two generators, the identity $[\mathbb{1}]_0$ and the so-called Powers-Rieffel projection $[e_{t_1 t_2}]_0$. From the normalisation of the trace we get $\mathcal{T}([\mathbb{1}]_0) = 1$ and the original Středa formula implies $\mathcal{T}([e_{t_1 t_2}]_0) = \Phi_{12}$. The image of $\text{Ch}_\emptyset$ is therefore $\mathbb{Z} + \Phi_{12}\mathbb{Z}$. The Fermi projection p_F for each spectral gap is determined by the two integer labels $n_\emptyset$ and $n_{t_1 t_2}$, which is known as *gap labelling*. Its image under $\text{Ch}_\emptyset$ is equal to the integrated density of states for all Fermi energies inside this gap.

Quantum Hall effect

For electronic systems which are described by observables belonging to a higher-dimensional non-commutative torus algebra, gap labelling is also possible. For our observable algebra $\mathcal{A} = M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta$ of spin-1/2 electrons in the presence of a magnetic field and coupled to a multi- q spin texture such that $K_0(\mathcal{A}_\Theta) \cong \mathbb{Z}^{2^{r+d-1}}$, there are 2^{r+d-1} gap labels n_J , $J \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\}$ with $|J|$ even. The image of the Chern cocycles is given by the following higher gap labelling formula [PS16, Cor. 5.7.2]:

Higher gap labelling

Theorem 3.9 (Higher gap labelling). *The image of $\text{Ch}_I : K_0(\mathcal{A}) \rightarrow \mathbb{C}$ with $I \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\}$ of even cardinality as defined in Eq. (3.51) is given by*

$$\text{Im}(\text{Ch}_I) = \mathbb{Z} + \sum_{\substack{|J| \text{ even} \\ I \subsetneq J}} \eta_{(J \setminus I) \cup I} \text{Pf}(\Theta_{J \setminus I}) \mathbb{Z}. \quad (3.59)$$

3.4. The Magnetic Multi-q Texture Tight-Binding Hamiltonian

The tight-binding Hamiltonian describing spin-1/2 electrons coupled to a multi- q spin texture on a d -dimensional lattice permeated by a constant magnetic field is a representation of an element from the observable algebra $\mathcal{A} = M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta$ as a bounded operator on the physical Hilbert space $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$.

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Tight-binding Hamiltonian

In Chap. 2.1, we discussed how the behaviour of interacting electrons in crystalline materials can be described using a series of approximations leading via an effective non-interacting one-electron Hamiltonian eventually to a tight-binding lattice Hamiltonian while preserving the key topological features of the energy spectrum. The basic toy model is given by the tight-binding Hamiltonian of the form

$$H = - \sum_{\langle \mathbf{i}, \mathbf{j} \rangle \in \mathbb{Z}^{2d}} \lambda_{\text{hop}}(\mathbf{i}, \mathbf{j}) |\mathbf{i}\rangle \langle \mathbf{j}| + \lambda_{\text{xc}} \sum_{\mathbf{i} \in \mathbb{Z}^d} \boldsymbol{\sigma} \cdot \mathbf{n}(\mathbf{x}_{\mathbf{i}}) |\mathbf{i}\rangle \langle \mathbf{i}|, \quad (3.60)$$

where $\langle \mathbf{i}, \mathbf{j} \rangle$ indicates the restriction of the sum to nearest-neighbour pairs in the d -dimensional lattice. The coefficient $\lambda_{\text{hop}}(\mathbf{i}, \mathbf{j}) \in M_2(\mathbb{C})$ is scalar in spin space and contains the hopping parameter λ_{hop} and the phase factor $e^{i\Gamma_A([\mathbf{i}, \mathbf{j}])}$ gathered by an electron moving from the site at $\mathbf{x}_{\mathbf{i}}$ to the site at $\mathbf{x}_{\mathbf{j}}$ in the constant magnetic field B . With the magnetic potential A in the symmetric gauge, the phase can be expressed in terms of the flux matrix Φ by

$$\Gamma_A([\mathbf{i}, \mathbf{j}]) = \frac{e}{\hbar} \int_{[\mathbf{x}_{\mathbf{i}}, \mathbf{x}_{\mathbf{j}}]} A = 2\pi(\mathbf{i} \wedge_{\Phi} \mathbf{j}),$$

in accordance with the conventions laid out in Sec. 3.1.2. The exchange parameter λ_{xc} describes the coupling strength of the electron spin to the magnetic texture $\mathbf{n} : \mathbb{R}^d \rightarrow \mathbb{R}^3$, with $\boldsymbol{\sigma}$ representing the vector of Pauli matrices. We assume the system to be in the strong coupling regime with $\frac{\lambda_{\text{hop}}}{\lambda_{\text{xc}}} \ll 1$ where the electron spins align with the texture. We want to stress that generalisations to further orbital and spin degrees of freedom as well as next-nearest neighbour coupling and beyond are possible to be expressed as part of the same observable algebra.

Section content

In the following, we rewrite the tight-binding Hamiltonian into its canonical form such that its affiliation to the observable algebra constructed in Sec. 3.1 becomes apparent. In doing so, we identify the corresponding abstract algebra element and verify that it is smooth and Itô-differentiable. This ensures that the Fermi projections associated with its spectral gaps are eligible for the treatment with the non-commutative geometry tools from Sec. 3.3 constructed from the differential calculus introduced in Sec. 3.2. With the newfound knowledge that the Chern numbers for the spectral gaps are well-defined, we present their decomposition into integer gap labels explicitly for the cases of $2q$ -spin waves and $3q$ -spin lattices. Additionally, we demonstrate that the magnetic Itô-derivatives also provide access to a non-commutative expression for orbital magnetisation in our model, that is a generalisation of the formula from modern theory introduced in Chap. 2.4.

3.4.1. Canonical Form of the Hamiltonian

The canonical form of the tight-binding Hamiltonian is that of the integrated Schrödinger representation of a generic element of the observable algebra. To unearth it, we consider the hopping term and the exchange term separately. The hopping term is translation invariant under the magnetic translations and its off-diagonal nature in lattice space can be expressed in terms of the dual magnetic translation operators. Since those are

3.4. The Magnetic Multi- q Texture Tight-Binding Hamiltonian

a representation of the lattice translation generators, the whole hopping term can be constructed from these generators. The exchange term is translation covariant, which is precisely the property modelled by our implementation of the non-commutative torus algebra. It is also diagonal in lattice space and can therefore be rewritten as a multiplication operator representing the texture's phase torus functions. In the following, we rewrite the two parts of the tight-binding Hamiltonian and identify the corresponding algebra element. In the end, we confirm that this algebra element is part of the smooth subalgebra and furthermore Itô-differentiable.

As established in Sec. 3.1.2 for the representation on a physical Hilbert space, we consider the family of covariant Schrödinger representations $\{(\ell^2(\mathbb{Z}^d), \pi_\varphi, \rho^A)\}_{\varphi \in T^r}$ of the twisted C^* -dynamical system $(C(T^r), \mathbb{Z}^d, \alpha, \gamma)$. From it, we obtain the family of integrated representations $\{(\ell^2(\mathbb{Z}^d), \pi_\varphi^\times = \pi_\varphi \rtimes \rho^A)\}_{\varphi \in T^r}$ of the twisted crossed product algebra $C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ that can be extended to a representation of the C^* -completion $\mathcal{A}_\Theta = C(T^r) \rtimes_\theta^\Phi \mathbb{Z}^d$ and finally to a representation of the observable algebra $\mathcal{A} = M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta$ on $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$. To recognise this representation in the Hilbert space operators, we rewrite the tight-binding Hamiltonian from Eq. (3.60) into the canonical form

*Covariant
representation*

$$H = \sum_{\mathbf{n}, \mathbf{m} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n}} h_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A = \pi_\varphi^\times(h) \quad (3.61)$$

and by that identify the coefficients $h_{\mathbf{m}} \in M_2(C(T^r))$ of the corresponding algebra element

$$h = \sum_{\mathbf{m} \in \mathbb{Z}^d} h_{\mathbf{m}} \otimes t^{\mathbf{m}}.$$

In case of ergodic textures, h is unique by the faithfulness of the representation.

Let us now first consider the hopping term H_{hop} of the tight-binding Hamiltonian H . From a given site $\mathbf{i} \in \mathbb{Z}^d$, we denote by $\mathbf{d}_1, \dots, \mathbf{d}_c \in \mathbb{Z}^d$ the relative position of its nearest neighbours (which we assume to be independent of $\mathbf{i}$), with c being the coordination number of the lattice. Further, we define $\varphi = \omega(\mathbf{x}_0)$ to denote the phase at the arbitrarily chosen origin site with label $\mathbf{0}$. The hopping term can then be rewritten the following way

Hopping term

$$\begin{aligned} H_{\text{hop}} &= - \sum_{\langle \mathbf{i}, \mathbf{j} \rangle \in \mathbb{Z}^{2d}} \lambda_{\text{hop}}(\mathbf{i}, \mathbf{j}) |\mathbf{i}\rangle \langle \mathbf{j}| = - \sum_{k=1}^c \sum_{\mathbf{i} \in \mathbb{Z}^d} \lambda_{\text{hop}}(\mathbf{i}, \mathbf{i} + \mathbf{d}_k) |\mathbf{i}\rangle \langle \mathbf{i} + \mathbf{d}_k| \\ &= -\lambda_{\text{hop}} \sum_{k=1}^c \sum_{\mathbf{i} \in \mathbb{Z}^d} \mathbb{1}_2 e^{2\pi i(\mathbf{i} \wedge_\Phi \mathbf{d}_k)} |\mathbf{i}\rangle \langle \mathbf{i}| \hat{T}_{-\mathbf{d}_k} \\ &= -\lambda_{\text{hop}} \sum_{k=1}^c \sum_{\mathbf{i} \in \mathbb{Z}^d} (\alpha_{-\mathbf{i}} \mathbb{1}_2)(\varphi) |\mathbf{i}\rangle \langle \mathbf{i}| \hat{U}_{-\mathbf{d}_k}^A \\ &= \pi_\varphi^\times \left(-\lambda_{\text{hop}} \sum_{k=1}^c \mathbb{1}_2 \otimes t^{-\mathbf{d}_k} \right), \end{aligned}$$

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which one recognises as the canonical form with coefficients $h_{\mathbf{m}}^{\text{hop}} = \mathbb{1}_2$ for $\mathbf{m} = \mathbf{d}_k$, $k = 1, \dots, c$ and $h_{\mathbf{m}}^{\text{hop}} = 0$ otherwise. The algebra element

$$\Delta = \sum_{k=1}^c \mathbb{1}_2 \otimes t^{-\mathbf{d}_k}, \quad (3.62)$$

is also referred to as the adjacency operator of the lattice. In case of a one-dimensional chain or a two-dimensional triangular lattice it is (suppressing the tensor product), respectively, given by

$$\begin{aligned} \Delta_{\text{chain}} &= t + t^{-1} \\ \Delta_{\text{triangular}} &= t_1 + t_2 + t_1 t_2 + t_1^{-1} + t_2^{-1} + t_1^{-1} t_2^{-1}. \end{aligned}$$

The hopping term in the canonical form is manifestly invariant under magnetic translations, which commute with the dual magnetic translation operators:

$$\hat{V}_{\mathbf{i}}^A H_{\text{hop}} \hat{V}_{\mathbf{i}}^{A-1} = H_{\text{hop}}.$$

Exchange term

In contrast, the exchange term denoted by $\mathcal{H}_{\text{xc}}(\boldsymbol{\varphi})$ is translation covariant with respect to the magnetic translations. For any covariant representation, this property is immediately implied by the compatibility condition for the algebra and group representations. $\mathcal{H}_{\text{xc}}(\boldsymbol{\varphi})$ is diagonal on the lattice Hilbert space and can therefore be interpreted as a multiplication operator representing a function in $M_2(C_b(\mathbb{Z}^d))$ in the sense of Eq. (3.11). We can reinterpret it as a function in $M_2(C(T^r))$ using the $\mathbb{Z}^d$ lattice action on the algebra $C(T^r)$ of phase torus functions:

$$\begin{aligned} \boldsymbol{\sigma} \cdot \mathbf{n}(\mathbf{x}_{\mathbf{i}}) &= \sum_{j=1}^3 \sigma_j \otimes n_j(\boldsymbol{\omega}(\mathbf{x}_{\mathbf{i}})) = \sum_{j=1}^3 \sigma_j \otimes n_j(\tau_{\mathbf{i}} \boldsymbol{\varphi}) = \sum_{j=1}^3 \sigma_j \otimes \alpha_{-\mathbf{i}} n_j(\boldsymbol{\varphi}) \\ &=: \alpha_{-\mathbf{i}}(\boldsymbol{\sigma} \cdot \mathbf{n})(\boldsymbol{\varphi}). \end{aligned}$$

Now, the exchange term is a multiplication operator in the sense of Eq. (3.12), and we obtain

$$\begin{aligned} \mathcal{H}_{\text{xc}}(\boldsymbol{\varphi}) &= \lambda_{\text{xc}} \sum_{\mathbf{i} \in \mathbb{Z}^d} \boldsymbol{\sigma} \cdot \mathbf{n}(\mathbf{x}_{\mathbf{i}}) |\mathbf{i}\rangle \langle \mathbf{i}| = \lambda_{\text{xc}} \sum_{\mathbf{i} \in \mathbb{Z}^d} \alpha_{-\mathbf{i}}(\boldsymbol{\sigma} \cdot \mathbf{n})(\boldsymbol{\varphi}) |\mathbf{i}\rangle \langle \mathbf{i}| \hat{U}_{\mathbf{0}}^A \\ &= \pi_{\boldsymbol{\varphi}}^{\times}(\lambda_{\text{xc}} \boldsymbol{\sigma} \cdot \mathbf{n} \otimes t^{\mathbf{0}}), \end{aligned}$$

which one recognises as the canonical form with coefficients $h_{\mathbf{0}}^{\text{xc}} = \boldsymbol{\sigma} \cdot \mathbf{n}$ and $h_{\mathbf{m}}^{\text{xc}} = 0$ otherwise.

Algebra element

Combined, we find that the Hamiltonian $H = H_{\text{hop}} + H_{\text{xc}}$ is given by the integrated Schrödinger representation $\pi_{\boldsymbol{\varphi}}^{\times}(h)$ of

$$h = -\lambda_{\text{hop}} \Delta + \lambda_{\text{xc}} \boldsymbol{\sigma} \cdot \mathbf{n}, \quad (3.63)$$

3.4. The Magnetic Multi-q Texture Tight-Binding Hamiltonian

which is an element of the observable algebra $M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta$. The canonical form of H is then that of Eq. (3.61) with coefficients

$$h_{\mathbf{m}}(\varphi) = \begin{cases} \lambda_{\text{xc}} \boldsymbol{\sigma} \cdot \mathbf{n}, & \mathbf{m} = 0 \\ -\lambda_{\text{hop}} \mathbb{1}_2, & \mathbf{m} \in \{\mathbf{d}_1, \dots, \mathbf{d}_c\} \\ 0, & \text{else} \end{cases} \quad (3.64)$$

The Hamiltonian in total is translation covariant with respect to the magnetic translations

$$\hat{V}_{\mathbf{m}}^A H(\varphi) \hat{V}_{\mathbf{m}}^{A^{-1}} = H(\tau_{-\mathbf{m}} \varphi)$$

or alternatively

$$\hat{V}_{\mathbf{m}}^A H(\varphi) \hat{V}_{\mathbf{m}}^{A^{-1}} = H(\varphi - 2\pi\theta\mathbf{m}).$$

It is easy to verify, that h lies in the smooth subalgebra $M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta$ and is beyond that also Itô-differentiable. For the former, we apply the smoothness criterium from Sec. 3.2.2. The Fourier coefficients $h_{\mathbf{m}}$ of h are elements in $M_2(C^\infty(T^r))$ and are zero for $\mathbf{m} \notin \{0, \mathbf{d}_1, \dots, \mathbf{d}_c\}$. The latter then follows from the fact, that the Fourier coefficients $h_{\mathbf{m}}$ are independent of the algebra parameters Θ and therefore smoothly differentiable with respect to them. This makes h also Itô-differentiable. As an immediate consequence, the Fermi projections $p_F = \chi(h \leq E_F)$ with Fermi energy $E_F \notin \sigma(h)$ located in a spectral gap of h , are smooth and Itô-differentiable as well.

Smoothness properties

3.4.2. Chern Number Decomposition

For all spectral gaps of the tight-binding Hamiltonian, the set of invariant Chern numbers can be decomposed into a set of invariant integer labels. Since the Fermi gap projections of the spectral gaps of h are smooth, we can use the Chern cocycles to compute the Chern numbers associated with their K_0 -equivalence classes. Since they are also Itô-differentiable, the generalised Středa formulas can be applied to extract the integer gap labels. In the following, we give the explicit form of the Chern number for the $2q$ spin waves and three different $3q$ skyrmion and vortex lattices introduced in Chap. 1.2.3 and present the corresponding Chern number decomposition in gap labels.

Let $h \in \mathcal{A}$ be the tight-binding Hamiltonian from Eq. (3.63) and let $p := \chi(h \leq E_F)$ be the Fermi projection with Fermi energy $E_F \notin \sigma(h)$ located in a spectral gap of h . Then the 2^{r+d-1} Chern numbers associated with this gap, can be obtained via the pairing of the K_0 -class $[p]_0$ with the Chern cocycles defined in Sec. 3.3.2

General expression

$$Ch_I([p]_0) = \frac{(2\pi i)^n}{n!} \sum_{\sigma \in S_{2n}} (-1)^\sigma \mathcal{T}(p \partial_{\sigma_1} p \dots \partial_{\sigma_{2n}} p),$$

for each $I \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\}$ with $|I| = 2n$, $n \in \mathbb{N}_0$. The projection equivalence class can be expressed as a linear combination of K_0 -group generators:

$$[p]_0 = \sum_{\substack{J \subseteq \{u_1, \dots, u_r, t_1, \dots, t_d\} \\ |J| \text{ even}}} n_J [e_J]_0.$$

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By linearity of the Chern cocycles, the same integer coefficients appear as coefficients of the Θ -dependent Chern number polynomials

$$Ch_I([p]_0) = n_I + \sum_{\substack{|J| \text{ even} \\ I \subsetneq J}} n_J \eta_{(J \setminus I) \cup I} \text{Pf}(\Theta_{J \setminus I}).$$

Explicit evaluation of the Chern numbers then yields 2^{r+d-1} polynomial equations with 2^{r+d-1} coefficients, which we can solve to obtain the integer gap labels.

On the right hand-side we already suppress the $[p]_0$ -dependence of the labels in the notation and from now on, we also suppress it in the Chern number expression on the left hand-side.

$2q$ spin wave

In the case of a one-dimensional chain with a $2q$ spin wave as described in Chap. 1.2.3.2, we have two linear dependent q -vectors. We choose for them to be rationally dependent such that we can describe the periodicity of the spin wave with a single Fourier generator. The generators of the non-commutative torus $\mathcal{A}_{\Theta_{2q}} = C(T) \rtimes_{\theta} \mathbb{Z}$ are then $\{u, t\}$ with the Θ_{2q} matrix given by

$$\Theta_{2q} = \begin{pmatrix} 0 & \vartheta \\ -\vartheta & 0 \end{pmatrix}. \quad (3.65)$$

The corresponding K_0 -group is $K_0(\mathcal{A}_{\Theta_{2q}}) = \mathbb{Z}^2$ and the eligible Fermi projections $p \in M_2(\mathcal{A}_{\Theta_{2q}})$ pair as follows with the Chern cocycles:

$$\begin{aligned} Ch_{\emptyset}([p]_0) &= \mathcal{T}(p) = n_{\emptyset} + \vartheta n_{\{u, t\}}, \\ Ch_{\{u, t\}}([p]_0) &= 2\pi i \mathcal{T}(p \partial^u p \partial^t p - p \partial^t p \partial^u p) = n_{\{u, t\}}. \end{aligned}$$

The integer gap labels can be extracted immediately and are given by

$$n_{\emptyset} = Ch_{\emptyset} - \vartheta Ch_{\{u, t\}} \quad \text{and} \quad n_{\{u, t\}} = Ch_{\{u, t\}}.$$

$3q$ spin lattice

For a two-dimensional lattice with a $3q$ spin lattice as described in Chap. 1.2.3.3 with two different skyrmion lattices and a vortex lattice, we have three linear dependent q -vectors. Since the three q -vectors compensate each other, we can describe the periodicity of the spin textures by just two Fourier generators. In the presence of a magnetic field $\mathbf{B} = B\hat{\mathbf{e}}_z$ perpendicular to the plane of the lattice with vector potential $\mathbf{A}(x, y) = \frac{B}{2}(x\hat{\mathbf{e}}_y - y\hat{\mathbf{e}}_x)$ in the symmetric gauge, we have the magnetic flux matrix $\phi = \frac{1}{2\pi} \frac{\sqrt{3}}{2} B \frac{e}{\hbar} = |\mathbf{a}_1 \times \mathbf{a}_2| B \phi_0$ with flux quantum $\phi_0 = \frac{\hbar}{e}$. The generators of the non-commutative torus $\mathcal{A}_{\Theta_{3q}} = C(T^2) \rtimes_{\theta}^{\Phi} \mathbb{Z}^2$ are then $\{u_1, u_2, t_1, t_2\}$ with the Θ_{3q} matrix given by

$$\Theta_{3q} = \begin{pmatrix} 0 & \theta \\ -\theta^T & \Phi \end{pmatrix} \quad \text{with} \quad \theta = \vartheta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \Phi = \phi \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (3.66)$$

The corresponding K_0 -group is $K_0(\mathcal{A}_{\Theta_{3q}}) = \mathbb{Z}^8$ and the eligible Fermi projections $p \in M_2(\mathcal{A}_{\Theta_{3q}})$ pair as follows with the Chern cocycles:

$$Ch_{\emptyset} = n_{\emptyset} + \phi n_{\{t_1, t_2\}} + \vartheta n_{\{u_1, t_1\}} + \vartheta n_{\{u_2, t_2\}} - \vartheta^2 n_{\{u_1, u_2, t_1, t_2\}},$$

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$$\begin{aligned}
Ch_{\{u_1, u_2\}} &= n_{\{u_1, u_2\}} + \phi n_{\{u_1, u_2, t_1, t_2\}}, \\
Ch_{\{u_1, t_1\}} &= n_{\{u_1, t_1\}} - \vartheta n_{\{u_1, u_2, t_1, t_2\}}, \\
Ch_{\{u_1, t_2\}} &= n_{\{u_1, t_2\}}, \\
Ch_{\{u_2, t_1\}} &= n_{\{u_2, t_1\}}, \\
Ch_{\{u_2, t_2\}} &= n_{\{u_2, t_2\}} - \vartheta n_{\{u_1, u_2, t_1, t_2\}}, \\
Ch_{\{t_1, t_2\}} &= n_{\{t_1, t_2\}}, \\
Ch_{\{u_1, u_2, t_1, t_2\}} &= n_{\{u_1, u_2, t_1, t_2\}}.
\end{aligned}$$

Solving this linear system for the gap label coefficients yields the following equations:

$$\begin{aligned}
n_\emptyset &= Ch_\emptyset - \phi Ch_{\{t_1, t_2\}} - \vartheta Ch_{\{u_1, t_1\}} - \vartheta Ch_{\{u_2, t_2\}} - \vartheta^2 Ch_{\{u_1, u_2, t_1, t_2\}}, \\
n_{\{u_1, u_2\}} &= Ch_{\{u_1, u_2\}} - \phi Ch_{\{u_1, u_2, t_1, t_2\}}, \\
n_{\{u_1, t_1\}} &= Ch_{\{u_1, t_1\}} + \vartheta Ch_{\{u_1, u_2, t_1, t_2\}}, \\
n_{\{u_1, t_2\}} &= Ch_{\{u_1, t_2\}}, \\
n_{\{u_2, t_1\}} &= Ch_{\{u_2, t_1\}}, \\
n_{\{u_2, t_2\}} &= Ch_{\{u_2, t_2\}} + \vartheta Ch_{\{u_1, u_2, t_1, t_2\}}, \\
n_{\{t_1, t_2\}} &= Ch_{\{t_1, t_2\}}, \\
n_{\{u_1, u_2, t_1, t_2\}} &= Ch_{\{u_1, u_2, t_1, t_2\}}.
\end{aligned}$$

3.4.3. Orbital Magnetisation

The orbital motion of electrons induces a contribution to the magnetisation. In Chap. 1.1.2, we discussed how the orbital magnetic moments in solids are often times suppressed by orbital quenching. In general, if the electron Hamiltonian is time-reversal invariant the orbital magnetisation vanishes. The time-reversal symmetry may be broken by the presence of an external magnetic field or an internal spin magnetisation, leading to a non-zero orbital contribution. The orbital magnetisation can then be defined as the response of the free energy per unit volume to the magnetic field.

Ordinary perturbation theory cannot be used for magnetic Hamiltonians since the magnetic vector potential is unbounded. Even in the case of periodic systems the derivative with respect to the magnetic field is not applicable due to the quantised magnetic flux. However, in the framework of fields of C^* -algebras it is well-defined in terms of the Itô derivatives. Since the thermodynamic potential at $T = 0$ can be expressed in terms of the canonical trace of an algebra element composed of the Hamiltonian and its Fermi projection, we can explicitly compute a non-commutative formula for orbital magnetisation. This was first described in [ST13] and extends to the presence of disorder in the media. In the following, we present the necessary quantities in our formalism and perform the derivation of the orbital magnetisation with the Itô-like rules of calculus. Then, we rewrite the expression into the form corresponding to the modern theory formula presented in Chap. 2.4 and thereby identify the local and itinerant circulation contributions.

3. C^* -Algebra Theory of Multi-q Textures

*Thermodynamic
definition*

The orbital magnetisation at finite temperature T is defined as the response of the thermodynamic grand potential $\Omega = E - TS - \mu N$ with inner energy E , entropy S , particle number N , and chemical potential μ , to the change of the magnetic field $\mathbf{B}$ per volume V [Shi+07]

$$\mathbf{M}_{\text{orb}} = -\frac{1}{V} \left(\frac{\partial \Omega}{\partial \mathbf{B}} \right)_{T, \mu}.$$

In the following, we consider our two-dimensional lattice system permeated by the constant magnetic field $\mathbf{B}$ in the infinite volume limit $V \rightarrow \infty$. Then, the orbital magnetisation can be expressed in our formalism in terms of the canonical partition function by [ST13]

$$\mathbf{M}_{\text{orb}} = \frac{1}{V_0} \frac{\partial}{\partial \mathbf{B}} \frac{1}{\beta} \mathcal{T} \left(\ln \left(1 + e^{-\beta(h-\mu)} \right) \right) = \frac{1}{\beta V_0} \int_0^\beta d\beta' \frac{\partial}{\partial \mathbf{B}} \mathcal{T} (f_{\beta', \mu}(h)(\mu - h)),$$

where $f_{\beta', \mu}(x) = (1 + e^{-\beta'(x-\mu)})^{-1}$ denotes the Fermi-Dirac distribution with the inverse temperature $\beta = \frac{1}{kT}$ and chemical potential μ , $\mathcal{T}$ is the canonical trace from Eq. (3.30) that coincides with the infinite volume limit of the trace per unit volume from Eq. (3.31), and $V_0 = |\mathbf{a}_1 \times \mathbf{a}_2|$ the volume of the unit cell.

We define the auxiliary quantity $\tilde{\mathbf{M}}_{\text{orb}} = \frac{1}{V_0} \frac{\partial}{\partial \mathbf{B}} \mathcal{T} (f_{\beta, \mu}(h)(\mu - h))$ such that $\frac{\partial(\beta \mathbf{M}_{\text{orb}})}{\partial \beta} = \tilde{\mathbf{M}}_{\text{orb}}$. For zero temperature $\beta \rightarrow \infty$ both quantities coincide. In this limit, we have $\lim_{\beta \rightarrow \infty} f_{\beta, \mu}(h) = \chi(h \leq \mu)$. For filled bands at zero temperature the chemical potential μ coincides with the Fermi energy at the middle of the corresponding band gap, and such we obtain a Fermi projection $p = \chi(h \leq \mu)$.

Zero temperature

The orbital magnetisation along the direction of the magnetic field $\mathbf{B} = B\hat{\mathbf{e}}_z$ with magnetic flux $\phi = \frac{V_0}{2\pi} \frac{e}{\hbar} B$ at zero temperature can then be expressed as

$$M_{\text{orb}}^z = \frac{e}{\hbar} \frac{1}{2\pi} \partial_\phi \mathcal{T}((\mu - h)p) = \frac{e}{\hbar} \frac{i}{2} \mathcal{T}(|\mu - h|[\partial_1^t p, \partial_2^t p]), \quad (3.67)$$

where the second equality was evaluated using the Itô-like rules of calculus from Sec. 3.2.3 following [ST13, Prop. 5] as presented in App. A11. The derived expression can be expanded into contributions corresponding to those from modern theory introduced in Chap. 2.4:

$$M_{\text{orb}}^z = \frac{e}{\hbar} \frac{-i}{2} \mathcal{T}(p \partial_1^t p h \partial_2^t p - p \partial_2^t p h \partial_1^t p + h p [\partial_1^t p, \partial_2^t p] - 2\mu p [\partial_1^t p, \partial_2^t p]) \quad (3.68)$$

$$= \frac{e}{\hbar} \text{Im} \mathcal{T}(p \partial_1^t p h \partial_2^t p + h p \partial_1^t p \partial_2^t p - 2\mu p \partial_1^t p \partial_2^t p). \quad (3.69)$$

The details of this expansion are presented in App. A11. From the derivation of the modern theory, we assign the interpretation of local-circulation and itinerant current contributions to

$$M_{\text{orb}}^{LC} = \frac{e}{\hbar} \text{Im} \mathcal{T}(p \partial_1^t p (h - \mu) \partial_2^t p),$$

$$M_{\text{orb}}^{IC} = \frac{e}{\hbar} \text{Im} \mathcal{T}((h - \mu) p \partial_1^t p \partial_2^t p).$$

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The derivative of the orbital magnetisation with respect to the chemical potentials is proportional to the first momentum space Chern number

Bulk-Boundary interpretation

$$\frac{dM_{\text{orb}}^z}{d\mu} = \frac{e}{\hbar} i\mathcal{T}(p[\partial_1^t p, \partial_2^t p]) = \frac{e}{\hbar} \frac{1}{2\pi} Ch_{t_1 t_2}([p]_0).$$

This can be interpreted in terms of the bulk-boundary correspondence as laid out in technical detail in [PS16] and discussed in the context of the orbital magnetisation in [ST13, Chap. 6-7]. In a finite system, the momentum space Chern number describes the current along the surface of the sample, which contributes to the orbital magnetisation as discussed in Chap. 2.4.1.

Remark 3.8 (Orbital Magnetisation in the presence of disorder). As presented above, the formula for the orbital magnetisation at zero temperature given in Eq. (3.67) is valid for Fermi energies inside gaps of the energy spectrum. It can be shown that this is still true in the presence of disorder and dynamically localised states as shown in [ST13, Thm. 3].

4 Approximate Computational Programme

For the C^* -algebraic formalism established in Chap. 3, there exists a series of approximations that provide access to finite volume algorithms for numerical evaluation of the physics formulas with fast decaying error estimates. This computational programme was developed in [Pro17] for disordered topological insulators and was adopted by the author in [Pra+24] for the application to multi- q magnets.

The tight-binding Hamiltonian from Eq. (3.60) operating on the infinite-dimensional Hilbert space $\mathbb{C}^2 \otimes \ell^2(\mathbb{Z}^d)$ cannot be implemented exactly for computational purposes. This can be circumvented using a model on a finite sample $V \subset \mathbb{Z}^d$ that can be described with a finite-dimensional Hilbert space $\mathbb{C}^2 \otimes \ell^2(V)$. An appropriate choice of boundary conditions is instrumental in preventing the spectrum from being contaminated by boundary modes and, thereby, in ensuring the integrity the spectral gaps. The conventional approach is the approximation of the Hamiltonian on a finite super-cell with periodic boundary conditions, for which it can be shown that the resolvent converges fast to the bulk limit as the size goes to infinity and that the spectral properties of the infinite volume Hamiltonian are being recovered. This has been demonstrated to hold for Hamiltonians from the lattice group algebra [LP23], from the non-commutative two-torus [PV80b; LLS01], and from the non-commutative torus incorporating disorder [Pro17].

Finite Volume

The observable algebra $\mathcal{A}$ for our system coupled to a multi- q spin texture and constant magnetic field requires a similar approach as the disordered observable algebra, where the algebra of continuous functions over the disorder configuration takes the place of the one over the phase torus. Even though $\mathcal{A}$ is also an ordinary non-commutative torus with $r + d$ generators, the usual approach for non-commutative tori cannot be employed, since the finite volume restriction only applies to the d real space dimensions.

Disorder vs. multi- q texture

The approximate Hamiltonian with periodic boundary conditions can be represented as an element from an approximating algebra. For that, *finite volume approximating algebras* are introduced with corresponding finite dimensional Hilbert space representations [Pro17, Chap. 4.4]. The differential calculus introduced in Chap. 3.2 needs to be modified to accommodate the finite approximations [Pro17, Chap. 4.5]. With that, we obtain explicit finite representations that can be implemented into a computer programme [Pro17, Chap. 5], and which are used in the upcoming chapters for the computation of the full set of Chern numbers, gap labels, and the orbital magnetisation. The formal description of the approximations in an algebraic setting facilitates the error estimations for the approximate physics formulas. One finds that the upper bounds on the errors decay to

Approximate algebras

4. Approximate Computational Programme

zero faster than any inverse power of the volume [Pro17, Chap. 6, 8]. This enables a good numerical accuracy with reasonable computing resources.

Chapter content

In this chapter, we introduce the formal approximations and present the explicit expressions used for implementation. First, we briefly discuss the convergence of the periodic boundary Hamiltonian, to then establish the approximate algebras and their representations. Next, we deal with the approximate calculus and derive its form in the representation. From this, we can finally construct the approximate formulas for the Chern numbers and the orbital magnetisation and discuss the implementation of the algorithm. At the end, we give the corresponding error bounds.

4.1. The Approximating Algebra for Computation

The finite volume approximating algebra generates the finite super-cell models with periodic boundary conditions and can be equipped with an approximate differential calculus. A suitable sequence of these approximating algebras has the infinite volume algebra as its projective limit. This algebraic formalisation of the finite volume approximation facilitates the identification of the proper finite computable expressions and the description of the convergence in the thermodynamic limit.

Group algebra

We want to start this section by comparing different strategies to obtain finite approximations for infinite volume lattice models of different complexity: Imposing periodic boundary conditions on a lattice group algebra Hamiltonian $h \in \mathbb{C}\mathbb{Z}$ on $\ell^2(\mathbb{Z})$ can for instance be understood mathematically by the description of the group $\mathbb{Z}$ as direct limit of normal subgroups

$$\mathbb{Z} = p^0\mathbb{Z} \triangleright p^1\mathbb{Z} \triangleright p^2\mathbb{Z} \triangleright \dots,$$

where p is a natural number greater than 1. The quotients $\mathbb{Z}/p^k\mathbb{Z}$ are the periodic groups of integers modulo p^k and are finite-dimensional, and the respective canonical homomorphisms $\phi_k : \mathbb{Z} \rightarrow \mathbb{Z}/p^k\mathbb{Z}$ induce $*$ -morphisms ϕ_k between the C^* -algebra completions $C^*(\mathbb{Z})$ of $\mathbb{C}\mathbb{Z}$ and $C^*(\mathbb{Z}/p^k\mathbb{Z})$ of $\mathbb{C}\mathbb{Z}/p^k\mathbb{Z}$. These morphisms are compatible with the functional calculus as $\phi_k(f(h)) = f(\phi_k(h))$ for any function $f \in C(\mathbb{R})$ and $h \in \mathbb{C}\mathbb{Z}$ self-adjoint. The spectrum of $\phi_k(h)$ is a subset of the spectrum of h [LP23, Chap. 3], and therefore all spectral gaps in $\sigma(h)$ are also present in $\sigma(\phi_k(h))$ and are not contaminated by the approximation.

The convergence of the spectral properties along the coherent sequence of subgroups has been demonstrated in [LP23] based on the algebraic scheme by Wolfgang Lück [Lüc94]. Although, the direct limit of the quotient groups $\mathbb{Z}/p^k\mathbb{Z}$ is in general much larger than $\mathbb{Z}$, the quotient morphisms ϕ_k together with the universal property of the limit imply the existence of an injective group morphism ϕ onto a dense subspace of the direct limit [LP23, Chap. 4.1]. One can then verify that any model Hamiltonians taken from the group C^* -algebra of $\mathbb{Z}$ can be delineated in terms of a sequence of finite-dimensional, approximate Hamiltonians with periodic boundary conditions such that the resolvents, density of states, etc., converge to the true bulk limit as $k \rightarrow \infty$ [LP23, Chap. 4.2-4.3].

4.1. The Approximating Algebra for Computation

The approximation of the non-commutative two-torus by finite-dimensional matrix algebras has been developed in [PV80b; LLS01] for rational and irrational parameters by embedding the non-commutative torus into an almost-finite algebra. In general, an *almost-finite (AF) algebra* is generated as the inductive limit of an inductive tower of finite C^* -algebras

Non-commutative torus

$$\mathcal{A} = \varinjlim \mathcal{A}_n, \quad \mathcal{A}_0 \xrightarrow{i_0} \mathcal{A}_1 \xrightarrow{i_1} \dots \xrightarrow{i_{n-1}} \mathcal{A}_n \xrightarrow{i_n} \dots$$

from which finite volume approximations of its subalgebras can be defined by finding explicit representations of the finite algebras and the connecting homomorphisms. Non-commutative tori themselves are not almost-finite, which can be recognised by their K_1 -groups that coincide with their K_0 -groups in contrast to being trivial as for AF algebras. Instead, similar to the introductory case of the group C^* -algebra, they can be embedded in a suitable AF algebra obtained as the limit of finite matrix algebras as first discovered for the irrational case in [PV80b]. The work of [LLS01] contributed the rational case and corroborated the previously observed continuous transition of physical quantities when going from rational to irrational action parameters.

In contrast, in [Pro17] a projective tower of (finite or not) C^* -algebras is used to generate a C^* -algebra as its projective limit

Disorder non-commutative torus

$$\mathcal{A} = \varprojlim \mathcal{A}_n, \quad \mathcal{A}_0 \xleftarrow{p_0} \mathcal{A}_1 \xleftarrow{p_1} \dots \xleftarrow{p_{n-1}} \mathcal{A}_n \xleftarrow{p_n} \dots,$$

that always exists and is essentially unique since the category of C^* -algebras is complete. This strategy aims to have the observable algebra as the limit of such a projective tower of algebras, which might be not finite, but accept canonical finite dimensional representations. As an advantage compared to the inductive tower, the resolvent set of an element from $\mathcal{A}$ is not contaminated by false spectrum while moving down the approximating tower.

Since the observable algebra in [Pro17] is the disordered non-commutative torus, it warrants the employment of two distinct approximations, one for the functions on the disorder configuration and one for the non-commutative torus. In the first step, the disorder configuration is constrained to periodic configurations from which the *periodic approximating algebra* can then be constructed [Pro17, Chap. 4.1-4.2]. Subsequently, in the second step, the finite volume disorder configurations are equipped with periodic group actions for the definition of the *finite volume approximating algebra* [Pro17, Chap. 4.3-4.4].

The projective tower can then be built for a sequence of super-cells with increasing sizes, each of which containing multiples of its predecessors, and a fixed rational flux, such that one has an integer flux in the smallest super-cell and therefore all super-cells. The $*$ -epimorphisms between the individual finite volume approximating algebras then restrict the periodic disorder configurations to the ones that are still periodic on the next smaller super-cell and the translation generators to lower powers [Pro17, Chap. 5.1].

4. Approximate Computational Programme

The projective limit of these finite volume approximating algebras is the disordered non-commutative torus with the chosen rational flux. The cases with irrational flux can be inferred, since the observables constructed from the functional calculus of the generic Hamiltonians are smooth functions with respect to the flux.

Multi- q non-commutative torus

The observable algebra incorporating multi- q spin textures and a constant magnetic field is a matrix algebra of the non-commutative torus, as demonstrated in Chap. 3.1.3. However, as the finite volume approximation is only enacted on the real space lattice and not on the space where the phase torus Fourier generators operate, the approximate scheme from [LLS01; PV80b] is not feasible, and the one from [Pro17] must be employed. Since the coefficient functions on the phase space torus are already periodic, they can be immediately equipped with the periodic action of the finite volume approximating algebra, and the first step is not required. As for the disordered non-commutative torus, the finite volume approximating algebras of the multi- q non-commutative torus are not themselves finite, but they accept canonical finite dimensional representations, since the phase torus functions are only evaluated at a finite number of points for each representation in the continuous family of covariant representations.

Differential calculus

The differential calculus and its representation must be modified to accommodate the finite volume approximations [Pro17, Chap. 4.5]. For instance, the construction of the $*$ -derivations from the continuous torus actions can no longer be performed in case of the translation generators since the finite volume approximations only accept discrete values for phase factors. As a consequence, one has to settle with approximate derivations that can be defined in a canonical way, but do not adhere to the Leibniz rule. Their representations then provide the proper canonical finite volume approximation for the commutator of an observable operator with the position operator, which is itself incompatible with the boundary conditions. The phase $*$ -derivations can still be generated from the continuous torus action, still adhere to the Leibniz rule, and are still represented as the derivation of the smooth representation.

Since the finite volume approximating algebras always require rational approximations, their lattice group action does not act ergodic on the phase torus functions, and thus the trace per unit volume does no longer exactly correspond to the proper canonical trace that contains the integral over the full phase space. Nevertheless, for numerical purposes, the physical trace per unit volume provides a satisfactory numerical accuracy, as increasingly large periodic super-cells increasingly sample the phase space in a sufficient manner.

Section Content

In this section, we present the finite volume approximating algebras, discuss the quantisation condition for the parameters, and set up the family of finite-dimensional covariant representations. With them, we can construct explicitly a projective tower that has the observable algebra with rational flux as its limit. Subsequently, we describe the approximate translation derivations and derive their canonical representations, and then complete the approximate differential calculus by describing the phase derivations and the canonical faithful trace on the approximating algebras.

4.1.1. Finite Volume Approximating Algebra

The finite volume approximating algebra is a C^* -algebra that accepts a finite representation on the physical Hilbert space with imposed periodic boundary conditions. These restrictions imply a quantisation condition on the parameters Θ of the twisted group action.

In the following, we present the finite volume approximating algebra as the universal C^* -algebra of the unitary generators of the phase torus functions and the translations with the additional relations imposed by the periodic boundary conditions. From that, we derive the quantisation condition and discuss the inverse procedure of assigning suitable super-cells to given rational parameters. Then, we present the family of finite Hilbert space representations and check the covariance condition. Eventually, we give an explicit construction of a projective tower of finite volume approximating algebras that has the observable algebra with rational flux as its limit.

Let $N_i \in \mathbb{N}$, $i = 1, \dots, d$, be the sizes of a finite super-cell $V_{\mathbf{N}} \in \mathbb{Z}^d$. We define the corresponding finite volume approximating algebra of the non-commutative torus algebra $\mathcal{A}_{\Theta}$ as the universal C^* -algebra

Finite volume algebra

$$\mathcal{A}_{\Theta}^{\mathbf{N}} = C^*(\langle \mu_1, \dots, \mu_{r+d} \mid \mu_a \mu_b = e^{2\pi i \Theta_{ab}} \mu_b \mu_a, \mu_{r+i}^{N_i} = 1 \rangle),$$

analogous to the description of $\mathcal{A}_{\Theta}$ in Eq. (3.23). The additional constraint of the periodic boundary conditions only applies to the d translation generators $\mu_{r+i} = t_i$, $i = 1, \dots, d$, and, therefore, $\mathcal{A}_{\Theta}^{\mathbf{N}}$ is clearly not finite since the r phase function generators $\mu_i = u_i$, $i = 1, \dots, r$, remain unrestricted. Consistency among the relations can only be achieved for certain quantised values of the parameter matrix Θ with respect to the system sizes N_i . For the $\frac{1}{2}d(d-1)$ magnetic flux parameters in the antisymmetric flux matrix Φ the identity

$$t_j = t_i^{N_i} t_j = e^{2\pi i \Phi_{ij} N_i} t_j t_i^{N_i} = e^{2\pi i \Phi_{ij} N_i} t_j,$$

with $i, j = 1, \dots, d$, implies $\Phi_{ij} N_i \in \mathbb{Z}$ and $\Phi_{ij} N_j = -\Phi_{ji} N_j \in \mathbb{Z}$. For the rd multi- q texture parameters in the matrix θ one has similarly

$$u_j = t_i^{N_i} u_j = e^{-2\pi i \theta_{ji} N_i} u_j t_i^{N_i} = e^{-2\pi i \theta_{ji} N_i} u_j,$$

with $i = 1, \dots, d$ and $j = 1, \dots, r$, which requires $\theta_{ji} N_i \in \mathbb{Z}$. This condition can also be obtained on the level of the phase torus functions $f \in C(T^r)$ that are generated by the u_j , $j = 1, \dots, r$. There it follows from the group action by $f = t_i^{N_i} f = \alpha_{N_i \hat{e}_i}(f)$ with $\alpha_{N_i \hat{e}_i}(f)(\varphi_j) = f(\varphi_j - 2\pi \theta_{ji} N_i)$. The entries of the parameter matrix Θ therefore need to satisfy the quantisation conditions

$$\Theta_{r+i, r+j} N_i \in \mathbb{Z}, \quad \Theta_{r+i, r+j} N_j \in \mathbb{Z} \quad \text{for } i, j = 1, \dots, d \quad \text{and} \quad (4.1)$$

$$\Theta_{r+j, i} N_i \in \mathbb{Z} \quad \text{for } i = 1, \dots, r \quad \text{and } j = 1, \dots, d. \quad (4.2)$$

For a given multi- q texture with parameter matrix $\theta \in M_{r \times d}(\mathbb{Q})$ one can always find a super-cell with sizes $N_1, \dots, N_d$ such that these requirements are met: If the θ_{ij} coefficients are rational, they can respectively be expressed with co-prime integers $a_{ij}, b_{ij} \in \mathbb{Z}$, such

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that $\theta_{ij} = \frac{a_{ij}}{b_{ij}}$. For each real space dimension, $j = 1, \dots, d$, there exists an N_j such that for each $i = 1, \dots, r$ there is an $m_{ij} \in \mathbb{Z}$ with $m_{ij}b_{ij} = N_j$. The smallest such N_j is the least common multiple of the b_{ij} , $i = 1, \dots, r$. Then we have $N_j\theta_{ij} = m_{ij}a_{ij} \in \mathbb{Z}$, in other words, $\theta_{ij}N_j \in \mathbb{Z}$. To accommodate additionally a magnetic field with rational flux matrix $\Phi \in M_d(\mathbb{Q})$, $\Phi_{ij} = \frac{c_{ij}}{d_{ij}}$, the smallest N_j need to be the least common multiple of the b_{ij} , $i = 1, \dots, r$, as well as the d_{ij} , $i = 1, \dots, d$, and d_{ji} , $i = 1, \dots, d$.

Balanced presentation In the following, we will only consider the case $N_j = 2L + 1$ for all $j = 1, \dots, d$ with $L \in \mathbb{N}$, which restricts the possibilities of the parameters to

$$\Theta_{ab} = \frac{n_{ab}}{2L + 1}, n_{ab} \in \mathbb{Z}. \quad (4.3)$$

We choose the corresponding finite super-cell to be balanced, which then refers to a cube V_L of the cardinality $|V_L| = (2L + 1)^d$ centred at the origin such that $|m_i| \leq L$, $i = 1, \dots, d$. This guarantees the property that $\mathbf{m} \in V_L$ always implies $-\mathbf{m} \in V_L$. Let us introduce some handy notation as used in [Pro17, Chap. 4.3.], by considering the following exact sequence of Abelian groups:

$$0 \longrightarrow ((2L + 1)\mathbb{Z})^d \xrightarrow{i} \mathbb{Z}^d \xrightleftharpoons[s]{ev} (\mathbb{Z}/(2L + 1))^d \longrightarrow 0. \quad (4.4)$$

We denote the quotient group by $\hat{\mathbb{Z}}^d$ and the class of an element $\mathbf{m} \in \mathbb{Z}^d$ by $\hat{\mathbf{m}}$. We choose the map s in such a way, that the image of a class $\hat{\mathbf{m}}$ is the unique point $\mathbf{n} \in V_L$ such that $\hat{\mathbf{n}} = \hat{\mathbf{m}}$. This map is not a homomorphism.

The choice of a balanced super-cell simplifies the presentation of the corresponding finite volume approximating algebra $\mathcal{A}_\Theta^L$. The finite number of translation elements $t^{\mathbf{m}}$, $\mathbf{m} \in V_L$, have the simple conjugated form $(t^{\mathbf{m}})^* = t^{-\mathbf{m}}$ and the commutation relation

$$t^{\mathbf{m}}t^{\mathbf{n}} = e^{4\pi i(\mathbf{m} \wedge \Phi \mathbf{n})} t^{\mathbf{n}}t^{\mathbf{m}} = e^{2\pi i(\mathbf{m} \wedge \Phi \mathbf{n})} t^{s(\widehat{\mathbf{m} + \mathbf{n}})}.$$

A generic element of $\mathcal{A}_\Theta^L$ can thus be presented as

$$a = \sum_{\mathbf{m} \in V_L} a_{\mathbf{m}} \otimes t^{\mathbf{m}} \quad (4.5)$$

with the familiar form of the product and conjugation

$$ab = \sum_{\mathbf{m} \in V_L} \sum_{\mathbf{n} \in V_L} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{s(\widehat{\mathbf{m} - \mathbf{n}})}) \otimes t^{\mathbf{m}}, \quad (4.6)$$

$$a^* = \sum_{\mathbf{m} \in V_L} \alpha_{\mathbf{m}}(a_{-\mathbf{m}}^*) \otimes t^{\mathbf{m}}. \quad (4.7)$$

While Eq. (4.5) showcases again by the coefficients $a_{\mathbf{m}} \in C(T^r)$, that $\mathcal{A}_\Theta^L$ is not finite, the coefficients of the product for a fixed $\varphi \in T^r$ only depend on the value of the first coefficient at φ and the values of the second coefficients at the finite number of translates $\tau_{\mathbf{m}}\varphi \in T^r$, $\mathbf{m} \in V_L$. This allows for the finite canonical representations presented in the next paragraph.

4.1. The Approximating Algebra for Computation

The canonical Hilbert space on the finite super-cell V_L is $\ell^2(V_L)$. By restricting the domain for the family of covariant $*$ -representations $\pi_\varphi^\times$ of $\mathcal{A}_\Theta$ on $\ell^2(\mathbb{Z}^d)$, we obtain the finite covariant $*$ -representations $\hat{\pi}_\varphi^\times: \mathcal{A}_\Theta^L \rightarrow \mathcal{B}(\ell^2(V_L))$ that represent a generic element $a = \sum_{\mathbf{m} \in V_L} a_{\mathbf{m}} \otimes t^{\mathbf{m}}$ as

Finite representation

$$\hat{\pi}_\varphi^\times(a) = \sum_{\mathbf{n}, \mathbf{m} \in V_L} (\alpha_{-\mathbf{n}} a_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A, \quad (4.8)$$

where $\hat{U}_{\mathbf{m}}^A$ is the dual magnetic translation operator on the finite lattice with periodic boundary conditions. The finite representations generate the finite super-cell models with periodic boundary conditions that are commonly used in super-cell computations of condensed matter systems. They are clearly no longer faithful, since the representation of a function $f \in C(T^r)$ is already zero if f is zero at the finite set of points $V_L \varphi = \{\tau_{\mathbf{m}} \varphi | \mathbf{m} \in V_L\}$. The covariance condition however is still satisfied, for the magnetic translation operators on the finite lattice with periodic boundary conditions one has

$$\hat{V}_{\mathbf{m}}^A \hat{\pi}_\varphi^\times(a) \hat{V}_{\mathbf{m}}^{A^{-1}} = \hat{\pi}_\varphi^\times(\tau_{-\mathbf{m}} a).$$

The group quotient map $\mathbb{Z}^d \rightarrow \hat{\mathbb{Z}}^d$ established by the short exact sequence Eq. (4.4) induces an $*$ -epimorphism

Connecting morphisms

$$\hat{p}: \mathcal{A}_\Theta \rightarrow \mathcal{A}_\Theta^L \quad t_i \mapsto t_i^L \quad \text{with} \quad (t_i^L)^{2L+1} = 1 \quad (4.9)$$

from the observable algebra to the finite volume approximating algebra with super-cell V_L [Pro17, Lem. 4.20]. A generic algebra element $a = \sum_{\mathbf{m} \in \mathbb{Z}^d} a_{\mathbf{m}} \otimes t^{\mathbf{m}}$ [Pro17, Prop. 4.22] is consequently mapped to

$$\hat{p}(a) = \sum_{\mathbf{m} \in V_L} \hat{a}_{\mathbf{m}} \otimes t^{\mathbf{m}} \quad \text{with} \quad \hat{a}_{\mathbf{m}} = \sum_{\substack{\mathbf{n} \in \mathbb{Z}^d \\ \hat{\mathbf{n}} = \mathbf{m}}} a_{\mathbf{n}}. \quad (4.10)$$

There are analogous $*$ -epimorphisms $\hat{p}': \mathcal{A}_\Theta^{L'} \rightarrow \mathcal{A}_\Theta^L$ between finite volume approximating algebras with compatible sizes, i.e. $(2L+1) = c(2L'+1)$ for some $c \in \mathbb{N}$ odd.

With this description of the finite volume approximating algebras $\mathcal{A}_\Theta^L$ and their connecting morphisms, we can now explicitly construct the projective tower that has the infinite volume algebra $\mathcal{A}_\Theta$ (with rational parameters) as its projective limit [Pro17, Chap. 5.1]. Let Θ adhere to Eq. (4.3) for a super-cell of size $2L_0+1$ and let us consider the increasing sequence $(L_n)_{n \in \mathbb{N}_0}$ with $L_{n+1} = cL_n + \frac{c}{2} - \frac{1}{2}$, $c \in \mathbb{N}$ odd, such that $2L_{n+1}+1 = c(2L_n+1)$. Then, we can generate a projective tower of C^* -algebras

Projective tower

$$\mathcal{U}_d^{L_0} \xleftarrow{\hat{p}_0} \mathcal{U}_d^{L_1} \xleftarrow{\hat{p}_1} \dots \xleftarrow{\hat{p}_{n-1}} \mathcal{U}_d^{L_n} \xleftarrow{\hat{p}_n} \dots$$

with $\mathcal{U}_d^L = C^*(\langle t_1^L, \dots, t_d^L \mid t_i^L t_j^L = e^{2\pi i \Phi_{ij}} t_j^L t_i^L, (t_i^L)^{2L+1} = 1 \rangle)$.

The limit $\varprojlim \mathcal{U}_d^{L_n}$ is then generated by the coherent sequences $t_i = \{t_i^{L_0}, t_i^{L_1}, \dots\}$, $i = 1, \dots, d$, that are unitary operators themselves which obey the commutation relation $t_i t_j = e^{2\pi i \Phi_{ij}} t_j t_i$. Therefore, by the universal property, they generate precisely the

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universal C^* -algebra $C^*(\langle t_1, \dots, t_d \mid t_i t_j = e^{2\pi i \Phi_{ij}} t_j t_i \rangle)$. Together with the unitary generators $u_1, \dots, u_r$ of the continuous functions on the phase torus T^r and their commutation relations with the translation generators, we obtain the projective tower

$$\mathcal{A}_\Theta^{L_0} \xleftarrow{\hat{p}_0} \mathcal{A}_\Theta^{L_1} \xleftarrow{\hat{p}_1} \dots \xleftarrow{\hat{p}_{n-1}} \mathcal{A}_\Theta^{L_n} \xleftarrow{\hat{p}_n} \dots$$

that recovers the non-commutative torus $\mathcal{A}_\Theta$ as its projective limit $\varprojlim \mathcal{A}_\Theta^{L_n}$. Consequently, the matrix algebras of the finite volume approximating algebras together with their canonical finite dimensional representations provide an appropriate finite approximation of the observable algebra.

For irrational parameters in Θ one can employ a sequence of rational approximations, such as an expansion in terms of continued fractions [LLS01, Sec. 2.2]. In the present case, the Hamiltonian and, thereby, all observables obtained from it by the smooth functional calculus are smooth with respect to the parameters. Thus, we can use the finite volume approximations along the sequence or rational approximations to converge towards the values at the irrational parameters.

4.1.2. Approximate Differential Calculus

The differential calculus on the non-commutative torus needs to be modified to be applicable to the finite volume approximating algebras. In particular, there exists no continuous torus group action on the translation generators since the phases of the generators need to adhere to the quantisation condition. As a consequence, the corresponding $*$ -derivations can only be approximated. In contrast, since the phase function generators are not affected by the finite volume restrictions, their respective $*$ -derivations can still be implemented exactly. The proper trace on the approximating algebra is still the canonical faithful trace from the infinite volume algebra, however, its representation no longer coincides with the physical trace per unit volume and can only be approximated by it. In the following, we present the approximated and exact $*$ -derivations that are defined on the finite volume approximating algebras and derive their form in the representation. Then, we discuss the canonical trace on the algebra and on the representations and the trace per unit volume approximation.

*Phase
derivations*

The r -torus Lie group action on $\mathcal{A}_\Theta$ as defined on the unitary generators of the phase torus functions in Eq. (3.26) can also be defined on the finite volume approximating algebras $\mathcal{A}_\Theta^L$. Therefore, the $*$ -derivations that are defined as the generators of the corresponding $*$ -automorphism group are well-defined on $\mathcal{A}_\Theta^L$ as well. For a generic element $a \in \mathcal{A}_\Theta^L$ they are given by

$$\hat{\partial}_i^u a = \sum_{\mathbf{m} \in V_L} \partial_{\varphi_i} a_{\mathbf{m}} \otimes t^{\mathbf{m}}. \quad (4.11)$$

Their representations in $\ell^2(V_L)$ are therefore given by

$$\hat{\pi}_\varphi^\times(\hat{\partial}_i^u a) = \sum_{\mathbf{n}, \mathbf{m} \in V_L} \partial_{\varphi_i}(\alpha_{-\mathbf{n}} a_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A = \partial_{\varphi_i} \hat{\pi}_\varphi^\times(a). \quad (4.12)$$

4.1. The Approximating Algebra for Computation

In contrast, due to the quantisation condition that restricts the permissible phase factors of the translation generators, the translation derivations cannot be defined this way on $\mathcal{A}_\Theta^L$. Instead, we have to settle for approximate derivations that can be defined in a canonical way by

*Translation
derivations*

$$\hat{\partial}_i^t a = i \sum_{\mathbf{m} \in V_L} m_i a_{\mathbf{m}} \otimes t^{\mathbf{m}}. \quad (4.13)$$

They are not $*$ -derivations in the sense of Def. 3.7, since they do not satisfy the Leibniz rule. Their representations on the physical Hilbert space are however less straight forward. If we consider the representation presented in Eq. (3.36) $\pi_\varphi^\times(\partial_i^t a) = i[\hat{x}_i, \pi_\varphi^\times(a)]$, we find the position operator $\hat{x}_i$ incompatible with the periodic boundary conditions. Instead, we can utilise the following identity

$$s(\hat{n}) = \sum_{\lambda^{2L+1}=1} c_\lambda \lambda^n, \quad \text{for } n \in \mathbb{Z} \quad \text{with} \quad c_\lambda = \begin{cases} \frac{\lambda^{L+1}}{1-\lambda}, & \text{if } \lambda \neq 1 \\ 0, & \text{if } \lambda = 1 \end{cases},$$

which is the discrete Fourier transformation of the sequence of the $2L+1$ complex numbers $c_{-L}, \dots, c_L$ onto the sequence $-L, \dots, L$, as verified in App. A12. Since s is periodic on this interval, we can use it to devise a physical representation on $\ell^2(V_L)$ that is compatible with the periodic boundary conditions as first reported in [Pro17, Prop 4.26]:

$$\hat{\pi}_\varphi^\times(\hat{\partial}_i^t a) = i \sum_{\lambda^{2L+1}=1} c_\lambda \lambda^{\hat{x}_i} \hat{\pi}_\varphi^\times(a) \lambda^{-\hat{x}_i}. \quad (4.14)$$

It is easy to check that this is consistent by plugging in the expression for $\hat{\pi}_\varphi^\times(a)$:

$$\begin{aligned} & i \sum_{\lambda^{2L+1}=1} c_\lambda \lambda^{n_i} \left(\sum_{\mathbf{n}, \mathbf{m} \in V_L} (\alpha_{-\mathbf{n}} a_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \right) \lambda^{-(n_i - m_i)} \\ &= \sum_{\mathbf{n}, \mathbf{m} \in V_L} \left(i \sum_{\lambda^{2L+1}=1} c_\lambda \lambda^{m_i} \right) (\alpha_{-\mathbf{n}} a_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \\ &= \sum_{\mathbf{n}, \mathbf{m} \in V_L} m_i (\alpha_{-\mathbf{n}}(a_{\mathbf{m}}))(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \\ &= \hat{\pi}_\varphi^\times(\hat{\partial}_i^t a). \end{aligned}$$

The last missing component is the appropriate trace for the finite-volume approximating observable algebra $\mathcal{A}^L = M_2(\mathbb{C}) \otimes \mathcal{A}_\Theta^L$. Since the trace on the observable algebra from Eq. (3.30) is itself given in terms of the Fourier coefficients of the torus function at the origin and since those are unaffected by the approximation, we obtain the analogue expression for typical elements of the finite-volume approximating algebra [Pro17, Def. 4.23]

Trace

$$\hat{\mathcal{T}}(a) = \int_{T^r} \frac{d\varphi}{(2\pi)^r} \text{tr}(a_0). \quad (4.15)$$

4. Approximate Computational Programme

On the finite representations it is therefore given by [Pro17, Prop. 4.26]

$$\hat{\mathcal{T}}(a) = \int_{T^r} \frac{d\varphi}{(2\pi)^r} \text{tr} \langle 0 | \hat{\pi}_{\varphi}^{\times}(a) | 0 \rangle. \quad (4.16)$$

The significant difference to the trace on the full observable algebra is, that it does no longer correspond to a trace per unit volume. Since the translation action τ describing rational rotations is not ergodic on T^r , we do not have access to Birkhoff's ergodic theorem again. However, T^r is still invariant under the action, which implies

$$\hat{\mathcal{T}}(a) = \int_{T^r} \frac{d\varphi}{(2\pi)^r} \frac{1}{|V_L|} \sum_{\mathbf{m} \in V_L} \text{tr} \langle \mathbf{m} | \hat{\pi}_{\varphi}^{\times}(a) | \mathbf{m} \rangle.$$

For increasing volume, the expression under the phase integral starts to self-average and become independent of φ . Therefore, for our numerical evaluation we omit the phase space average and merely compute the finite trace per unit volume

$$\hat{\mathcal{T}}_{V_L}^{\varphi}(a) = \frac{1}{|V_L|} \sum_{\mathbf{m} \in V_L} \text{tr} \langle \mathbf{m} | \hat{\pi}_{\varphi}^{\times}(a) | \mathbf{m} \rangle \quad (4.17)$$

for one fixed phase space origin φ . In the limit of $L \rightarrow \infty$ ergodicity is restored and (4.17) converges to the trace in the non-commutative torus. We argue that the finite trace per unit volume is physically motivated, as long as there is no physical averaging mechanism.

4.2. Canonical Finite Volume Algorithms

By implementing the representations of the finite volume approximating algebra for computation, we gain access to algorithms for the numerical approximations of physical quantities. In this work, the focus lies in particular on the Chern numbers and the Orbital Magnetisation.

Algorithm For a given model in dimension d which includes the model parameters λ_{hop} and λ_{xc} , and the multi- q texture $\hat{\mathbf{n}}$ of the tight-binding Hamiltonian Eq. (3.60) the computation of a numerical approximation to a physical quantity takes the following steps:

1. Choose system size $N = 2L + 1$, texture parameters θ and flux parameters Φ (such that the quantisation condition Eq. (4.3) is met), and phase φ at the origin site of the lattice.
2. Construct $2N^d$ -dimensional vector space.
3. Set up the Hamiltonian as a $(2N^d \times 2N^d)$ -matrix with periodic boundary conditions applied to nearest neighbours.
4. Diagonalise the Hamiltonian.
5. Compute observables using the spectral theorem.

6. Evaluate the phase derivations approximately as difference quotients and the translation derivations using the representation Eq. (4.14)

7. Evaluate the trace as matrix trace normalised by the system volume $|V_L| = N^d$.

This procedure follows along the lines of [Pro17, Chap. 5.2]. In this section, we present the explicit expressions for the finite approximation of physics formulas and discuss the details of their implementation.

Section Content

4.2.1. Physics Formulas

The formulas that describe physical quantities are expressed as correlation functions which are traces of algebra elements constructed from the Hamiltonian $h \in \mathcal{A}$ using the functional and differential calculus:

General formulas

$$\mathcal{T}\left(\partial^{\alpha_1} G_1(h) \partial^{\alpha_2} G_2(h) \dots\right), \quad (4.18)$$

where ∂^{α_i} denote the $*$ -derivations with the multi-indices α_i , and the functions $G_i : \mathbb{R} \rightarrow \mathbb{C}$ are smooth on the spectrum $\sigma(h)$. In particular, in case of the Chern numbers and Orbital Magnetisation these functions are the identity and the indicator function $\chi(\cdot \leq E_F)$ with Fermi energy $E_F \notin \sigma(h)$ positioned in a spectral gap such that we obtain the Fermi projection p_F .

If the Hamiltonian $h \in \mathcal{A}$ has rational parameters Θ , we can use the $*$ -epimorphism from Eq. (4.9) to project it to $\hat{h} := \hat{p}(h) \in \mathcal{A}^L$ in the finite volume approximating algebra with appropriate super-cell size. For a Hamiltonian in the canonical form with coefficients as established in Eq. (3.64), $\hat{h}$ has the same coefficients as h . The formulas for the physical quantities can then be approximated by

Approximate formulas

$$\hat{\mathcal{T}}\left(\hat{\partial}^{\alpha_1} G_1(\hat{h}) \hat{\partial}^{\alpha_2} G_2(\hat{h}) \dots\right). \quad (4.19)$$

The functions are smooth over $\sigma(\hat{h})$, because $\sigma(\hat{h}) \subset \sigma(h)$. In the next section Sec. 4.3, we derive an upper bound for the error introduced by this restriction. Here, we give the explicit formulas for the numerical computation of the Chern numbers and the Orbital Magnetisation using the finite trace per unit volume on top of the approximations discussed above.

Let $h, p \in M_2(\mathcal{A}^L)$ denote the Hamiltonian and a Fermi projection in the finite volume approximate algebra. The approximate formula for the n th Chern numbers as introduced in Eq. (3.51) can be expressed as

Chern numbers

$$\widehat{Ch}_I^\varphi(p) = \frac{(2\pi i)^n}{n!} \sum_{\sigma \in S_{2n}} (-1)^\sigma \frac{1}{|V_L|} \sum_{\mathbf{m} \in V_L} \text{tr} \langle \mathbf{m} | \hat{\pi}_\varphi^\times(p) \hat{\pi}_\varphi^\times(\hat{\partial}_{\sigma_1} p) \dots \hat{\pi}_\varphi^\times(\hat{\partial}_{\sigma_{2n}} p) | \mathbf{m} \rangle. \quad (4.20)$$

For the orbital magnetisation Eq. (3.67) the approximate expression is given by

Orbital Magnetisation

$$\begin{aligned} \hat{M}_{\text{orb}}^z{}^\varphi &= \frac{e}{\hbar} \text{Im} \frac{1}{|V_L|} \sum_{\mathbf{m} \in V_N} \text{tr} \langle \mathbf{m} | \hat{\pi}_\varphi^\times(p) \hat{\pi}_\varphi^\times(\hat{\partial}_1^t p) \hat{\pi}_\varphi^\times(h) \hat{\pi}_\varphi^\times(\hat{\partial}_2^t p) \\ &\quad + \hat{\pi}_\varphi^\times(h) \hat{\pi}_\varphi^\times(p) \hat{\pi}_\varphi^\times(\hat{\partial}_1^t p) \hat{\pi}_\varphi^\times(\hat{\partial}_2^t p) - 2\mu \hat{\pi}_\varphi^\times(p) \hat{\pi}_\varphi^\times(\hat{\partial}_1^t p) \hat{\pi}_\varphi^\times(\hat{\partial}_2^t p) | \mathbf{m} \rangle. \end{aligned} \quad (4.21)$$

4. Approximate Computational Programme

4.2.2. Implementation

The individual components of the physics formulas are implemented separately and combined at the end to obtain a numerical value. In the introduction of this Sec. 4.2, a broad overview over this process is given. Here, we discuss the details of the specific implementation and refer to App. B for the corresponding Python code used for the calculations performed in this work (for 3q-textures in dimension $d = 2$).

Hilbert space At first the $2N^d$ -dimensional complex Hilbert space $\mathcal{H} = \mathbb{C}^{2N^d}$ is constructed with the labels

$$\mathcal{H} = \left\{ |m_1, \dots, m_d, s\rangle \mid 1 \leq m_i \leq N, 1 \leq s \leq 2 \right\}, \quad (4.22)$$

and implemented as in App. B1.

Hamiltonian The Hamiltonian can be defined on $\mathcal{H}$ as the complex $2N^d \times 2N^d$ -matrix

$$\begin{aligned} H^\varphi = & - \sum_{m_1, \dots, m_d=1}^N \sum_{s=1}^2 \sum_{k=1}^c \lambda_{\text{hop}}(\mathbf{m}, \mathbf{m} + \mathbf{d}_k) |m_1, \dots, m_d, s\rangle \langle m_1 + d_1^k, \dots, m_d + d_d^k, s| \\ & + \sum_{m_1, \dots, m_d=1}^N \sum_{s,t=1}^2 \sum_{i=1}^3 \lambda_{\text{xc}} \sigma_{st}^i n_i(\mathbf{x}_{\mathbf{m}}, \varphi) |m_1, \dots, m_d, s\rangle \langle m_1, \dots, m_d, t| \end{aligned} \quad (4.23)$$

where $d_1^k, \dots, d_d^k$, $k = 1, \dots, c$, encode the relative position of the c nearest neighbours as introduced in Sec. 3.4.1 while maintaining periodic boundary conditions, and σ^i , $i = 1, \dots, 3$, denotes the i th Pauli matrix. The implementation is given in App. B2. The Hamiltonian H^φ is the finite representation $\hat{\pi}_\varphi^\times(\hat{h})$ of the element $\hat{h} \in \mathcal{A}^L$ in the finite volume approximating algebra of the physical observable algebra $\mathcal{A}$.

Spectral projection Next, we need to determine the representation of the spectral projection $p_F \in \mathcal{A}^L$ as defined in Eq. (3.37). Since the representations $\hat{\pi}_\varphi^\times$ are homomorphisms, they commute with the functional calculus

$$\hat{\pi}_\varphi^\times(p_F) = \hat{\pi}_\varphi^\times(\chi(\hat{h} \leq E_F)) = \chi(\hat{\pi}_\varphi^\times(\hat{h}) \leq E_F),$$

and thus we can use the spectral theorem to construct the representation of the spectral projection from the eigenvectors and eigenvalues of the Hamiltonian $H^\varphi = \hat{\pi}_\varphi^\times(\hat{h})$. Let ϵ_i and $|\epsilon_i\rangle$, $i = 1, \dots, 2N^d$, be the (energy) eigenvalues and eigenvectors of H^φ in $\mathcal{H}$, then the spectral projection can be computed as

$$P_F^\varphi = \chi(H^\varphi \leq E_F) = \sum_{i=1}^{2N^d} \chi(\epsilon_i \leq E_F) |\epsilon_i\rangle \langle \epsilon_i|. \quad (4.24)$$

The functions for the diagonalisation and the projection are given in App. B3. Within the code, a distinction is made between the Fermi projection, which projects onto states below a specified Fermi energy E_F and the spectral projection, which projects onto a predetermined number of occupied states (fixed integrated density of states). Both versions are useful for different use cases: The Fermi projection allows for sweeping

over an energy range, while the spectral projection facilitates following a gap over a system/texture parameter range.

The translation derivations $\hat{\partial}_i^t P_F^\varphi := \hat{\pi}_\varphi^\times(\hat{\partial}_i^t p_F)$ can be implemented immediately following the expression given in Eq. (4.14). The entries of the projection matrix are multiplied by the difference between the corresponding site labels with periodic boundary conditions:

*Differential
Calculus*

$$\hat{\partial}_i^t P_F^\varphi = i \sum_{|\mathbf{m}, s\rangle, |\mathbf{n}, t\rangle \in \mathcal{H}} s(\widehat{m_i - n_i}) \langle \mathbf{m}, s | P_F^\varphi | \mathbf{n}, t \rangle |\mathbf{m}, s\rangle \langle \mathbf{n}, t|. \quad (4.25)$$

The periodic coefficient $s(\widehat{m_i - n_i}) = ((m_i - n_i + L \bmod N) - L)$ is hereby evaluated as $(m_i - n_i) - \lfloor \frac{m_i - n_i}{0.5N} \rfloor N$ which is equivalent in the cases $-N < m_i - n_i < N$ and more efficient. The phase derivations $\hat{\partial}_i^u P_F^\varphi := \hat{\pi}_\varphi^\times(\hat{\partial}_i^u p)$ which are given by derivatives with respect to φ_i can be implemented as difference quotient using finite steps $\Delta\varphi > 0$ to approximate

$$\hat{\partial}_i^u P_F^\varphi = \lim_{\Delta\varphi \rightarrow 0} \frac{P_F^{\varphi_i + \Delta\varphi} - P_F^\varphi}{\Delta\varphi}. \quad (4.26)$$

For this, it is important to guarantee the projections at φ and $(\varphi_1, \dots, \varphi_i + \Delta\varphi, \dots, \varphi_r)$ have the same rank. Therefore, a fixed filling is achieved by using the spectral projection or modifying the Fermi energy of the displaced Fermi projection. The python code is presented in App. B4. The trace per unit volume is further implemented as the normalised trace

$$\hat{\mathcal{T}}_{V_L}(\cdot) = \frac{1}{|V_L|} \sum_{|\mathbf{m}, s\rangle \in \mathcal{H}} \langle \mathbf{m}, s | \cdot | \mathbf{m}, s \rangle, \quad (4.27)$$

as seen in App. B5.

The calculation of the approximate Chern numbers can then be performed by computing the trace of the right combination of the projection and its derivations as seen in Eq. (4.20). For efficiency, several matrix products can be avoided by combining each term (corresponding to permutation σ) with its complex conjugate (that corresponds to its transposition and therefore to the reverse permutation $r(\sigma)$). If the sign of this permutation is negative, the imaginary part remains, whereas if the sign is positive the real part remains. This alternates with $n = |I|/2$:

Chern numbers

$$\widehat{Ch}_I^\varphi(p) = \frac{(2\pi i)^n}{n!} \begin{cases} 2i \operatorname{Im} X, & \text{for } n \bmod 2 = 1 \\ 2 \operatorname{Re} X, & \text{for } n \bmod 2 = 0 \end{cases} \quad (4.28)$$

$$X = \frac{1}{|V_L|} \sum_{\mathbf{m}, s \in \mathcal{H}} \langle \mathbf{m}, s | \sum_{\sigma \in R_{2n}} (-1)^\sigma P_F^\varphi \hat{\partial}_{\sigma_1} P_F^\varphi \dots \hat{\partial}_{\sigma_{2n}} P_F^\varphi | \mathbf{m}, s \rangle$$

Here, the set $R_{2n} = S_{2n}/\sim$ with $\sigma \sim r(\sigma)$ denotes the permutations of $2n$ elements modulo reversal. For simplicity, we choose the lexicographically smaller representative. The implementation is presented in App. B6.

4. Approximate Computational Programme

*Orbital
Magnetisation*

The approximate orbital magnetisation is similarly computed and involves additionally the Hamiltonian:

$$\begin{aligned} \frac{\hbar}{e} \hat{M}_{\text{orb}}^z = \text{Im} \frac{1}{|V_L|} \sum_{\mathbf{m}, s \in \mathcal{H}} \langle \mathbf{m}, s | & 2H^\varphi P_F^\varphi \hat{\partial}_1^t P_F^\varphi \hat{\partial}_2^t P_F^\varphi - H^\varphi \hat{\partial}_1^t P_F^\varphi \hat{\partial}_2^t P_F^\varphi \\ & - 2\mu P_F^\varphi \hat{\partial}_1^t P_F^\varphi \hat{\partial}_2^t P_F^\varphi | \mathbf{m}, s \rangle. \end{aligned} \quad (4.29)$$

Here, the identity

$$\begin{aligned} \text{Im} \mathcal{T}(p \partial_1^t p h \partial_2^t p) &= -\text{Im} \mathcal{T}(p \partial_2^t p h \partial_1^t p) = -\text{Im} \mathcal{T}(h \partial_1^t p p \partial_2^t p) \\ &= -\text{Im} \mathcal{T}(h (1-p) \partial_1^t p \partial_2^t p) = \text{Im} \mathcal{T}(h p \partial_1^t p \partial_2^t p - h \partial_1^t p \partial_2^t p) \end{aligned}$$

is used to avoid evaluating redundant matrix products. The corresponding code is given in App. B7.

4.3. Error Bounds

The disparity between the values for the physical quantities computed with the finite-volume approximating algebra and their true values as calculable from the proper observable algebra can be estimated by deriving upper bounds on the error. Indeed, one finds the finite volume approximation converging faster than any inverse power of the volume. However, we need to stress that this only includes the finite-volume approximation as established in Sec. 4.1 with the proper trace from Eq. (4.16) containing the phase average. The finite trace per unit volume of Eq. (4.17) and the numerical approximations discussed in Sec. 4.2, such as the difference quotient, are not included.

Section Content

In this section, we present the error bound of the finite volume approximation with its proof in App. A13. We then discuss the error of our implementation and visualise the convergence with numerical results.

Error bounds

The discrepancy between physics formulas of the form Eq. (4.18) and their approximations of the form Eq. (4.19) can be attributed to two sources: Firstly, the restriction of the algebra elements to the finite volume approximating algebra must be considered. Secondly, the approximate formula for the translation derivations must be taken into account. If the Hamiltonian belongs to the smooth subalgebra $\mathcal{A}$, both can be accounted for with the following error estimation:

Theorem 4.1 (Error bounds). *Let $h \in \mathcal{A}$ be a Hamiltonian and $\hat{h} = \hat{p}(h) \in \mathcal{A}^L$ the corresponding element in an appropriate finite volume approximating algebra. Then, for any $K \in \mathbb{N}$, there exists a finite positive constant A_K such that:*

$$\left| \mathcal{T} \left(\partial^{\alpha_1} G_1(h) \dots \partial^{\alpha_n} G_n(h) \right) - \hat{\mathcal{T}} \left(\hat{\partial}^{\alpha_1} G_1(\hat{h}) \dots \hat{\partial}^{\alpha_n} G_n(\hat{h}) \right) \right| \leq \frac{A_K}{(1 + |V_L|)^K},$$

where $G_i : \mathbb{R} \rightarrow \mathbb{C}$ are smooth functions over $\sigma(h)$ and the α_i 's are multi-indices.

The proof of this theorem follows the proof of [Pro17, Thm. 6.4] and is presented in App. A13.

4.3. Error Bounds

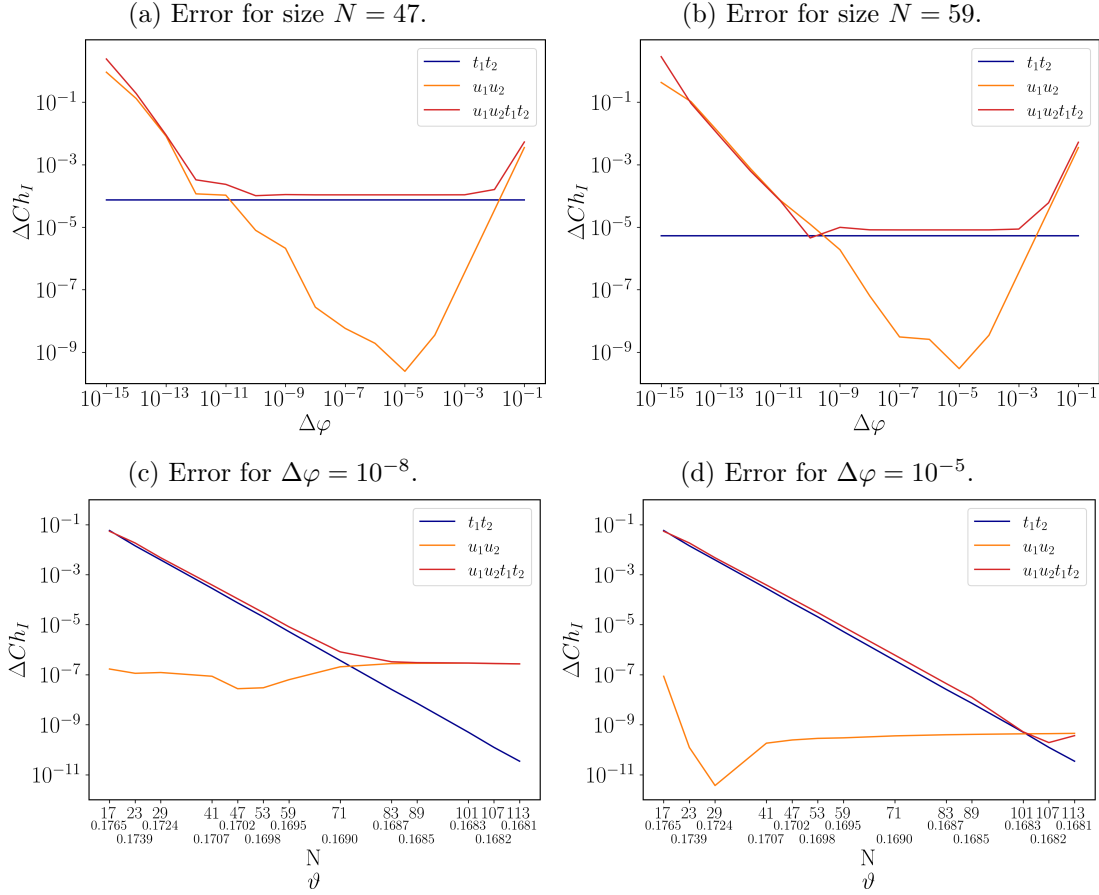


Figure 4.1.: **Error estimates for different sizes and finite differences.** Difference between some indicative Chern number results and their true integer value for different system sizes N and finite differences $\Delta\varphi$. The considered system is coupled to the helical skyrmion lattice with system and texture parameters as indicated in Fig. 5.5 and Fermi energy fixed to Gap U_1 in Fig. 5.5. The pitch in Fig. 4.1(a) is $\vartheta = \frac{8}{47} \approx 0.1702$ and in Fig. 4.1(b) it is $\vartheta = \frac{10}{59} \approx 0.1695$.

For numerical computations implemented as specified in Sec. 4.2.2, the finite trace per unit volume, the finite difference approximation for the phase derivations, the numerical methods used for the diagonalisation, and the machine accuracy introduce additional sources of error. Nevertheless, the computational programme still provides commendable accuracy as can be demonstrated in the example in Fig. 4.1. Here, we choose some approximate Chern numbers out of the results presented in Chap. 5 and plot their difference $\Delta Ch_I = |Ch_I - \widehat{Ch}_I^\varphi|$ to the integral algebraic value against the finite difference step $\Delta\varphi$ and systems size N .

As expected since the Chern number $\widehat{Ch}_{\{t_1 t_2\}}^\varphi$ does not contain the phase derivation, we find it independent of $\Delta\varphi$, while the error of $\widehat{Ch}_{\{u_1 u_2\}}^\varphi$ exhibits a minimum for $\Delta\varphi \approx 10^{-5}$. The error of the mixed second Chern number $\widehat{Ch}_{\{u_1 u_2 t_1 t_2\}}^\varphi$ is bounded from below by the maximum error of the two first Chern numbers.

Numerical results

4. Approximate Computational Programme

Considering the behaviour against the system size N , we find $\widehat{Ch}_{\{t_1 t_2\}}^\varphi$ converging exponentially, which matches the predictions from Thm. 4.1. The Chern number $\widehat{Ch}_{\{u_1 u_2\}}^\varphi$, that only contains the phase derivations, stays largely independent of the system size, but the impact of the insufficient self-averaging property of the finite trace per unit volume for smaller system sizes is visible. Here, the error of $\widehat{Ch}_{\{u_1 u_2 t_1 t_2\}}^\varphi$ also converges with the system size, but it is bounded from below by the precision of $\widehat{Ch}_{\{u_1 u_2\}}^\varphi$.

Disorder *Remark 4.1* (Error bounds with disorder). For the disordered non-commutative torus, those error bounds can also be established using an additional first round of approximations, which deals with the restriction of the disorder configuration to a periodic one [Pro17, Chap. 6]. For this, they require an additional assumption on the Hamiltonians coefficients, which demands that their dependence on the disorder at distant sites decays fast with the distance. Physics formulas that are constructed from smooth functions on the spectrum of the Hamiltonian are applicable for all finite-temperature scenarios and those zero temperature ones, where the Fermi energy is located inside a spectral gap.

However, in the presence of strong disorder, these gaps are usually closed and replaced by mobility gaps where the energy spectrum has a localised character. In [Pro17, Chap. 8], it is proven that even for the case where the functions of the Hamiltonian are only piece-wise continuous and possess discontinuities, which occur inside the mobility gap, the error displays the same kind of rapid decay.

5 | Chern Hierarchy of Multi- q Textures

Multi- q textures coupled to the spin of electrons can introduce topological features into the electronic structure. This has been known to happen in the strong coupling limit $|\lambda_{xc}/\lambda_{hop}| \gg 1$ of two-dimensional skyrmionic crystals in the tight-binding approximation [HEN15]. The emergent topological spectral gaps can be classified in terms of Chern numbers and K -theoretic gap labels by applying the C^* -algebraic formalism developed in Chap. 3 and using the approximate computational programme laid out in Chap. 4.

The pitch of the $1q$ -spin waves that generate the texture by superposition assumes a role similar to that of a magnetic flux in scaling the topological features. From Thm. 3.9 we know, that the integrated density of states (IDS) is a polynomial in the pitch parameters that has the integer Chern labels as coefficients. By computing the density of states (DOS), we can fit the fingerprints of the gaps in the IDS and thereby extract the coefficients with minimal computational effort. As explicitly presented in Chap. 3.4.2, in one dimension the IDS is linear and in two dimensions it is quadratic in the pitch. However, not all Chern numbers and gap labels are accessible from the IDS alone. Using the approximate computational programme we can compute the full hierarchy of Chern numbers for all possible Fermi energies and the formulas yield integer values with high accuracy whenever the Fermi energy is located in a gap of the electronic spectrum. This allows us to determine at which energies the electronic states carry contributions to the different Chern numbers. In particular, we find large compensating contributions at the energies at which the DOS features Van Hove singularities.

A major motivation for this work was the question of the relationship between the topological features in the multi- q textures and the topological features of the electronic spectrum. If the texture is normalised, we can induce a topological transition in its smooth vector field by continuously tuning the relative phase between the spin waves and by continuously adding a constant component in the z direction. This can cause a destructive interference in the superposition at a point in space, leading to a discontinuity in the normalised field, which can be interpreted as a spin flip. Computing the Chern numbers of interest for a fixed gap along such a transition allows us to observe their behaviour at these critical points. We find that not all spectral topological features correspond to the topology of the underlying texture. Although the Chern numbers are invariant under changes that keep the spectral gaps open, we observe that some of them change without visible gap crossings. This is due to the singular nature of the topological transitions of the texture. By introducing a regularisation, the spectral flow through the gaps can be revealed.

*Scaling
behaviour*

Chern hierarchy

*Topological
phase transitions*

Spectral flow

5. Chern Hierarchy of Multi- q Textures

Chapter content

In the author's previous work [Lux+24], the IDS of a helical spin wave superposition, a helical skyrmion lattice, and a vortex lattice were evaluated and analysed. Then, in the author's subsequent work [Pra+24], the Chern numbers, the topological phase transitions, and the spectral flow were explicitly computed for the helical skyrmion lattice. In this chapter, we consider and compare all the above textures and an additional sinusoidal skyrmion texture, the form of which is explicitly presented and visualised in Chap. 1.2.3. This chapter is therefore partially adapted from [Lux+24] and [Pra+24, Chap. 5]. The analysis of the IDS and the computation of the Chern numbers is performed in Sec. 5.1 and Sec. 5.2. In the absence of any two-dimensional topological features in the spin superposition and the vortex lattice, the phase transitions and the spectral flow are computed exclusively for the helical and sinusoidal skyrmion lattices in Sec. 5.3 and Sec. 5.4, respectively. For the whole chapter we assume the absence of external magnetic fields, $\mathbf{B} = 0$.

Preliminary analysis

Before we consider any explicit computations, we want to comment on which topological invariants can be expected to arise from very general arguments. First, we know that all higher Chern numbers carried by all states together are zero. This follows immediately by considering the trivial Fermi projection $P_F = \mathbb{1}$ that projects onto all states and has vanishing derivations. Consequently, for all states contributing to a Chern number there need to exist states with a compensating contribution. Only the zeroth Chern number carried by all states is non-zero. It corresponds to the number of all states, therefore the IDS, and with our choice of normalisation it is 2.

For the $2q$ spin wave superposition in one dimension there are only two Chern numbers, while the electronic system coupled to the $3q$ lattices exhibit eight distinct Chern numbers. Their relations have been explored explicitly in Chap. 3.4.2. Since the vector fields of the two skyrmion lattices are normalised, we can construct two additional analytic projection operators, p and $p^\perp$, that do not exist for the vortex lattice:

$$p = \frac{1}{2}(\mathbb{1}_2 \otimes t^0 - \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}(\boldsymbol{\varphi}) \otimes t^0). \quad (5.1)$$

The idempotence of p depends on the normalisation of the magnetic texture $\hat{\mathbf{n}} \in C^\infty(T^2, S^2)$. Then, the tight-binding Hamiltonian H from Eq. (3.60) is the covariant representation of an element h of the non-commutative torus $C(T^2) \rtimes_\theta^\Phi \mathbb{Z}^2$ tensored with the operators in $M_2(\mathbb{C})$ acting on the internal spin degree of freedom, that can be expressed in terms of p by

$$h/\lambda_{\text{xc}} = (\mathbb{1}_2 \otimes t^0 - 2p) + \epsilon\Delta. \quad (5.2)$$

Here, we assume $\lambda_{\text{xc}} > 0$ and $\epsilon = \lambda_{\text{hop}}/\lambda_{\text{xc}}$, and Δ is the adjacency operator of the lattice which couples nearest neighbours with unit strength, as defined in Eq. (3.62). At $\epsilon = 0$, the Hamiltonian H has a gap at zero energy, referred to as the zero energy gap in the following. For $0 < |\epsilon| \ll 1$, this gap remains open, and the gap projection operator changes continuously as a function of ϵ . For a topological classification of the zero energy gap, we can thus conveniently focus on the limit of $\epsilon \rightarrow 0$. Thereby, we

5.1. Topological Fingerprints in the Integrated Density of States

reduce the situation to the two-band scenario of Eq. (1.32) with $\Sigma = T^2$, as explored in Chap. 1.3.2. The occupied subspace below zero energy belongs to the eigenspace of p with an eigenvalue equal to one, characterised by a perfect anti-alignment of the electron spin with the vector field specified by $\hat{\mathbf{n}}$. We compute the Chern labels

$$n_\emptyset = Ch_\emptyset([p]_0) = 1, \quad (5.3)$$

and

$$n_{\{u_1, u_2\}} = Ch_{\{u_1, u_2\}}([p]_0) = -2\pi i \int_{T^2} \frac{d\varphi}{(2\pi)^2} \frac{1}{8} \text{tr}(\boldsymbol{\sigma} \cdot \hat{\mathbf{n}})[(\boldsymbol{\sigma} \cdot \partial_{\varphi_1} \hat{\mathbf{n}}), (\boldsymbol{\sigma} \cdot \partial_{\varphi_2} \hat{\mathbf{n}})] \quad (5.4)$$

$$= \frac{1}{4\pi} \int_{T^2} d\varphi \hat{\mathbf{n}} \cdot (\partial_{\varphi_1} \hat{\mathbf{n}} \times \partial_{\varphi_2} \hat{\mathbf{n}}) = \deg \hat{\mathbf{n}}. \quad (5.5)$$

All remaining Chern numbers for this gap are zero since p commutes with the position operator. Since the trivial projection $\mathbb{1}_2 \otimes t^0$ has the trace 2 and maps to 0 if paired with any other Chern cocycle, we can also infer that the unoccupied subspace above zero energy, which is the eigenspace of

$$p^\perp = \mathbb{1}_2 \otimes t^0 - p = \frac{1}{2}(\mathbb{1}_2 \otimes t^0 + \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}(\varphi) \otimes t^0), \quad (5.6)$$

carries $n_\emptyset = 1$, $n_{\{u_1, u_2\}} = -\deg \hat{\mathbf{n}}$, and 0 for all remaining Chern numbers. Another relevant quantity is the spin magnetisation which has the expectation value

$$\mathbf{S} = \mathcal{T}(\boldsymbol{\sigma}p) = -\frac{1}{(2\pi)^2} \int_{T^2} d\varphi \hat{\mathbf{n}}(\varphi), \quad (5.7)$$

in units of $\hbar/2$. This reproduces Eq. (1.21) from Sec. 1.2.3.3. The spin magnetisation follows the phase diagrams shown in Fig. 1.4(b) and Fig. 1.6(b) for the respective textures.

5.1. Topological Fingerprints in the Integrated Density of States

The integrated density of states for any spectral gap coincides with the zeroth Chern number and is therefore a polynomial in the pitch parameter of the multi- q texture. The spectral gaps appear as discontinuity lines in IDS plots, and by fitting these fingerprints of the underlying K -theory description with an appropriate polynomial, we gain access to integer coefficients which consist of higher gap labels. This technique was first applied to electronic spin systems coupled to multi- q textures in the author's work [Lux+24]. In this section, we apply the analysis of the IDS to the $2q$ helical spin wave superposition, the $3q$ helical and sinusoidal skyrmion lattices, and the $3q$ vortex lattice.

First, we consider the case of the $2q$ spin wave as described in Chap. 1.2.3.2. There, we give the explicit form of the texture's vector field in Eq. (1.14) and depict an example of the phase space, the two helical spin waves, and their superposition in Fig. 1.2(b).

2q spin wave

5. Chern Hierarchy of Multi- q Textures

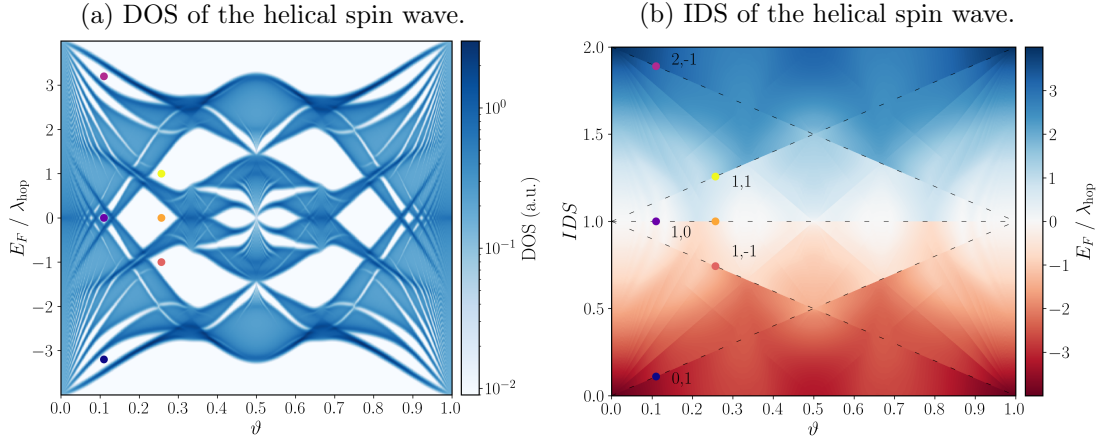


Figure 5.1.: **Spectrum of the helical 2 q spin wave superposition.** DOS (a) and IDS (b) at $k_B T = 0.01 \lambda_{\text{hop}}$ and $\lambda_{\text{xc}} / \lambda_{\text{hop}} = 1$ for a system with $N = 6421$ sites and periodic boundary conditions coupled to the $2q$ spin wave from Eq. (1.14) with $\theta_1 = \vartheta = \frac{i}{N}$, $i = 1, \dots, N-1$, $\theta_2 = 2\theta_1 = 2\vartheta$, and $\varphi_1 = \varphi_2 = 0$. Coloured bullets are used to match some gaps in the DOS with the corresponding line features in the IDS. This figure was adapted from [Lux+24, Fig. 1].

For the case $\theta_1 = \vartheta$, $\theta_2 = 2\vartheta$ the texture is periodic, and we can describe the observable algebra of the corresponding electronic system by $M_2(\mathcal{A}_{\Theta_{2q}})$ as defined in Chap. 3.4.2. Then, the IDS for all spectral gaps is of the form

$$n_\emptyset + n_{\{u,t\}}\vartheta. \quad (5.8)$$

We can diagonalise the finite Hamiltonian from Eq. (4.23) coupled to this spin wave for pitches ϑ in the range $(0, 1)$, to obtain a graph of the DOS and IDS against ϑ . From the scaling behaviour of the gaps in the IDS, we can extract the integer coefficients. In Fig. 5.1, we present the result for a very large system with interpolated spectrum at finite temperature $k_B T = 0.01 \lambda_{\text{hop}}$, such that $\text{DOS}(E_F) = \sum_{i=1}^{2N} \partial_{E_F} f(\epsilon_i - E_F)$ with the Fermi-Dirac distribution $f(\epsilon) = \left(\exp\left(\frac{\epsilon}{k_B T}\right) + 1 \right)^{-1}$. For the qualitative and quantitative analysis, the size of the system can be chosen significantly smaller. The large N was chosen purely to obtain an aesthetic and clear high-resolution picture.

In the DOS depicted in Fig. 5.1(a) the spectrum branches into a fractal shape and gaps open up as ϑ increases from zero. This is an instance of a Hofstadter butterfly [Hof76], where the pitch of the spin waves assumes the role of the magnetic flux. The IDS in Fig. 5.1(b) exhibits clear line features with integer slopes and intercepts that correspond to the spectral gaps in the DOS. The gaps can be grouped by the intercept label $n_\emptyset$ which takes the values 0, 1 and 2. For each of them there exists a sequence of gaps with ascending size of slope $n_{\{u,t\}}$ and decreasing width. This indicates, that there are ϑ states per unit cell at the energies between those gaps. Since the IDS is restricted to above 0 and to below 2, only the centre gap group has gaps with positive and negative slopes.

5.1. Topological Fingerprints in the Integrated Density of States

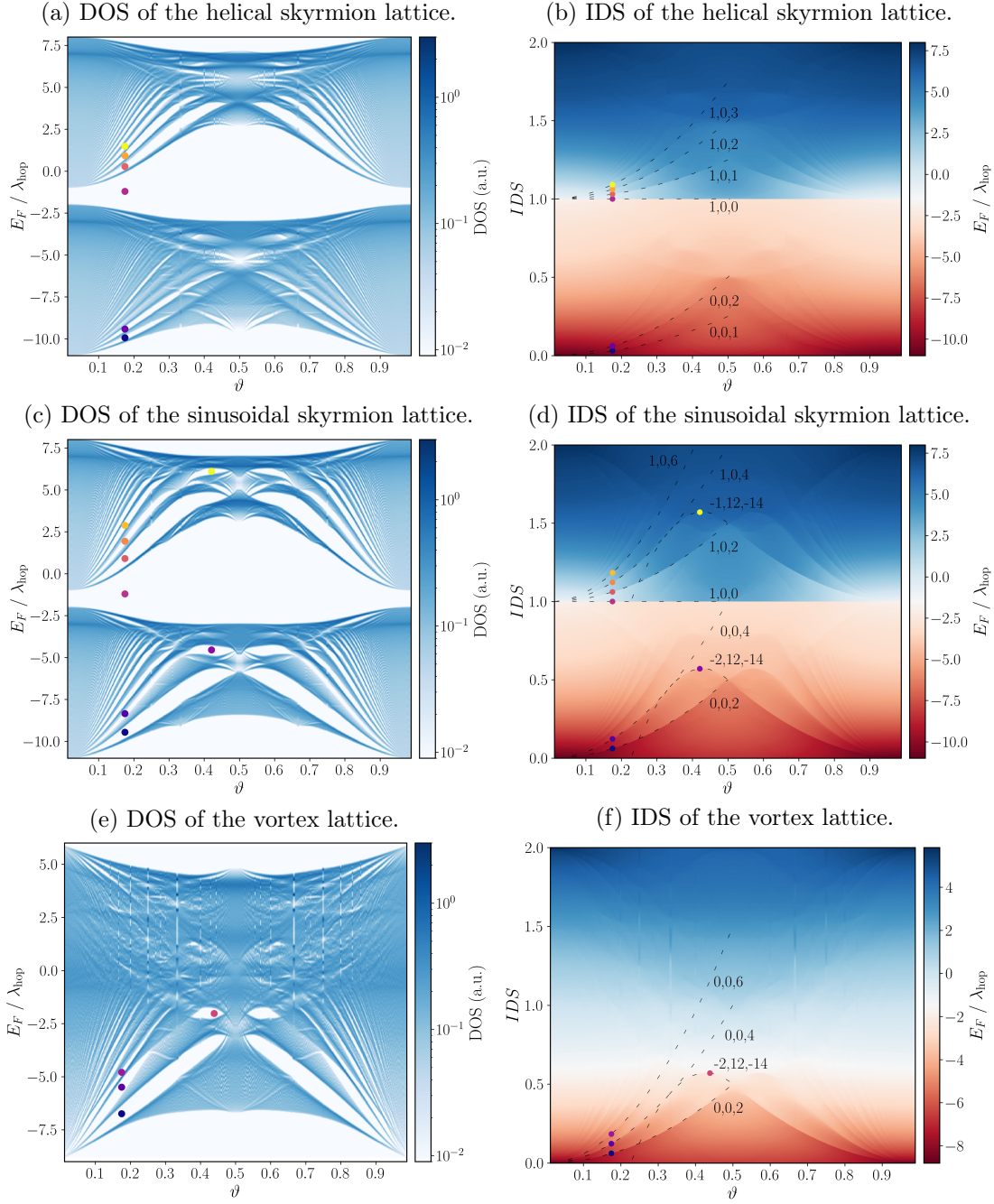


Figure 5.2.: **Spectrum of the 3q skyrmion and vortex lattices.** DOS and IDS at $k_B T = 0.01\lambda_{\text{hop}}$ and $\lambda_{\text{xc}}/\lambda_{\text{hop}} = 5$ for systems with N^2 sites and periodic boundary conditions, where $N \in [19, 79] \cap \mathbb{N}$ and $\vartheta \in (0, 1)$ such that $N\vartheta \in \mathbb{N}$ for some N , coupled to the helical skyrmion texture from Eq. (1.19) in Fig. (a) and (b), the sinusoidal skyrmion texture from Eq. (1.23) in Fig. (c) and (d), and the vortex texture from Eq. (1.25) in Fig. (e) and (f) with $\varphi_1 = \varphi_2 = \varphi_3 = 0$. Coloured bullets are used to match some gaps in the DOS with the corresponding line features in the IDS. The figures (a), (b), (e), and (f) were adapted from [Lux+24, Fig. 2].

5. Chern Hierarchy of Multi- q Textures

$3q$ spin lattices

For $3q$ spin textures, we have the three separate examples introduced in Chap. 1.2.3.3. Two of them are skyrmion lattices with a spin vector field that is the normalisation of the superpositions given in Eq. (1.19) and Eq. (1.23), respectively, and the other one is a vortex lattice with the spin vector field given by the superposition in Eq. (1.25).

In the case of Eq. (1.15), where the three q -vectors sum up to zero, the texture is periodic, and the observable algebra of the corresponding electronic system on a two-dimensional triangular lattice is $M_2(\mathcal{A}_{\Theta_{3q}})$, as defined in Chap. 3.4.2. Here, the real and reciprocal space lattice vectors are of the form in Eq. (1.16), which allows us to define $\mathbf{q}_1 = \vartheta \mathbf{b}_1$, $\mathbf{q}_2 = \vartheta \mathbf{b}_2$, and $\mathbf{q}_3 = \vartheta(-\mathbf{b}_1 - \mathbf{b}_2)$. Therefore, the matrix Θ_{3q} has the components shown in Eq. (3.66). Then, the IDS for all spectral gaps is of the form

$$n_\emptyset + (n_{\{u_1, t_1\}} + n_{\{u_2, t_2\}})\vartheta - n_{\{u_1, u_2, t_1, t_2\}}\vartheta^2. \quad (5.9)$$

As before, we diagonalise the finite Hamiltonian from Eq. (4.23) coupled to the different spin textures for ϑ in the range $(0, 1)$ and obtain a graph of the DOS and IDS against ϑ , from which we can extract the integer coefficients. In Fig. 5.2, we present the interpolated spectrum at finite temperature $k_B T = 0.01 \lambda_{\text{hop}}$ for a range of system sizes, which are chosen to compromise between precision and cost of computation. The total number of sites N^2 in the super-cell (and therefore the dimension of the finite Hilbert space $2N^2$) is comparable to the one chosen in the one-dimensional case, however, the quantisation condition from Eq. (4.2) for ϑ only allows for a significantly smaller number of values in the range $(0, 1)$ for each system size.

Similar to the one-dimensional case, for the DOS depicted in Fig. 5.2 (a), (c), and (e) the spectrum branches into a fractal shape and gaps open up as ϑ increases from zero. For the two skyrmion textures in (a) and (c), the spectrum is divided into two blocks, which is not the case for the vortex texture in (e). This matches our prediction from general arguments and is due to the normalisation of the skyrmion textures' vector fields. The large central gap in the DOS is visible as a prominent horizontal line in the IDS in (b) and (d). Consequently, the central gap possesses the labels $(1, 0, 0)$, meaning $n_\emptyset = 1$, $n_{\{u_1, t_1\}} + n_{\{u_2, t_2\}} = 0$, and $-n_{\{u_1, u_2, t_1, t_2\}} = 0$.

The line features corresponding to the remaining gaps are visibly quadratic in ϑ , and the large gaps that open up for small ϑ can be labelled by $n_\emptyset$, specifying the block, and $-n_{\{u_1, u_2, t_1, t_2\}}$ counting the gaps. We refer to these gaps as connected to the adiabatic limit $\vartheta \rightarrow 0$ of smooth textures. For the helical skyrmion lattice (b) they are labelled by increasing integer numbers, whereas for the sinusoidal skyrmion lattice (d) and the vortex lattice (f) they possess only even integer labels. Since all of them have $n_{\{u_1, t_1\}} + n_{\{u_2, t_2\}} = 0$ as their linear coefficient, there are ϑ^2 or, respectively, $2\vartheta^2$ states per unit cell at the energy levels between these gaps.

Relation to winding number

For the skyrmion lattices this may be explained by the emergent magnetic field picture for smooth textures in analogy with the Landau levels of the ordinary quantum Hall effect. There, the number of states per unit area at each Landau level is proportional to the number of flux quanta per unit area. This can be visualised in symmetric gauge as the states occupying orbits around the flux tubes of the magnetic field [Lau81] [Dav97, Chap. 6.4.2]. In the emergent magnetic field picture, the emergent magnetic field flux

is proportional to the skyrmion winding number, and for finite commensurate ϑ there are $(\vartheta N)^2$ texture unit cells in each super-cell with N^2 lattice unit cells. Therefore, the energy levels in the sinusoidal skyrmion lattice with winding number $\deg \hat{\mathbf{n}} = -2$ would include twice as many states as for the helical skyrmion lattice with winding number $\deg \hat{\mathbf{n}} = 1$. This is, however, not applicable to explain the number of states between the gaps in the vortex lattice with winding number $\deg \hat{\mathbf{n}} = 0$.

There are also gaps opening up towards $\vartheta \rightarrow 0.5$ that exhibit more complex labels. Prominent examples are the gaps in (d) and (f) with labels $(-1, 12, -14)$ and $(-2, 12, -14)$. Since those gaps are not connected to the adiabatic limit of smooth textures and are as such not treatable with commutative geometry, we coin them the *non-commutative spectral gaps*.

Non-commutative gaps

5.2. Full Chern Hierarchy

The multi- q spin textures introduce non-commutativity into the electronic system, manifesting in energy gaps that can be classified by K -theoretic integer labels. In the case of the $2q$ spin wave system, both existing gap labels enter the IDS, and thus can be accessed by analysing the scaling behaviour of the gaps. In contrast, for the $3q$ textures, only four of the gap labels enter, in the form of only three coefficients. In order to obtain the full hierarchy of gap labels, we can extract them from the Chern numbers computed explicitly with the formula in Eq. (3.51) utilising the approximate computational programme described in Chap. 4.

Only for Fermi energies located inside spectral gaps the Chern numbers are defined and the approximation formulas for the labels converge to integers with high accuracy. Nevertheless, scanning over the full range of energies gives valuable insight into which energy states contribute to which Chern numbers. In particular, we find large compensating contributions carried by the states at the van Hove singularities (VHS).

In this section, we present and discuss the explicitly computed Chern numbers and labels for the marked gaps in all the textures of the previous section. Further, we display the Fermi energy dependence for all labels of the $2q$ system and for a selection of main labels, i.e. the zeroth labels $n_\emptyset$, the real- and momentum space first labels $n_{\{u_1, u_2\}}$ and $n_{\{t_1, t_2\}}$, and the mixed space second labels $n_{\{u_1, u_2, t_1, t_2\}}$, for the $3q$ system. The analysis for the skyrmion systems is partially adapted from [Pra+24, Chap. 5.1].

Since we no longer need to compute the IDS, we use a sophisticated approximation method to create high-resolution pictures of the DOS, rather than computing the spectrum via exact diagonalisation. For the remainder of the chapter, we use the *Kernel Polynomial Method* (KPM) [Wei+06], which makes it computationally viable to evaluate much larger supercells, and is especially valuable for two-dimensional and even potentially higher-dimensional systems. For the KPM algorithm, we choose 2048 energy values, 2048 Chebyshev moments, and 10 random states, and use Jackson damping of high-frequency oscillations before the reconstruction of the Chebyshev polynomials.

Kernel Polynomial Method

5. Chern Hierarchy of Multi-q Textures

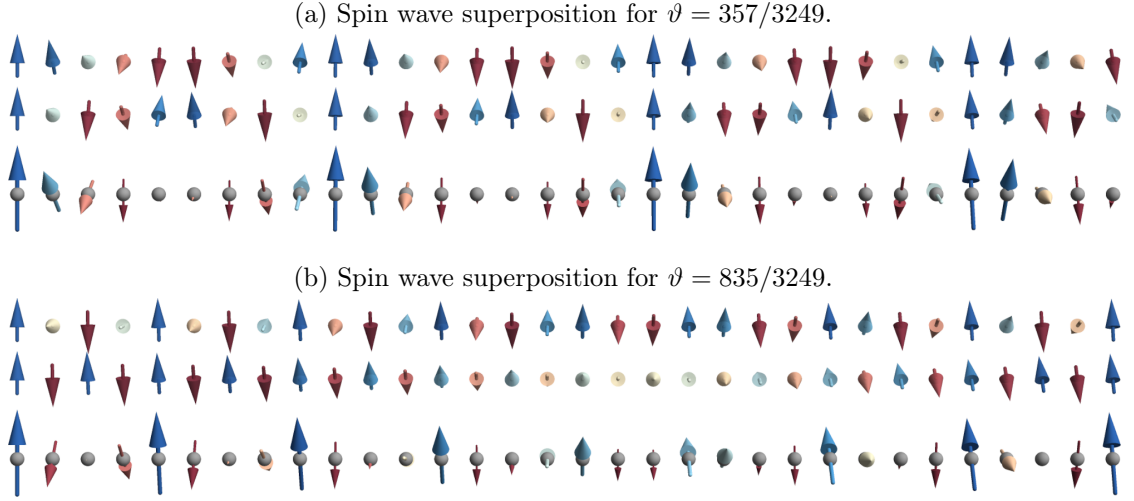


Figure 5.3.: **2q spin wave superposition.** The figure shows 32 sites of the spin wave textures for $\theta_1 = \vartheta$, $\theta_2 = 2\vartheta$, and $\varphi_1 = \varphi_2 = 0$, with $\vartheta = 357/3249$ in (a) and $\vartheta = 835/3249$ in (b), for which the labels were evaluated in Fig. 5.4.

2q spin wave

We evaluate the Chern numbers and extract the labels for a $2q$ spin wave superposition in a system of size $N = 3249$ for the two pitch values at which we placed the coloured bullets before. The correspondingly scaled spin wave superpositions are depicted in Fig. 5.3 and the resulting labels are presented in Fig. 5.4 and Tbl. 5.1. They corroborate the observation on the gap labels we made from Fig. 5.1: The gaps can be grouped into the lower group (L_i) with $n_\emptyset = 0$, the centre group (C_i) with $n_\emptyset = 1$, and the upper group (U_i) with $n_\emptyset = 2$. In each group the gaps are distinguished by the second label $n_{\{u,t\}}$. For the higher ϑ value, we can now see additionally that the gaps L'_2 and C'_{-2} as well as C'_2 and U'_{-2} crossed over each other and changed their order.

For the gaps marked by coloured bullets, the numerical values for the Chern numbers and labels listed in Tbl. 5.1 are very close to their predicted integer values, which indicates great accuracy of our approximation method.

3q skyrmion lattices

Next, we consider the two $3q$ skyrmion textures on a triangular lattice with a system size of $N = 57$ for two pitch values, respectively. The corresponding helical skyrmion lattices are depicted in Fig. 5.7 with the resulting Chern numbers and labels compiled in Fig. 5.5 and Tbl. 5.2, and the sinusoidal skyrmion lattices are shown in Fig. 5.8 with the results presented in Fig. 5.6 and Tbl. 5.3. Again, the numerical results corroborate the gap labels we extracted visually from the IDS in Fig. 5.2. The numerically determined values for the labels have good accuracy that seems to decrease with the narrowness of the gaps.

The centre gaps C_0 in Fig. 5.5 and in Fig. 5.6 fulfil our predictions from general arguments in having the labels $n_\emptyset = 1$, $n_{\{u_1, u_2\}} = \deg \hat{\mathbf{n}}$, and otherwise 0. Here, the difference between the two textures is very apparent, as the helical skyrmion lattice has winding number $\deg \hat{\mathbf{n}} = 1$ whereas the sinusoidal skyrmion lattice has winding number $\deg \hat{\mathbf{n}} = -2$.

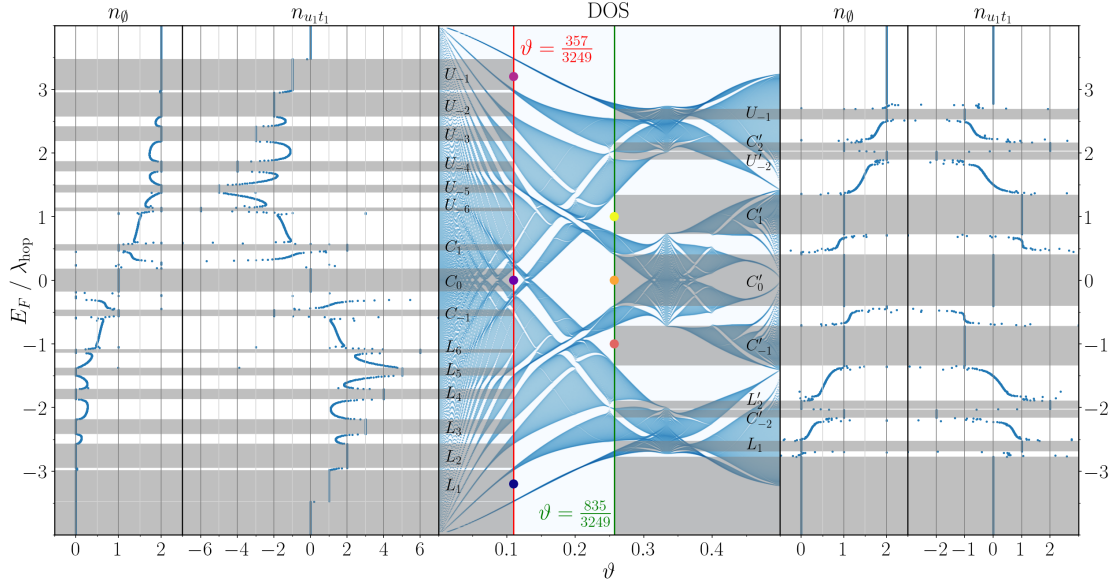


Figure 5.4.: **Main gap labels of the spin wave.** We evaluate the gap labels for $\lambda_{\text{xc}}/\lambda_{\text{hop}} = 1$ in a system of size $N = 3249$ at $\vartheta = \frac{357}{3249}$ and $\vartheta = \frac{835}{3249}$ with $\theta_1 = \vartheta$, $\theta_2 = 2\vartheta$, $\varphi_1 = \varphi_2 = 0$, and $\Delta\varphi = 10^{-5}$ for Fermi energies in the full energy range. The DOS is computed via KPM for a system of size $N = 160000$ with $\vartheta = (1 + \sqrt{N}i)/N$, $i \in \{0, \dots, \sqrt{N}/2\}$. For the gaps marked with coloured bullets all Chern numbers and labels are listed in Tbl. 5.1.

(a) Chern numbers at $\vartheta = \frac{357}{3249}$ and $\vartheta = \frac{835}{3249}$.						
Ch_J	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●
Ch_{n_0}	0.10987996	1.00000000	1.89012004	0.74299785	1.00000000	1.25700215
$Ch_{n_{u_1 t_1}}$	1.00000000	-0.00000000	-1.00000000	-1.00000000	0.00000000	1.00000000

(b) Labels of K -theory class in $K_0(\mathcal{A}) = \mathbb{Z}^2$.						
n_J	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●
n_0	$0+3.5 \times 10^{-11}$	$1+9.1 \times 10^{-13}$	$2-3.4 \times 10^{-11}$	$1+3.6 \times 10^{-10}$	$1-4.9 \times 10^{-13}$	$1-3.6 \times 10^{-10}$
$n_{u_1 t_1}$	$1-3.2 \times 10^{-10}$	$0-8.3 \times 10^{-12}$	$-1+3.1 \times 10^{-10}$	$-1-1.4 \times 10^{-9}$	$0+1.9 \times 10^{-12}$	$1+1.4 \times 10^{-9}$

Table 5.1.: **Full topological classification of the 2q spin wave.** For the gaps labelled by the coloured bullets in the density of states in Fig. 5.4, we compute all possible Chern numbers at $\vartheta = \frac{357}{3249}$ and $\vartheta = \frac{835}{3249}$ in Tbl. (a) and extract the corresponding K -theory class in Tbl. (b).

While the general considerations assigned $n_{\{u_1, u_2\}} = \deg \hat{\mathbf{n}}$ to the entire lower block of anti-aligned states, it now becomes revealed, that the label takes this value already around $E_F = -3\lambda_{\text{hop}}$ and is 0 before. Apparently only the states at this energy carry a contribution to the real space Chern number $Ch_{\{u_1, u_2\}}$. Similarly, for the upper block the compensating contribution is only carried by the states around $E_F = 7\lambda_{\text{hop}}$ from where on $n_{\{u_1, u_2\}}$ jumps back to 0. These two energies are correlated with an increased density of states. Indeed, the DOS shows a pronounced peak persisting in

5. Chern Hierarchy of Multi-q Textures

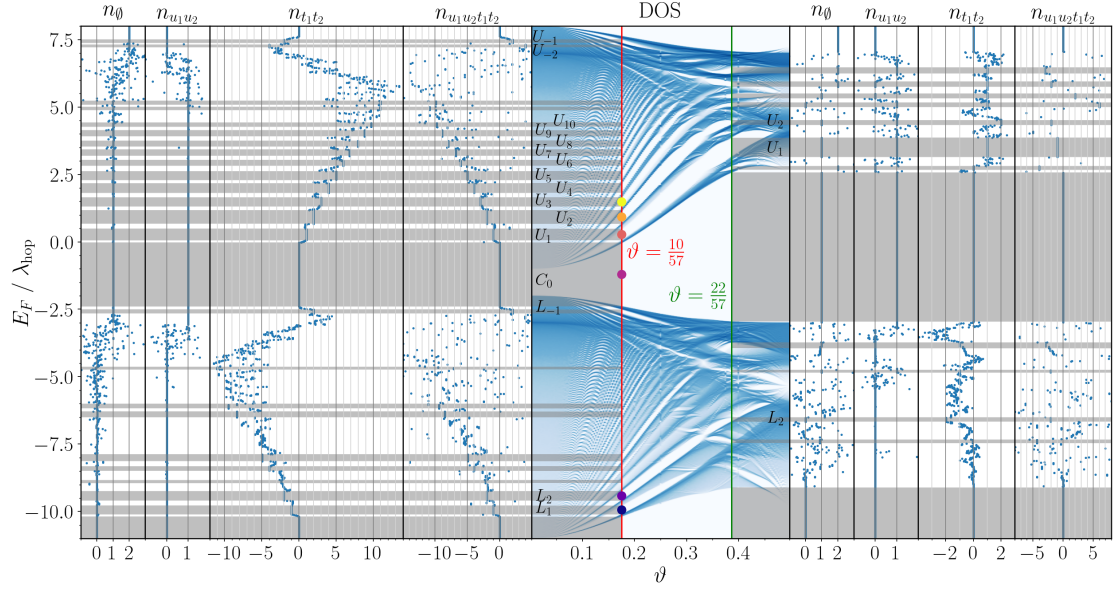


Figure 5.5.: **Main gap labels of the helical skyrmion crystal at zero shift and net magnetisation.** We evaluate gap labels in a system of size $N = 57$ at $\nu = \frac{10}{57}$ and $\nu = \frac{22}{57}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = 0$ and $m = 0$, and numeric parameter $\Delta\varphi = 10^{-5}$. The DOS is computed via KPM for a system of size $N = 400$ with $\nu = i/N$, $i \in \{0, \dots, N/2 - 1\}$. For the gaps marked with coloured bullets all Chern numbers and labels are listed in Tbl. 5.2. This figure was adapted from [Pra+24, Fig. 5].

(a) Chern numbers at $\nu = \frac{10}{57}$.

Ch_J	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●
Ch_0	0.03077870	0.06155740	1.00000000	1.03077870	1.06155740	1.09233610
$Ch_{u_1 u_2}$	0.00000000	-0.00000000	1.00000000	1.00000000	1.00000000	1.00000000
$Ch_{u_1 t_1}$	0.17543859	0.35084664	-0.00000000	0.17543819	0.35087550	0.52593783
$Ch_{u_1 t_2}$	0.00000000	0.00000000	-0.00000000	0.00000000	0.00000000	0.00000000
$Ch_{u_2 t_1}$	0.00000000	0.00000000	-0.00000000	0.00000000	0.00000000	0.00000000
$Ch_{u_2 t_2}$	0.17543859	0.35084664	-0.00000000	0.17543819	0.35087550	0.52593783
$Ch_{t_1 t_2}$	-0.99999991	-1.99963888	0.00000000	0.99999435	1.99998349	2.99508127
$Ch_{u_1 u_2 t_1 t_2}$	-0.99999986	-1.99938394	0.00000000	-0.99999147	-1.99998070	-2.99653480

(b) Labels of K -theory class in $K_0(\mathcal{A}) = \mathbb{Z}^8$.

n_J	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●
n_0	$0 - 1.5 \times 10^{-9}$	$0 - 8.2 \times 10^{-6}$	$1 + 6.1 \times 10^{-14}$	$1 - 1.2 \times 10^{-7}$	$1 - 1.5 \times 10^{-9}$	$1 + 2.6 \times 10^{-5}$
$n_{u_1 u_2}$	$0 + 2.8 \times 10^{-14}$	$0 - 1.8 \times 10^{-13}$	$1 + 3.0 \times 10^{-10}$	$1 + 3.0 \times 10^{-10}$	$1 + 2.9 \times 10^{-10}$	$1 + 2.9 \times 10^{-10}$
$n_{u_1 t_1}$	$0 + 1.7 \times 10^{-8}$	$0 + 7.8 \times 10^{-5}$	$0 - 7.9 \times 10^{-14}$	$0 + 1.1 \times 10^{-6}$	$0 + 1.7 \times 10^{-6}$	$0 + 2.3 \times 10^{-4}$
$n_{u_1 t_2}$	$0 + 7.0 \times 10^{-12}$	$0 + 2.0 \times 10^{-11}$	$0 - 2.7 \times 10^{-15}$	$0 + 7.2 \times 10^{-12}$	$0 + 1.3 \times 10^{-11}$	$0 + 3.1 \times 10^{-11}$
$n_{u_2 t_1}$	$0 + 6.1 \times 10^{-12}$	$0 + 1.2 \times 10^{-11}$	$0 - 1.9 \times 10^{-13}$	$0 + 1.3 \times 10^{-11}$	$0 + 1.5 \times 10^{-11}$	$0 + 1.9 \times 10^{-11}$
$n_{u_2 t_2}$	$0 + 1.7 \times 10^{-8}$	$0 + 7.8 \times 10^{-5}$	$0 - 2.1 \times 10^{-13}$	$0 + 1.1 \times 10^{-6}$	$0 + 1.7 \times 10^{-6}$	$0 + 2.3 \times 10^{-4}$
$n_{t_1 t_2}$	$-1 + 8.9 \times 10^{-8}$	$-2 + 3.6 \times 10^{-4}$	$0 + 2.0 \times 10^{-17}$	$1 - 5.6 \times 10^{-6}$	$2 - 1.7 \times 10^{-5}$	$3 - 4.9 \times 10^{-3}$
$n_{u_1 u_2 t_1 t_2}$	$-1 + 1.4 \times 10^{-7}$	$-2 + 6.2 \times 10^{-4}$	$0 + 1.6 \times 10^{-13}$	$-1 + 8.5 \times 10^{-6}$	$-2 + 1.9 \times 10^{-5}$	$-3 + 3.5 \times 10^{-3}$

Table 5.2.: **Full topological classification of the 3q helical skyrmion crystal.** For the gaps labelled by the coloured bullet points in the density of states in Fig. 5.5, we compute all possible Chern numbers at $\nu = \frac{10}{57}$ in Tbl. (a) and extract the corresponding K -theory class in Tbl. (b). This table was adapted from [Pra+24, Tbl. 1].

5.2. Full Chern Hierarchy

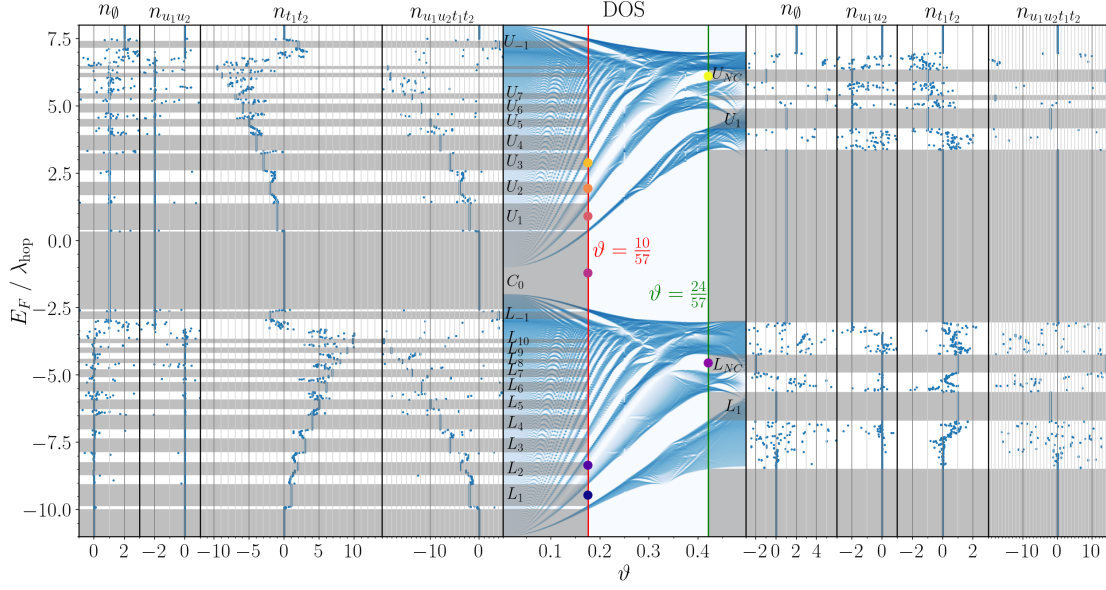


Figure 5.6.: **Main gap labels of the sinusoidal skyrmion crystal at zero shift and net magnetisation.** We evaluate gap labels in a system of size $N = 57$ at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{24}{57}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{\text{hop}} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = 0$ and $m = 0$, and numeric parameter $\Delta\varphi = 10^{-5}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$, $i \in \{0, \dots, N/2 - 1\}$. For the gaps marked with coloured bullets all Chern numbers and labels are listed in Tbl. 5.3.

(a) Chern numbers at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{24}{57}$.

Ch_J	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●
Ch_0	0.06155740	0.12311480	0.57063712	1.00000000	1.06155740	1.12311480	1.18467221	1.57063712
$Ch_{u_1 u_2}$	-0.00000000	-0.00000000	-0.00000000	-2.00000000	-2.00000000	-2.00000000	-2.00000000	-2.00000003
$Ch_{u_1 t_1}$	0.35087718	0.70072136	0.10526727	-0.00000000	0.35087719	0.70166749	1.05263148	0.10526316
$Ch_{u_1 t_2}$	0.00000000	0.00000000	-0.00000000	-0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
$Ch_{u_2 t_1}$	0.00000000	0.00000000	-0.00000000	-0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
$Ch_{u_2 t_2}$	0.35087718	0.70072136	0.10526727	-0.00000000	0.35087719	0.70166749	1.05263148	0.10526316
$Ch_{t_1 t_2}$	0.99999995	1.98701407	0.99998459	-0.00000000	-1.00000000	-1.99922345	-2.99999962	-1.00000000
$Ch_{u_1 u_2 t_1 t_2}$	-1.99999982	-3.94671888	13.99971250	-0.00000000	-2.00000000	-3.99866369	-6.00000378	14.00000072

(b) Labels of K -theory class in $K_0(\mathcal{A}) = \mathbb{Z}^8$.

n_J	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●	Gap ●
n_0	$0-2.4 \times 10^{-9}$	$0-1.3 \times 10^{-3}$	$-2+4.8 \times 10^{-5}$	$1+6.8 \times 10^{-14}$	$1+1.1 \times 10^{-12}$	$1-1.1 \times 10^{-5}$	$1+1.5 \times 10^{-7}$	$-1-1.3 \times 10^{-7}$
$n_{u_1 u_2}$	$0-1.3 \times 10^{-13}$	$0-6.0 \times 10^{-12}$	$0-5.9 \times 10^{-10}$	$-2-6.4 \times 10^{-10}$	$-2-6.4 \times 10^{-10}$	$-2-6.2 \times 10^{-10}$	$-2-5.9 \times 10^{-10}$	$-2-3.5 \times 10^{-8}$
$n_{u_1 t_1}$	$0+2.2 \times 10^{-8}$	$0+8.3 \times 10^{-3}$	$6-1.2 \times 10^{-4}$	$0-1.3 \times 10^{-13}$	$0-2.4 \times 10^{-11}$	$0+1.5 \times 10^{-4}$	$0-7.6 \times 10^{-7}$	$6+3.0 \times 10^{-7}$
$n_{u_1 t_2}$	$0+1.4 \times 10^{-11}$	$0+3.6 \times 10^{-11}$	$0-6.8 \times 10^{-12}$	$0-1.1 \times 10^{-13}$	$0+1.8 \times 10^{-11}$	$0+3.4 \times 10^{-11}$	$0+5.0 \times 10^{-11}$	$0+3.6 \times 10^{-12}$
$n_{u_2 t_1}$	$0+1.4 \times 10^{-11}$	$0+2.9 \times 10^{-11}$	$0-2.5 \times 10^{-11}$	$0-1.8 \times 10^{-13}$	$0+1.8 \times 10^{-11}$	$0+2.9 \times 10^{-11}$	$0+4.0 \times 10^{-11}$	$0+5.0 \times 10^{-12}$
$n_{u_2 t_2}$	$0+2.2 \times 10^{-8}$	$0+8.3 \times 10^{-3}$	$6-1.2 \times 10^{-4}$	$0-2.3 \times 10^{-13}$	$0-2.5 \times 10^{-11}$	$0+1.5 \times 10^{-4}$	$0-7.6 \times 10^{-7}$	$6+3.0 \times 10^{-7}$
$n_{t_1 t_2}$	$1-5.3 \times 10^{-8}$	$2-1.3 \times 10^{-2}$	$1-1.5 \times 10^{-5}$	$0-7.8 \times 10^{-17}$	$-1+1.4 \times 10^{-10}$	$-2+7.8 \times 10^{-4}$	$-3+3.8 \times 10^{-7}$	$-1+4.4 \times 10^{-10}$
$n_{u_1 u_2 t_1 t_2}$	$-2+1.8 \times 10^{-7}$	$-4+5.3 \times 10^{-2}$	$14-2.9 \times 10^{-4}$	$0-1.3 \times 10^{-14}$	$-2-2.5 \times 10^{-10}$	$-4+1.3 \times 10^{-3}$	$-6-3.8 \times 10^{-6}$	$14+7.2 \times 10^{-7}$

Table 5.3.: **Full topological classification of the 3q sinusoidal skyrmion crystal.** For the gaps labelled by the coloured bullet points in the density of states in Fig. 5.6, we compute all possible Chern numbers at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{24}{57}$ in Tbl. (a) and extract the corresponding K -theory class in Tbl. (b).

5. Chern Hierarchy of Multi-q Textures

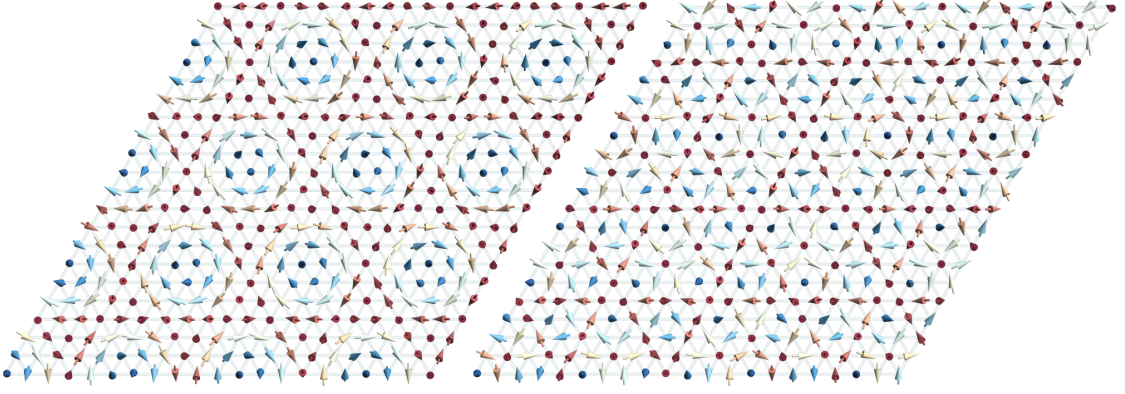


Figure 5.7.: **3q Helical skyrmionic texture at $\vartheta = 10/57$ and $\vartheta = 22/57$.** The figure shows 21×21 sites of the helical skyrmionic $3q$ texture with $\deg \hat{\mathbf{n}} = 1$ ($\varphi = 0$, $m = 0$) for $\vartheta = 10/57$ (left) and for $\vartheta = 22/57$ (right) at which the labels were evaluated in Fig. 5.5.

the limit of $\vartheta \rightarrow 0$, consistent with the van Hove singularities (VHS) of the triangular electronic lattice, located at the respective energies $E_{VHS} \approx 2\lambda_{\text{hop}} + \lambda_{\text{xc}} = 7$ and $E_{VHS} \approx 2\lambda_{\text{hop}} - \lambda_{\text{xc}} = -3$ [Göb+17b].

Likewise, the remaining depicted labels seem to receive a significant contribution from the states around the VHS as well. The $n_{\emptyset}$ label jumps from 0 to 1 and 1 to 2, respectively, and the $n_{\{t_1, t_2\}}$ and $n_{\{u_1, u_2, t_1, t_2\}}$ labels change their sign. The latter implies that the states at the VHS carry a large compensating contribution to all other contributing states, such that the cumulated contribution of each block is 0. Let us consider the labels $n_{\{t_1, t_2\}}$ and $n_{\{u_1, u_2, t_1, t_2\}}$ separately for both textures.

Helical skyrmions

For the helical skyrmion lattice each band between the $U_1, U_2, \dots$ gaps in the upper, spin-aligned block of energy states carries a contribution of 1 to $n_{\{t_1, t_2\}}$ which for $\vartheta = 10/57$ is well discernible up to U_{10} at the present numerical accuracy. Then, while passing the VHS the label changes sign and takes negative values. Eventually, the bands between the $U_{-1}, U_{-2}, \dots$ gaps contribute 2 until all contributions are fully compensated. For the lower, anti-aligned block we witness the same behaviour with opposite sign, although the gaps are less discernible. This is consistent with the known findings from mapping the bands in skyrmion systems to Landau levels which one finds to contribute 1 to the momentum space Chern number when below and 2 when above the VHS [Göb+17b]. The contributions to the $n_{\{u_1, u_2, t_1, t_2\}}$ label follow the same pattern but without the sign change between the blocks. This is consistent with their role of counting the ϑ^2 or $2\vartheta^2$ additional states between each of the gaps that connect to the adiabatic limit $\vartheta \rightarrow 0$.

Sinusoidal skyrmions

For the sinusoidal skyrmion lattice the behaviour of the labels $n_{\{t_1, t_2\}}$ and $n_{\{u_1, u_2, t_1, t_2\}}$ is similar, with some significant differences: The $n_{\{t_1, t_2\}}$ label also receives contributions of size 1 below and of size 2 above the VHS, but with the opposite sign, while the states in between the gaps contribute -2 to the $n_{\{u_1, u_2, t_1, t_2\}}$ label below and -4 above the VHS.

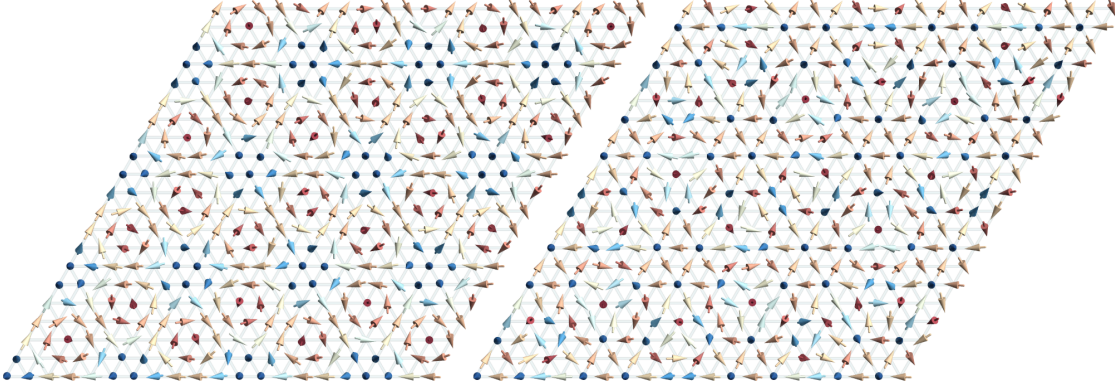


Figure 5.8.: **3q Sinusoidal skyrmionic texture at $\vartheta = 10/57$ and $\vartheta = 24/57$.** The figure shows 21×21 sites of the sinusoidal skyrmionic textures with $\deg \hat{\mathbf{n}} = -2$ ($\varphi = 0$, $m = 0$) for $\vartheta = 10/57$ (left) and for $\vartheta = 24/57$ (right) at which the labels were evaluated in Fig. 5.6.

For the larger pitch values $\vartheta = 22/57$ and $\vartheta = 24/57$, the gap formation is less pronounced in both systems, however, several non-commutative gaps open. These are not connected to the limit $\vartheta \rightarrow 0$ of smooth textures and can, therefore, not be treated with commutative geometry. They generally seem to behave differently from the rules we observe for the connected gaps.

Non-commutative gaps

While for lower pitch values $\vartheta \rightarrow 0$ the labels follow a rather predictable pattern from gap to gap, the same cannot be said for $\vartheta \rightarrow 0.5$, where no clear pattern can be identified. A look at the real space distribution of the spins in Fig. 5.7 and Fig. 5.8 reveals textures that, at first sight, do no longer resemble skyrmion lattices. Yet, the electrons' real space Chern number $Ch_{\{u_1, u_2\}}$ still exhibits quantisation and corresponds to the winding number of the texture's smooth vector field. The skyrmionic nature of the texture can thus only reveal itself through (approximate) ergodicity.

In conclusion, we can deduce from these results that for the skyrmionic textures the bands at the VHS carry the whole $\pm \deg \hat{\mathbf{n}}$ contribution to the real space first Chern number of the whole block, as well as the whole contribution to the momentum space first and the mixed space second Chern numbers that compensates the accumulated contributions from all the other bands. Electrons at the VHS are characterised by a vanishing group velocity. Their spin can thus align perfectly with the texture $\hat{\mathbf{n}}$. Notably, those seem to be the only states with non-trivial real space spin winding.

Conclusion skyrmion textures

The differences between the two skyrmion textures hint towards a relationship between the electronic space topology and the real space winding number that (at least for the gaps connected to the adiabatic limit $\vartheta \rightarrow 0$) goes beyond its concordance with the real space first Chern number. The sign of the momentum space first Chern number changes with the sign of the winding number (even though it does not change in size) and the mixed space second Chern number changes in size in accordance with the winding number (but not in sign). The latter suggests that the number of states at each energy level is proportional to the winding number, as discussed already in the last section.

5. Chern Hierarchy of Multi-q Textures

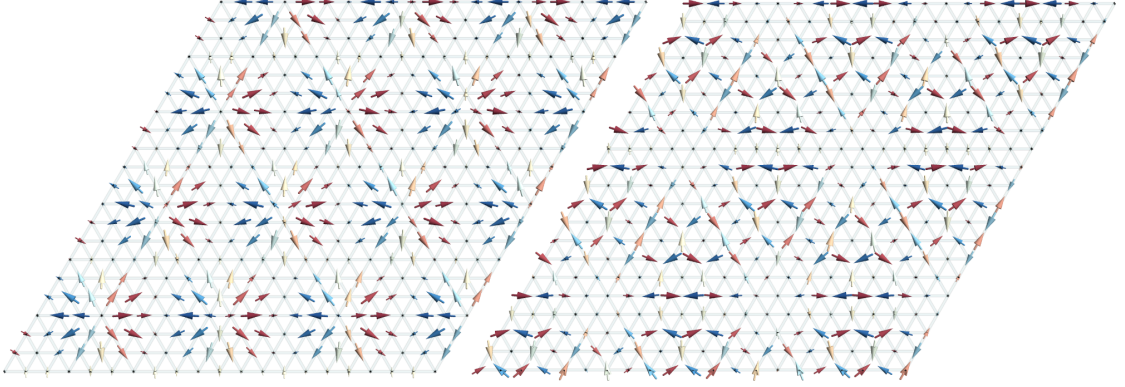


Figure 5.9.: **3q vortex texture at $\vartheta = 10/57$ and $\vartheta = 25/57$.** The figure shows 21×21 sites of the vortex texture for $\vartheta = 10/57$ (left) and for $\vartheta = 25/57$ (right) at which the labels were evaluated in Fig. 5.10.

As an attempt to explain the behaviour of the momentum space Chern number, one might try to map the bands from the skyrmionic system onto Landau levels created by the emergent magnetic field [Göb+17b] with strength equal to the winding number. However, we find that this analogy does not hold for all scenarios we consider. In the upcoming section, we seek to substantiate this relation and to illuminate the relationship for all possible winding numbers of these two textures.

3q vortex lattice

Lastly, we consider the 3q vortex lattice on a triangular lattice with system size $N = 57$ for two pitch values depicted in Fig. 5.9 and compile the results for the Chern numbers and labels in Fig. 5.10 and Tbl. 5.4. As before, the labels for the gaps marked by the coloured bullets have good accuracy and verify the IDS analysis of Fig. 5.2.

As a noticeable difference besides the missing centre gap both real- and moment space labels are zero over the full range of energies. This can be explained by the peculiar nature of the vortex lattice, which is unnormalised and in-plane with the underlying atomic lattice. As a result, the scalar spin chirality $\mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_y \mathbf{n})$ is zero everywhere, such that the texture has no winding number, which then also pertains to the real space Chern number $Ch_{\{u_1, u_2\}} = n_{\{u_1, u_2\}}$. Furthermore, the net magnetisation $\langle n_z \rangle$ is zero, which renders the system time reversal invariant, such that the momentum space Chern number $Ch_{\{t_1, t_2\}} = n_{\{t_1, t_2\}}$ is suppressed [CNM14].

The mixed space second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ that counts the number of states between each L_i gap in the DOS is, by its nature, non-zero and takes even integer values similar to the system with the sinusoidal skyrmion texture. We attribute this to the missing spin separation, which doubles the states at each energy level.

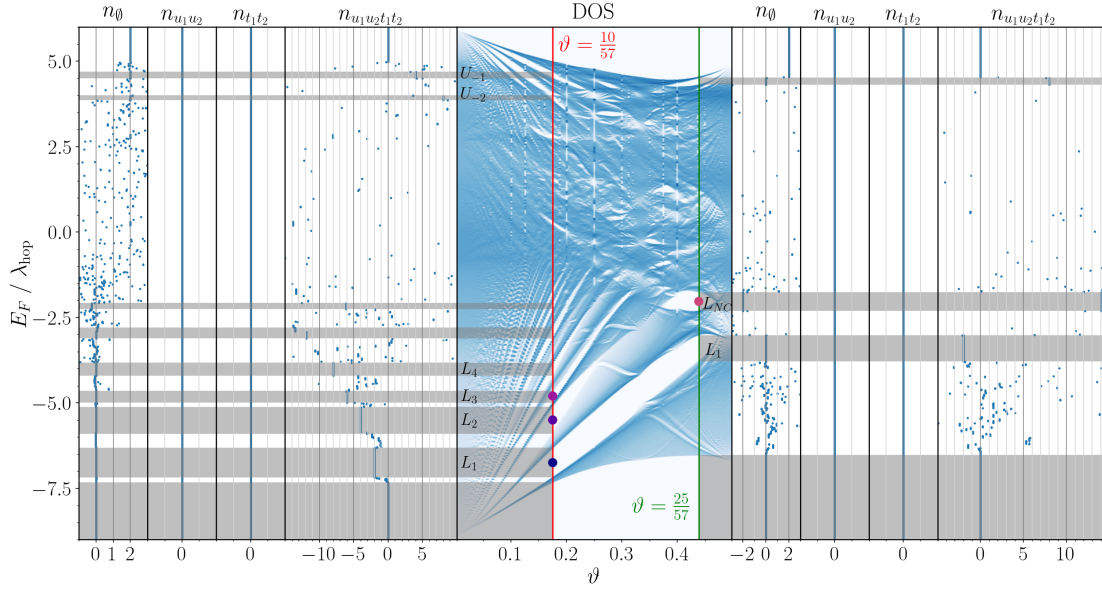


Figure 5.10.: **Main gap labels of the vortex crystal.** We evaluate gap labels in a system of size $N = 57$ at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{25}{57}$ for Fermi energies in the full energy range, with system parameters $\lambda_{\text{xc}}/\lambda_{\text{hop}} = 5$ and numeric parameter $\Delta\varphi = 10^{-5}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$, $i \in \{0, \dots, N/2 - 1\}$. For the gaps marked with coloured bullets all Chern numbers and labels are listed in Tbl. 5.4.

(a) Chern numbers at $\vartheta = \frac{10}{57}$.

Ch_J	Gap ●	Gap ●	Gap ●	Gap ●
$Ch_\emptyset$	0.06155740	0.12311480	0.18467221	0.57002155
$Ch_{u_1 u_2}$	-0.00000000	-0.00000000	-0.00000000	0.00000000
$Ch_{u_1 t_1}$	0.35087718	0.70174821	1.05259320	-0.14030075
$Ch_{u_1 t_2}$	0.00000000	0.00000000	0.00000000	0.00000000
$Ch_{u_2 t_1}$	0.00000000	0.00000000	0.00000000	0.00000000
$Ch_{u_2 t_2}$	0.35087718	0.70174821	1.05259320	-0.14030075
$Ch_{t_1 t_2}$	0.00000000	0.00000000	0.00000000	0.00000000
$Ch_{u_1 u_2 t_1 t_2}$	-1.99999963	-3.99961807	-5.99918000	13.99647796

(b) Labels of K -theory class in $K_0(\mathcal{A}) = \mathbb{Z}^8$.

n_J	Gap ●	Gap ●	Gap ●	Gap ●
$n_\emptyset$	$0-5.1 \times 10^{-9}$	$0-9.6 \times 10^{-6}$	$0-1.2 \times 10^{-5}$	$-2+6.3 \times 10^{-4}$
$n_{u_1 u_2}$	$0-1.5 \times 10^{-13}$	$0-8.2 \times 10^{-13}$	$0-1.2 \times 10^{-12}$	$0+1.5 \times 10^{-12}$
$n_{u_1 t_1}$	$0+4.7 \times 10^{-8}$	$0+6.1 \times 10^{-5}$	$0+1.1 \times 10^{-4}$	$6-1.5 \times 10^{-3}$
$n_{u_1 t_2}$	$0+1.8 \times 10^{-11}$	$0+2.7 \times 10^{-11}$	$0+4.0 \times 10^{-11}$	$0+7.8 \times 10^{-12}$
$n_{u_2 t_1}$	$0+1.9 \times 10^{-11}$	$0+3.5 \times 10^{-11}$	$0+6.2 \times 10^{-11}$	$0+8.8 \times 10^{-12}$
$n_{u_2 t_2}$	$0+4.7 \times 10^{-8}$	$0+6.1 \times 10^{-5}$	$0+1.1 \times 10^{-4}$	$6-1.5 \times 10^{-3}$
$n_{t_1 t_2}$	$0+4.7 \times 10^{-17}$	$0+1.9 \times 10^{-16}$	$0+8.5 \times 10^{-17}$	$0+2.0 \times 10^{-16}$
$n_{u_1 u_2 t_1 t_2}$	$-2+3.7 \times 10^{-7}$	$-4+3.8 \times 10^{-4}$	$-6+8.2 \times 10^{-4}$	$14-3.5 \times 10^{-3}$

Table 5.4.: **Full topological classification of the 3q vortex crystal.** For the gaps labelled by the coloured bullet points in the density of states in Fig. 5.10, we compute all possible Chern numbers at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{25}{57}$ in Tbl. (a) and extract the corresponding K -theory class in Tbl. (b).

5.3. Topological Phase Transitions following a Change in Real Space Winding

Continuous variation of texture parameters can induce discontinuities in the texture's normalised vector field $\hat{\mathbf{n}}$, which may cause a change in its winding number $\deg \hat{\mathbf{n}}$, as discussed in detail in Chap. 1.3.4. To investigate how the electronic state topology in form of the spectral gap labels is related to the real space topology in form of the winding number, we compute the main Chern numbers for different winding numbers and along the topological phase transitions between them. From our four example textures only the two $3q$ skyrmion lattices are eligible for this treatment since they have non-trivial winding. The parameter dependence of the winding number and the net magnetisation is visualised in Fig. 1.4 and Fig. 1.6.

In this section, we consider the helical skyrmion lattice and the sinusoidal skyrmion lattice in phases with different topological winding number and compare the real space Chern number $Ch_{\{u_1, u_2\}} = n_{\{u_1, u_2\}}$, the momentum space Chern number $Ch_{\{t_1, t_2\}} = n_{\{t_1, t_2\}}$, and the mixed space second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}} = n_{\{u_1, u_2, t_1, t_2\}}$. Then, we analyse the evolution of the Chern numbers in the U_1 gaps along the transitions and compile the results over the full parameter range in phase diagrams. The analysis for the helical skyrmion system is partially adapted from [Pra+24, Chap. 5.2].

DOS Evolution

Before we compute the Chern numbers for different points in the texture parameter space (m, φ) , we need to explore the evolution of the DOS between them. For that we choose line cuts in the winding number diagrams in Fig. 1.4(a) and 1.6(a) that cross areas of interest and use the KPM to compute the DOS along them. We choose system sizes $N = 401$ with pitch $\vartheta = \frac{70}{401}$, which is close to the pitch $\vartheta = \frac{10}{57}$ at which we evaluate Chern numbers in systems of size $N = 57$.

Helical skyrmions

For the helical skyrmion lattice, we choose three lines: The first line at net magnetisation parameter $m = 0$ for phase shifts φ between 0 and π for which the winding number changes from 1 to -1 at $(0, 0.5\pi)$. The second line at $\varphi = 0$ for m between 0 and 1 for which the winding number changes from 1 to -2 at $(\frac{1}{\sqrt{3}}, 0)$ and then to 0 at $(\frac{\sqrt{3}}{2}, 0)$. The third and last line at $m = 0.7$ from $\varphi = 0$ to π along which the winding number goes from -2 to -1 at around $(0.7, 0.1\pi)$.

Since we are particularly interested in the response to the discontinuities in the texture, we choose a phase space origin position $\boldsymbol{\varphi}$ with $\varphi_1 + \varphi_2 + \varphi_3 = \varphi$ to move the singularity onto the site at $\mathbf{x}_0$. For the paths along $m = 0$ and $m = 0.7$ we choose $\boldsymbol{\varphi} = (\varphi + \pi + \arccos \frac{m}{\sqrt{3}}, \pi + \arccos \frac{m}{\sqrt{3}}, -2 \arccos \frac{m}{\sqrt{3}})$ and for $\varphi = 0$ we choose $\boldsymbol{\varphi} = (\pi, \pi, 0)$. The DOS along these lines is presented in Fig. 5.11.

$m = 0$

The spectrum along the $m = 0$ line is symmetric, as the texture at the end point is obtained by the time-reversal of the texture at the starting point. For $\varphi \rightarrow 0.5\pi$, at which point the winding number $\deg \hat{\mathbf{n}}$ jumps from 1 to -1 , all gaps inside the blocks of aligned and anti-aligned states close and reopen again.

$\varphi = 0$

The $\varphi = 0$ line starts at the same parameter point with $\deg \hat{\mathbf{n}} = 1$. At $m = \frac{1}{\sqrt{3}}$ the texture's winding number jumps to $\deg \hat{\mathbf{n}} = -2$ and at $m = \frac{\sqrt{3}}{2}$ to $\deg \hat{\mathbf{n}} = 0$, however

5.3. Topological Phase Transitions following a Change in Real Space Winding

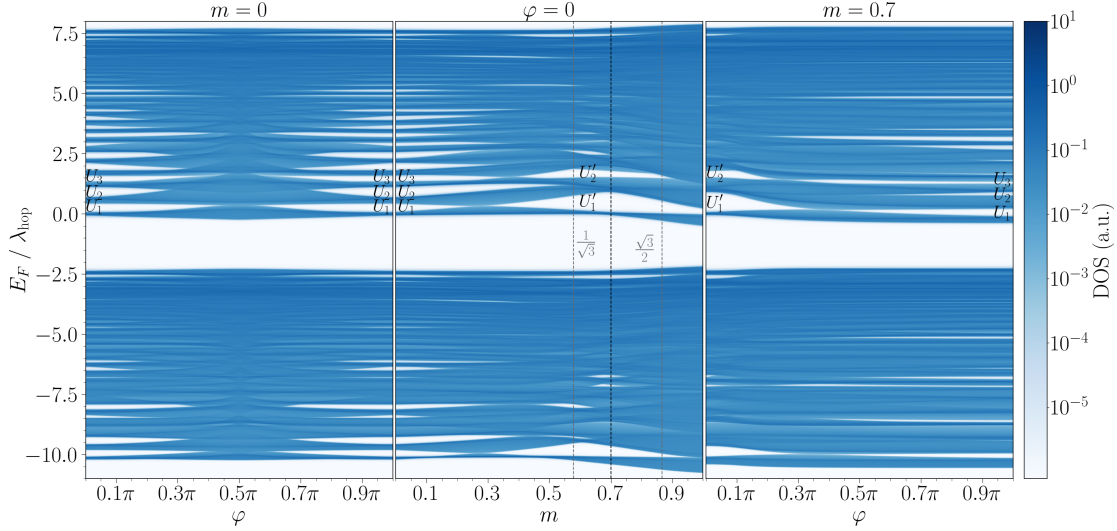


Figure 5.11.: **Density of states evolution across real space phase transitions for the helical skyrmion lattice.** We perform three different line cuts through the phase space spanned by the texture parameters (m, φ) and compute the DOS along them using the KPM for a system of size $N = 401$ with $\vartheta = \frac{70}{401}$ with system parameters $\lambda_{\text{xc}}/\lambda_{\text{hop}} = 5$. This figure was adapted from [Pra+24, Fig. 9].

this is not apparent from the spectrum. The U_1 gap closes at an earlier m value and reopens afterwards to U'_1 , and the U_2 gap closes and stays closed. This makes the U'_2 a factual continuation of gap U_3 . For $m \rightarrow 1$ all gaps except U_1 have closed.

The last line cut we follow starts with the spectrum which is at $m = 0.7$ in the previous DOS plot, where the U'_1 and U'_2 gaps are wide open and clear in the upper block. At the start we have $\deg \hat{\mathbf{n}} = -2$ that jumps to $\deg \hat{\mathbf{n}} = -1$ around $\varphi = 0.1\pi$, but the gaps seemingly stay open. The U'_1 gap closes briefly around $\varphi = 0.4\pi$ and the second energy band splits to reopen the U_2 gap we had before at $m = 0$ and $\varphi = 0$. Also, multiple higher gaps open. This is consistent with our expectations as the spectrum at the endpoint is in the same area of the winding number phase diagram from Fig. 1.4(a) as the spectrum at $m = 0$ and $\varphi = \pi$.

The winding number diagram of the sinusoidal skyrmion lattice in Fig. 1.6(a) differs a lot from the one of the helical skyrmions. Again, we choose three lines: The first line at net magnetisation parameter $m = 0$ for phase shifts φ between 0 and π for which the winding number changes from -2 to $+2$ at $(0, \frac{\pi}{2})$. The second line at $\varphi = 0$ for m between -1 and 1 for which the winding number changes from -2 to 0 at $(0.5, 0)$. The third and last line at $m = 0.25$ from $\varphi = 0$ to π along which the winding number goes from -2 to -1 at around $(0.25, 0.25\pi)$ and from -1 to $+2$ at around $(0.25, 0.6\pi)$. For the paths along $m = 0$ and $m = 0.25$ we choose $\varphi = (\varphi + \pi + \arccos m, \pi + \arccos m, -2 \arccos m)$ and for $\varphi = 0$ we choose $\varphi = (\pi + \arccos 0.5, \pi + \arccos 0.5, -2 \arccos 0.5)$. The DOS along these lines is presented in Fig. 5.12.

$m = 0.7$

Sinusoidal skyrmions

5. Chern Hierarchy of Multi-q Textures

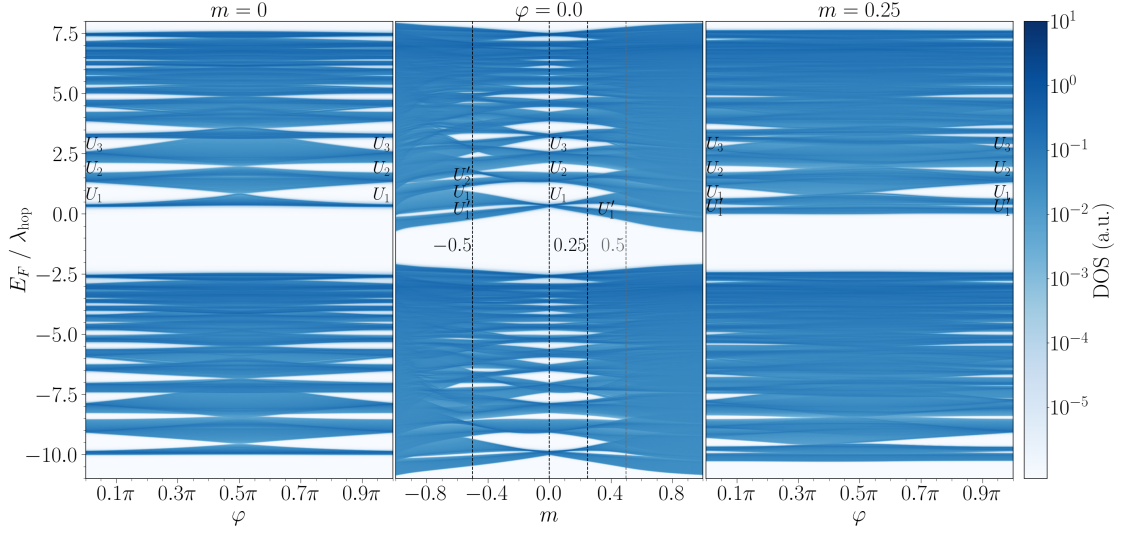


Figure 5.12.: **Density of states evolution across real space phase transitions for the sinusoidal skyrmion lattice.** We perform three different line cuts through the phase space spanned by the texture parameters (m, φ) and compute the DOS along them using the KPM for a system of size $N = 401$ with $\vartheta = \frac{70}{401}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$.

$m = 0$ Similar to the helical case, the spectrum along the $m = 0$ line is symmetric and at $\varphi = 0.5\pi$ where the winding number $\deg \hat{\mathbf{n}}$ jumps from -2 to $+2$ all gaps inside the blocks of aligned and anti-aligned states close and reopen again.

$\varphi = 0$ The $\varphi = 0$ line cut starts with $\deg \hat{\mathbf{n}} = -2$ that only jumps to $\deg \hat{\mathbf{n}} = 0$ at $m = 0.5$. The gaps that are open at $m = 0$ close for larger m values, but there is a new lowest gap, which closes for $m = 0$ and opens for non-zero m in the range. For $m = 0.5$, where the texture becomes trivial, most gaps are closed, whereas for $m = -0.5$, where the central gaps also close, new gaps open up. This seems unrelated to any of the texture properties that we considered in Fig. 1.6.

$m = 0.25$ Let us now consider the line starting with the spectrum at $m = 0.25$ in the previous DOS plot. At the start, we have $\deg \hat{\mathbf{n}} = -2$ that jumps to $\deg \hat{\mathbf{n}} = -1$ around $\varphi = 0.25\pi$, around which point all gaps narrow and close. Then, around $\varphi = 0.6\pi$ where $\deg \hat{\mathbf{n}} = -1$ jumps to $\deg \hat{\mathbf{n}} = +2$, similar gaps open back up. Apparently, the gaps close for the parameter area in which the winding number is $\deg \hat{\mathbf{n}} = -1$.

Chern Hierarchy Next, we choose two points in parameter space for each texture to evaluate how the Chern numbers differ for different winding numbers over the full range of Fermi energies. For both textures, we choose the point $(0, \pi)$ for which the phase shift inverts the direction of all spins in the texture while shifting the relative position of the magnetic unit cell, as displayed in Fig. 5.13(a) and Fig. 5.18(a). As a consequence, the winding number has the inverted sign, but the DOS is the same due to the time-reversal invariance of the spectrum.

Further, for the helical skyrmion lattice, we choose the point $(0.7, 0)$, where the net magnetisation parameter $m = 0.7$ raises the spins in z -direction, as shown in Fig. 5.13(b). This changes the winding number to -2 , as can be seen by the small skyrmions in the

5.3. Topological Phase Transitions following a Change in Real Space Winding

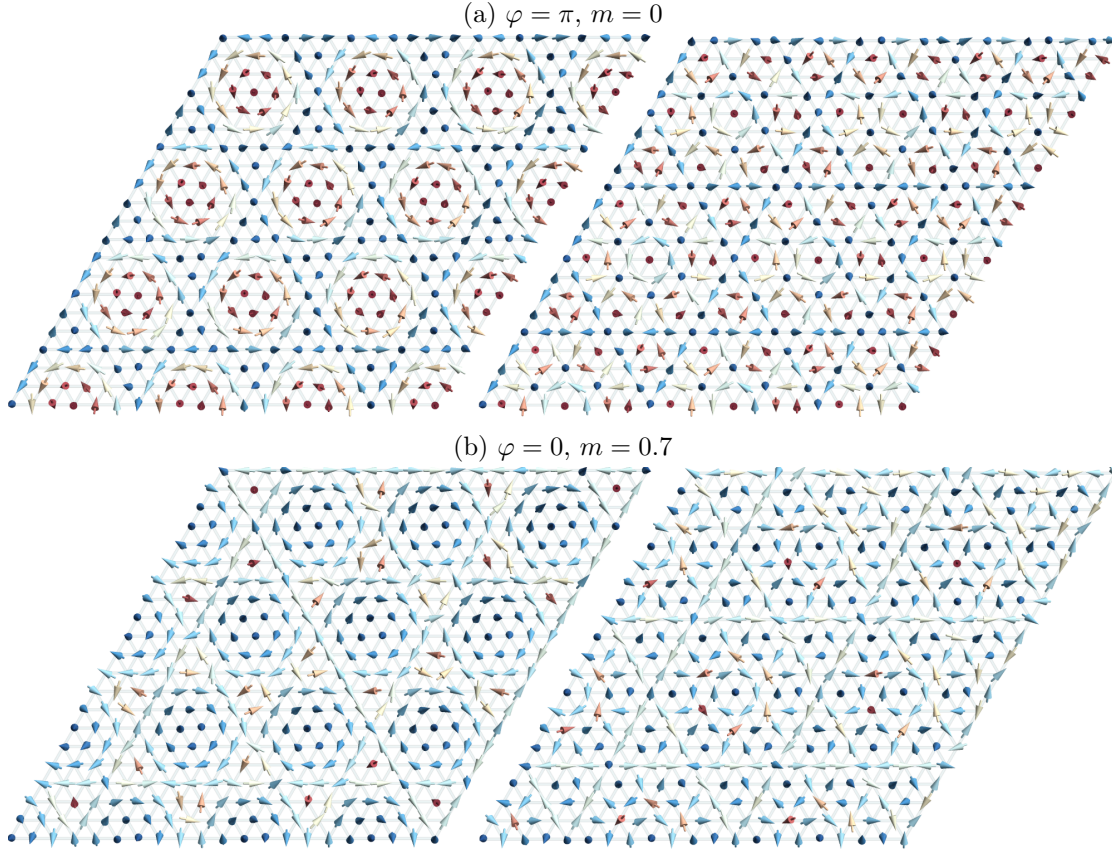


Figure 5.13.: **Helical 3q skyrmion textures for different parameters.** The figure shows 21×21 sites of the helical 3q skyrmion texture with $\deg \hat{\mathbf{n}} = -1$ ($\varphi = \pi, m = 0$) in (a) and $\deg \hat{\mathbf{n}} = -2$ ($\varphi = 0, m = 0.7$) in (b) for $\vartheta = 10/57$ and for $\vartheta = 20/53$, respectively. This figure was adapted from [Pra+24, Fig. 6].

sharp corners of the rhombic magnetic unit cell, and closes several gaps, as we observed in Fig. 5.11. As the second point for the sinusoidal skyrmion lattice, we choose $(-0.5, 0)$, where we have observed several additional gaps in Fig. 5.12, although the winding number is the same as at $(0, 0)$. The corresponding textures are shown in Fig. 5.18(b).

We begin, in Fig. 5.14, with the helical skyrmion lattice with shift $\varphi = \pi$ and net magnetisation parameter $m = 0$, for which we get $\deg \hat{\mathbf{n}} = -1$. Accordingly, we find the real space first Chern number $Ch_{\{u_1, u_2\}}$ flipped, with the states at the VHS carrying the opposite contribution as before. Similarly, the momentum space first Chern number $Ch_{\{t_1, t_2\}}$ exhibits a changed sign, with each band contributing the opposite amount as in the system with the inverted spin texture. Only the mixed-space second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ appears unaltered. This is consistent with the invariance of the DOS under time reversal, since $Ch_{\{u_1, u_2, t_1, t_2\}} = n_{\{u_1, u_2, t_1, t_2\}}$ is the coefficient of the quadratic term of the IDS in dependence of the length scale parameter.

Next, we consider the second parameter point $\varphi = 0$ and $m = 0.7$ for which we get $\deg \hat{\mathbf{n}} = -2$ as displayed in Fig. 5.15. Here, the texture is not obtained from a global

*Helical
skyrmions*

5. Chern Hierarchy of Multi-q Textures

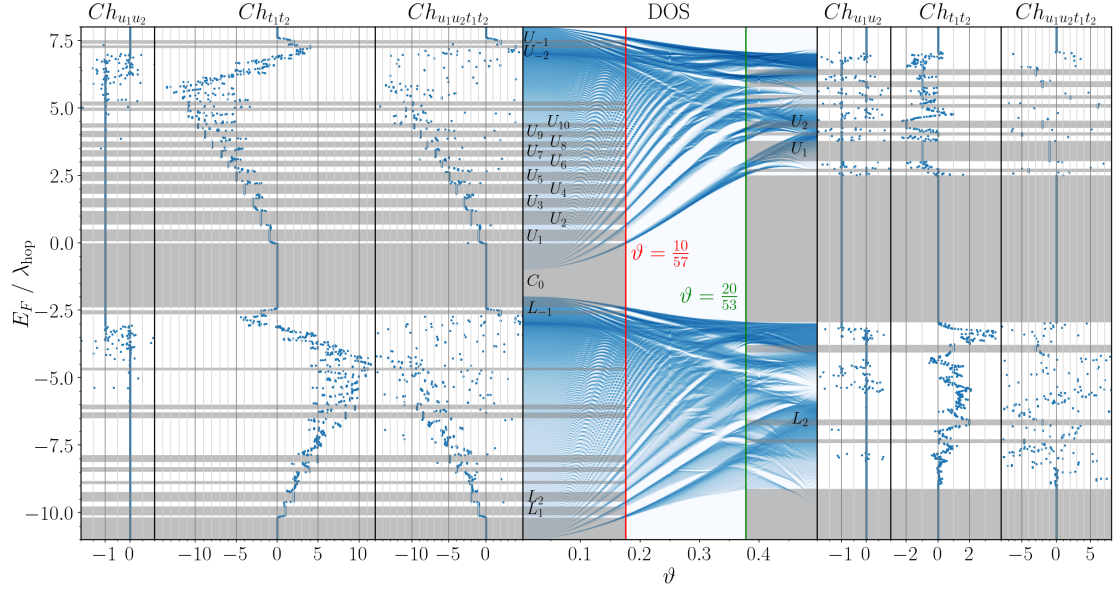


Figure 5.14.: **Main Chern numbers of the helical skyrmion crystal at π shift and zero net magnetisation.** We evaluate gap labels in a system of size $N = 57$ and $N = 53$ at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{20}{53}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = \pi$ and $m = 0$, and numeric parameter $\Delta\varphi = 10^{-8}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$, $i \in \{0, \dots, N/2 - 1\}$. This figure was adapted from [Pra+24, Fig. 7].

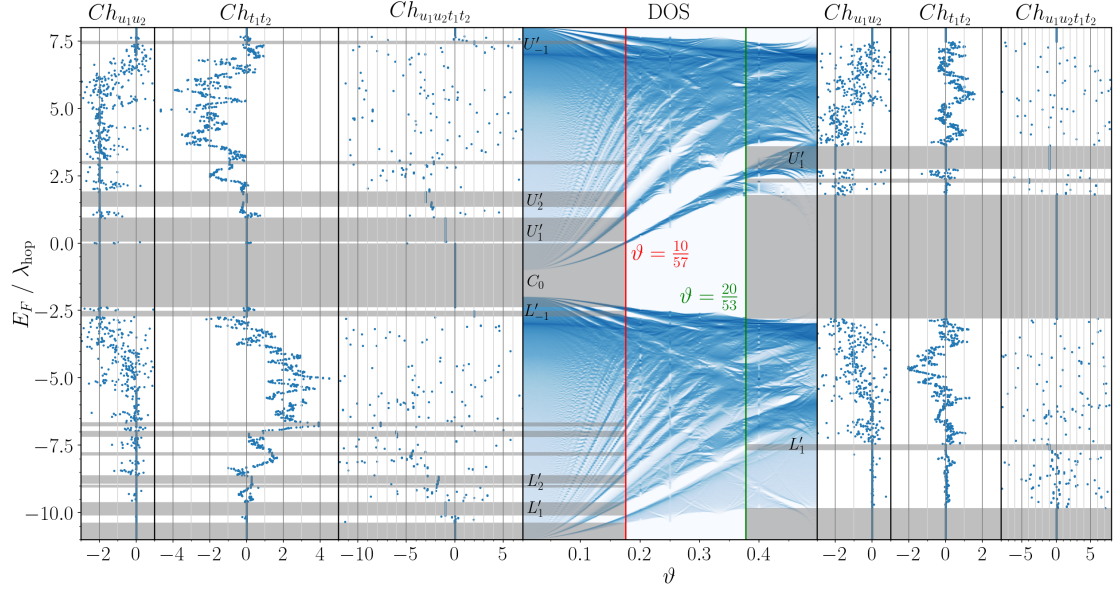


Figure 5.15.: **Main Chern numbers of the helical skyrmion crystal at zero shift and 0.7 net magnetisation.** We evaluate gap labels in a system of size $N = 57$ and $N = 53$ at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{20}{53}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = 0$ and $m = 0.7$, and numeric parameter $\Delta\varphi = 10^{-8}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$, $i \in \{0, \dots, N/2 - 1\}$. This figure was adapted from [Pra+24, Fig. 8].

5.3. Topological Phase Transitions following a Change in Real Space Winding

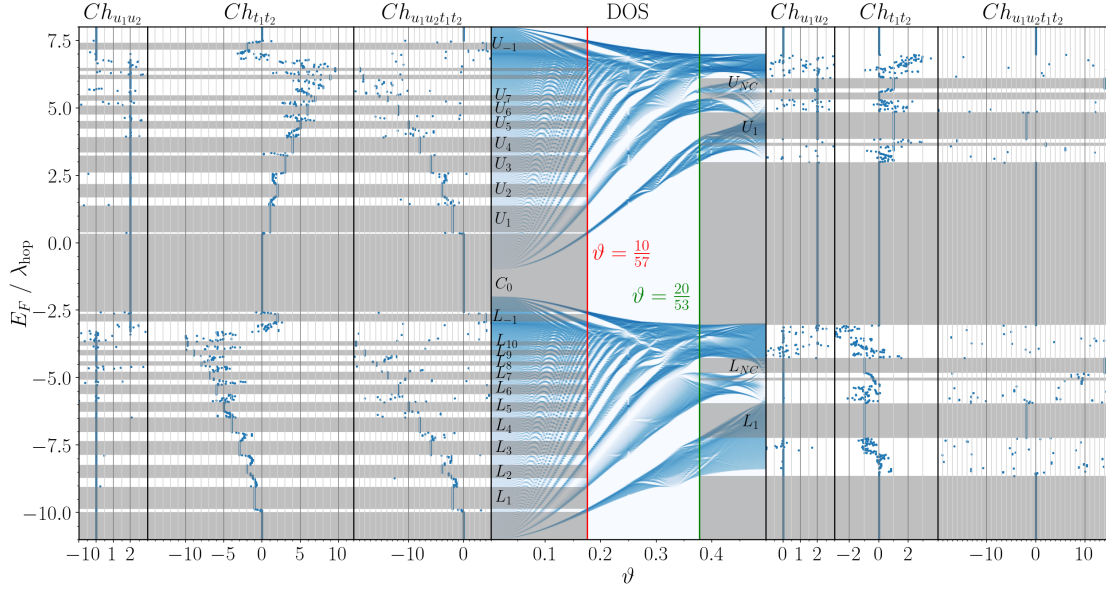


Figure 5.16.: **Main Chern numbers of the sinusoidal skyrmion crystal at π shift and zero net magnetisation.** We evaluate gap labels in a system of size $N = 57$ and $N = 53$ at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{20}{53}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = \pi$ and $m = 0$, and numeric parameter $\Delta\varphi = 10^{-8}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$, $i \in \{0, \dots, N/2 - 1\}$.

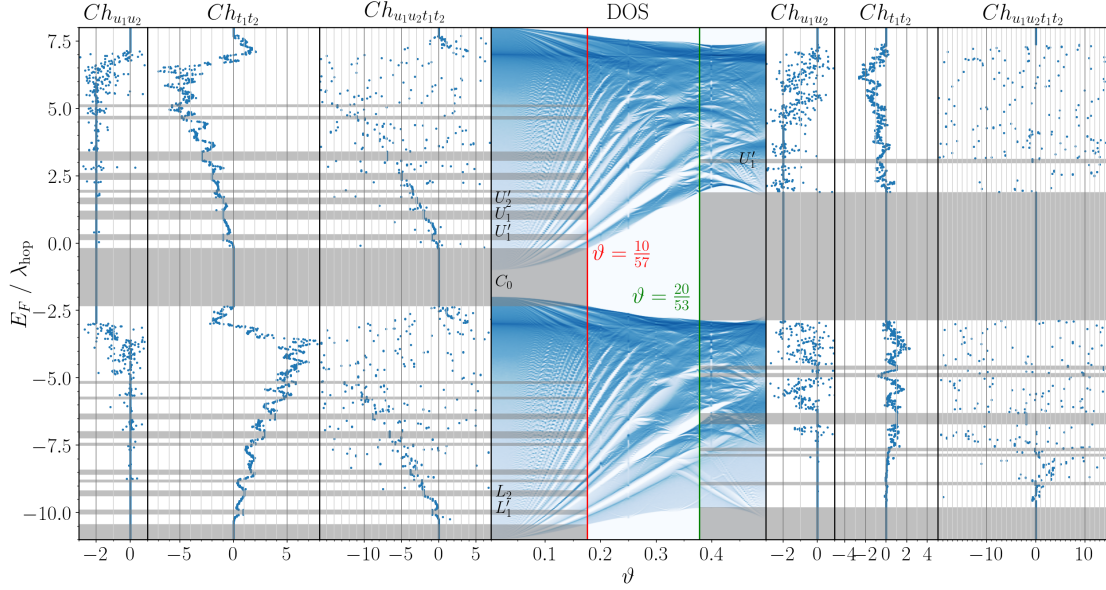


Figure 5.17.: **Main Chern numbers of the sinusoidal skyrmion crystal at zero shift and -0.5 net magnetisation.** We evaluate gap labels in a system of size $N = 57$ and $N = 53$ at $\vartheta = \frac{10}{57}$ and $\vartheta = \frac{20}{53}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = 0$ and $m = -0.5$, and numeric parameter $\Delta\varphi = 10^{-8}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$, $i \in \{0, \dots, N/2 - 1\}$.

5. Chern Hierarchy of Multi-q Textures

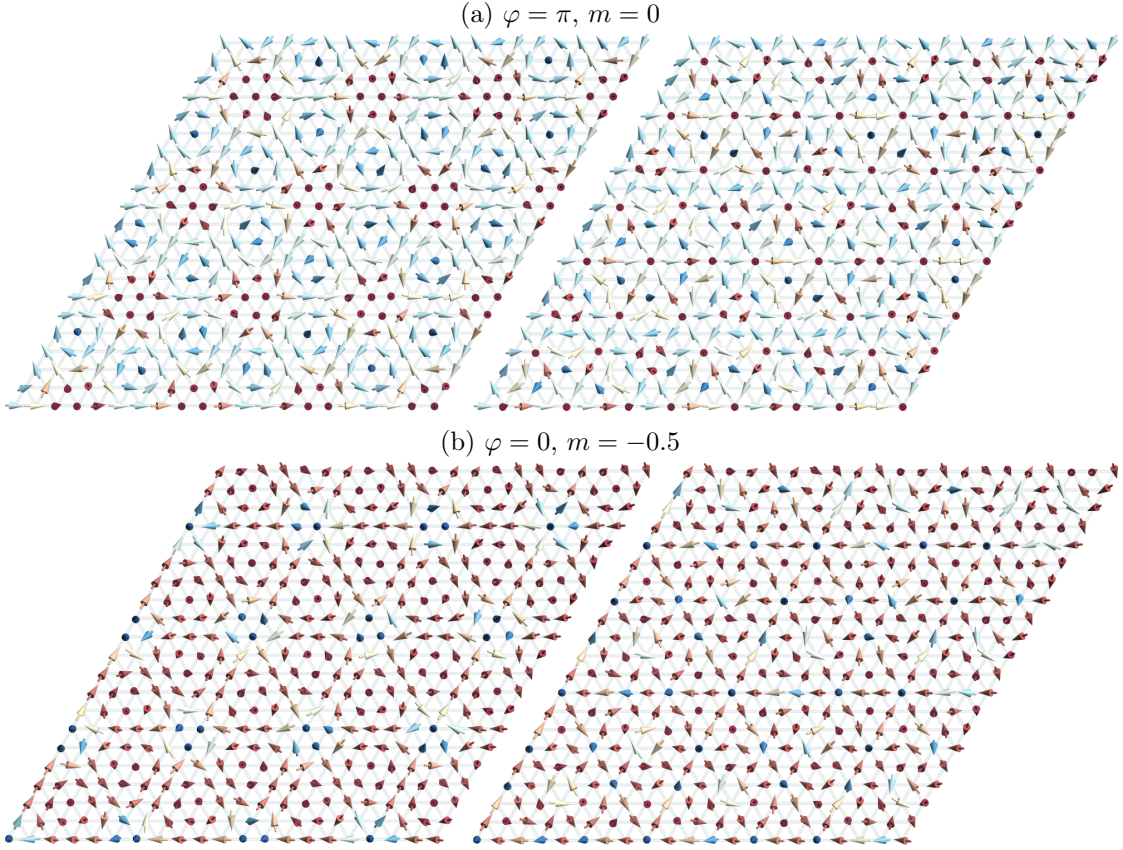


Figure 5.18.: **Sinusoidal 3q skyrmion textures for different parameters.** The figure shows 21×21 sites of the sinusoidal $3q$ skyrmion texture with $\deg \hat{\mathbf{n}} = 2$ ($\varphi = \pi, m = 0$) in (a) and $\deg \hat{\mathbf{n}} = -2$ ($\varphi = 0, m = -0.5$) in (b) for $\vartheta = 10/57$ and for $\vartheta = 20/53$, respectively.

symmetry operation and the result is thus less predictable from general considerations. In the DOS, only the lowest gaps of each block are sufficiently clear, which gives us less energy range at which our Chern number calculations converge to integers. We find $Ch_{\{u_1, u_2\}}$ is far less stable than before, but again only converges to $\deg \hat{\mathbf{n}}$ between the van Hove singularities. However, unexpectedly $Ch_{\{t_1, t_2\}}$ is 0 in the gaps U'_1, U'_2 , and U'_{-1} as well as in the gaps L'_1, L'_2 , and L'_{-1} . Apparently, none of the states carry a contribution to the momentum space first Chern number.

The mixed space second Chern number $Ch_{\{t_1, t_2, u_1, u_2\}}$ is -1 in U'_1 , -3 in U'_2 , and 2 in U'_{-1} . This implies that the first energy band of the block carries a contribution of -1 to the mixed space second Chern number, the second band however carries -2 , and the last band carries -2 as well. We can explain this with our observation from Fig. 5.11 that the gap U_2 closes once we increase the parameter m beyond $\frac{1}{\sqrt{3}}$. Therefore, the states between gap U'_1 and U'_2 are the same as between gap U_1 and U_3 , and thus they carry a contribution of -2 . For the lower block, the L'_1 and L'_{-1} gaps have the same mixed space second Chern numbers as in the upper block, but in the L'_2 gap this Chern number does not converge properly.

5.3. Topological Phase Transitions following a Change in Real Space Winding

For the sinusoidal skyrmion lattice with parameters $\varphi = \pi$ and $m = 0$, we have the same changes as for the helical skyrmion lattice, as seen in Fig. 5.16. The two first Chern numbers change sign together with the real space winding number and the mixed space second Chern number stays unchanged.

Sinusoidal skyrmions

At the second parameter point with $\varphi = 0$ and $m = -0.5$ the situation is different, as shown in Fig. 5.17. Since the texture winding number is the same as for $m = 0$, the real space first Chern number $Ch_{\{u_1, u_2\}}$ is unchanged. However, several new gaps open up that split the contribution to $Ch_{\{u_1, u_2, t_1, t_2\}}$ between each gap in half (from -2 to -1). Most striking is the behaviour of $Ch_{\{t_1, t_2\}}$ which stays at 1 throughout the gaps U'_1 , U_1 , and U'_2 . Apparently, only the states below the new U'_1 gap carry the contribution to this. We can see a similar behaviour for the gaps L'_1 and L_1 .

Next, we examine how the main Chern numbers of the first gap U_1 or, respectively, U'_1 , which are the gaps that stay open for most of the parameter range, change along the paths through the parameter space. The results for the helical skyrmion lattice are displayed in Fig. 5.19 and for the sinusoidal skyrmion lattice in Fig. 5.20. For the top row, we compute the exact diagonalisation of the tight-binding Hamiltonian with $\lambda_{xc}/\lambda_{hop} = 5$ on a supercell of size $N = 57$ with $\vartheta = \frac{10}{57}$, and plot the individual energy eigenvalues. From this diagonalisation, we also compute the corresponding main Chern numbers for the Fermi energy fixed to the centre of the U_1/U'_1 gap as indicated by the dashed lines.

Chern Transitions

For the helical skyrmion lattice, we only consider the first gap of the block of aligned states, that we marked as U_1 or U'_1 depending on the parameter range. This gap stays open for all three line cuts.

Helical skyrmions

Along the $m = 0$ line depicted in Fig. 5.19(a), we have a sharp jump from 1 to -1 in $Ch_{\{u_1, u_2\}}$ at $\varphi = 0.5\pi$, where the winding number switches from 1 to -1 . $Ch_{\{t_1, t_2\}}$ follows this behaviour, but the transition is less sharp and nearly continuous over a wider parameter range. The Chern number transition coincides with two states crossing the first gap. The second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ remains mostly constant at -1 but exhibits a peak in the vicinity of the winding number transition.

$m = 0$

Similarly, following the $\varphi = 0$ line in parameter space, shown in Fig. 5.19(b), $Ch_{\{u_1, u_2\}}$ matches the winding number of the texture. The first jump from 1 to -2 at $m = \frac{1}{\sqrt{3}}$ coincides with a singularity of $Ch_{\{u_1, u_2\}}$, while the second transition from -2 to 0 at $m = \frac{\sqrt{3}}{2}$ appears continuous. This is caused by the real space position of the lattice sites and whether the singularity of the magnetisation vector field occurs close to one of them. If we would additionally average over the phase space, the Chern number would exhibit a singularity at both parameter points. However, $Ch_{\{t_1, t_2\}}$ does not follow suit with the winding number and changes at a lower value of m . Already at $m \approx 0.27$ a band crossing in the first gap occurs and $Ch_{\{t_1, t_2\}}$ changes nearly continuously from 1 to 0. The second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ remains again mostly constant at -1 but exhibits a peak in the vicinity of the band crossing and a singularity at the point of the singularity of $Ch_{\{u_1, u_2\}}$. However, it does not respond to the second continuous change of $Ch_{\{u_1, u_2\}}$.

$\varphi = 0$

5. Chern Hierarchy of Multi-q Textures

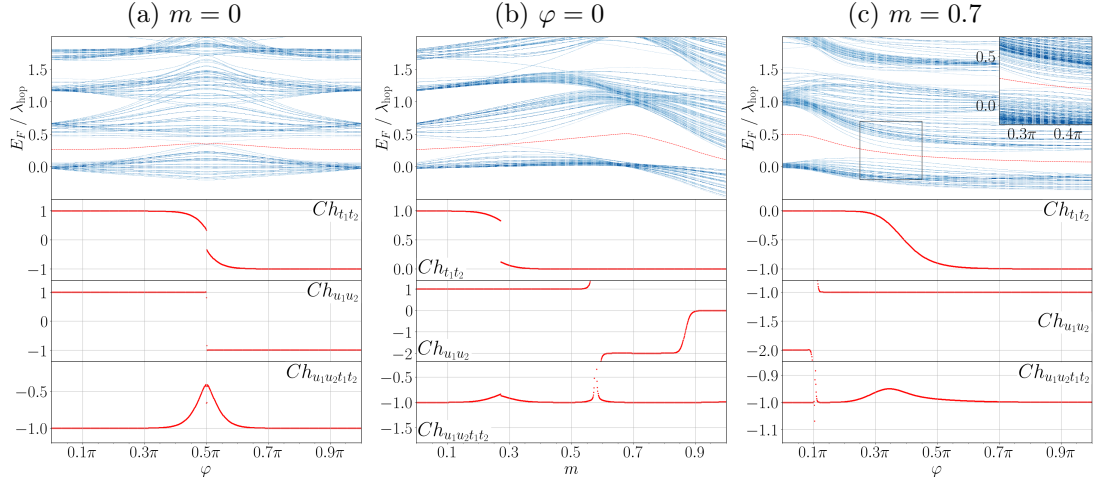


Figure 5.19.: **Chern number evolution across real space phase transitions for the helical skyrmion crystal.** We perform three line cuts through the phase space spanned by the texture parameters (m, φ) and fix the IDS to $1 + 1 \cdot \left(\frac{10}{57}\right)^2$ with the red dashed line marking the Fermi energy positioned in the middle of the gap. We compute the main Chern numbers of the first gap in a system with 57×57 sites at $\vartheta = \frac{10}{57}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$ and numeric parameter $\Delta\varphi = 10^{-8}$. The inset in Fig. 5.19(c) displays the energy eigenvalues computed in a larger system with 137×137 sites and $\vartheta = \frac{24}{137}$. This figure was adapted from [Pra+24, Fig. 10].

$m = 0.7$ The behaviour of the Chern numbers along the $m = 0.7$ line in Fig. 5.19(c) holds more unexpected features. While $Ch_{\{u_1, u_2\}}$ exhibits a singularity around $\varphi = 0.1\pi$ and jumps from -2 to -1 following the winding number, $Ch_{\{t_1, t_2\}}$ changes continuously over a wide range around $\varphi = 0.4\pi$ from 0 to -1 , while none of the eigenvalues in the system of size $N = 57$ cross the gap.

However, for a change in Chern number to occur in a system there must be a gap closing in the spectrum [Bel95], and indeed for a system size of $N = 137$, we observe a suitable crossing in the eigenvalues. At this point we need to remark, that this is not purely dependent on the system size, but rather on the ergodicity condition. For some sizes the crossing does appear, while for others it does not. This could also be resolved by computing the phase space average. Again, for this path the second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ remains mostly constant at -1 with a peak around the band crossing and a singularity at the singularity position of $Ch_{\{u_1, u_2\}}$.

Sinusoidal skyrmions For the sinusoidal skyrmion lattice, the first gap U_1 in the upper block of aligned states at $\varphi = 0$ and $m = 0$ closes for larger m while a second even lower gap U'_1 opens up for $m \neq 0$. Therefore, we consider the behaviour of the main Chern numbers of both of these gaps.

$m = 0$ Tuning the phase shift φ at $m = 0$ yields similar results to the helical skyrmion crystal, as shown in Fig. 5.20(a). Both first Chern numbers $Ch_{\{u_1, u_2\}}$ and $Ch_{\{t_1, t_2\}}$ switch their sign at $\varphi = 0.5\pi$ where the winding number changes from -2 to 2 . The second Chern number stays mostly constant, but exhibits a strange artefact at the winding number

5.3. Topological Phase Transitions following a Change in Real Space Winding

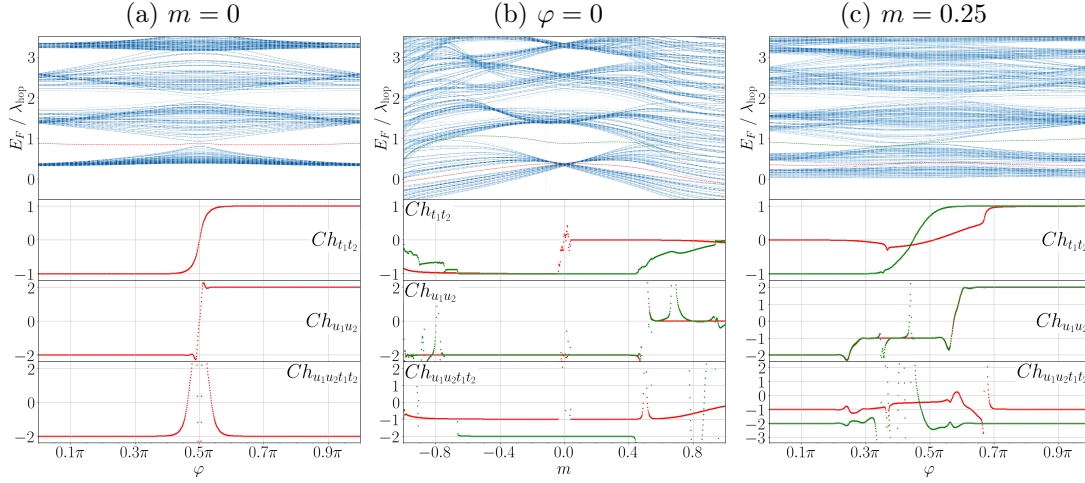


Figure 5.20.: **Chern number evolution across real space phase transitions for the sinusoidal skyrmion crystal.** We perform three line cuts through the phase space spanned by the texture parameters (m, φ) and fix the IDS to $1 + 1 \cdot (\frac{10}{57})^2$ and $1 + 2 \cdot (\frac{10}{57})^2$ with the green and red dashed lines marking the Fermi energy positioned in the middle of the gaps. We compute the main Chern numbers of the first gaps in a system with 57×57 sites at $\vartheta = \frac{10}{57}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$ and numeric parameter $\Delta\varphi = 10^{-5}$.

transition point where it briefly jumps back and forth between -2 and 2 . Since we do not observe states crossing the gap for $N = 57$, our Fermi energy is most likely positioned off centre in a way, such that the passing states would cross it one by one in an appropriately sized system.

Varying the net magnetisation parameter m for fixed $\varphi = 0$ reveals more surprising behaviour of the Chern numbers of the two first gaps, as presented in Fig. 5.20(b). While the real space Chern numbers $Ch_{\{u_1, u_2\}}$ converge to the winding number for those parameters where the respective gaps are open, and the mixed space Chern numbers $Ch_{\{u_1, u_2, t_1, t_2\}}$ stay mostly constant at -1 and -2 in this range, the momentum space Chern number $Ch_{\{t_1, t_2\}}$ seems to be affected by the sign of m . In gap U'_1 it converges to -1 for $m \leq 0$ and transitions to 0 for $m \geq 0$. In contrast, in U_1 it stays at -1 as long as the gap stays open.

The line cut at $m = 0.25$ crosses from the parameter area at which the winding number is -2 through the -1 area into the $+2$ area. We already have seen before, that the gaps close in the -1 area. In Fig. 5.20(c) we see that the momentum space Chern number $Ch_{\{t_1, t_2\}}$ in the U'_1 gap, that is 0 at $\varphi = 0$ for $m \geq 0$ changes to $+1$ once the parameter reaches the winding number $+2$ area, where the gap reopens. In the U_1 gap it seems to continuously transition from -1 to $+1$. The real space Chern number $Ch_{\{u_1, u_2\}}$ follows the texture winding number remarkably well through the closed gap, which we can explain with the fact that all of its contributions are carried by the states with energies at the van Hove singularities between which the gap does not close. This is not true for the mixed space Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$, which only converges to its values -1 and -2 while the gaps stay open.

5. Chern Hierarchy of Multi-q Textures

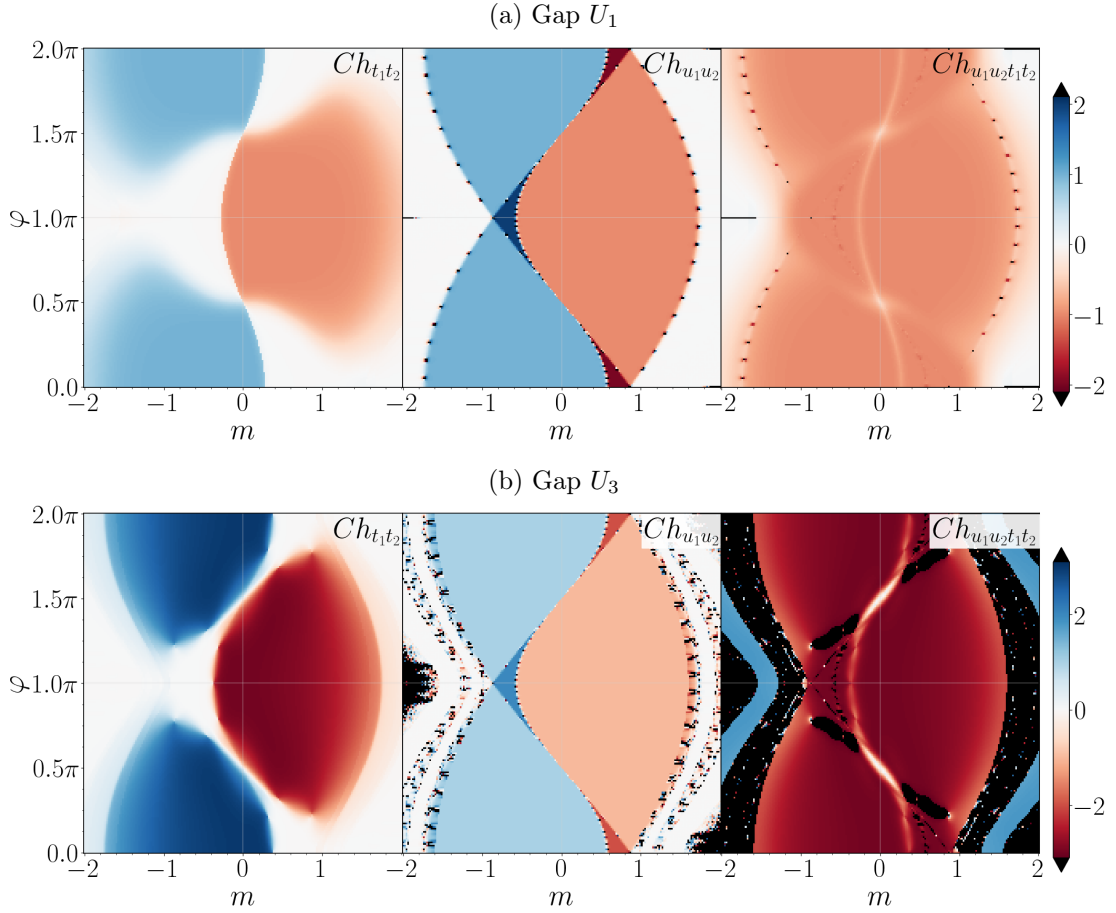


Figure 5.21.: **Topological phase diagrams for the helical skyrmion lattice.** For constant IDS $1 + 1 \cdot \left(\frac{10}{57}\right)^2$ in Fig. 5.21(a) and $1 + 3 \cdot \left(\frac{10}{57}\right)^2$ in Fig. 5.21(b), these diagrams trace the Chern numbers across the phase space spanned by (m, φ) . We compute them in a system with 57×57 sites at $\vartheta = \frac{10}{57}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$ and numeric parameter $\Delta\varphi = 10^{-8}$. Fig. 5.21(a) was adapted from [Pra+24, Fig. 11].

Chern Diagram

Since the parameter positions of the band crossings at which $Ch_{\{t_1, t_2\}}$ changes do not in general match the parameter position of the jumps in winding number, except for at $m = 0$, we further scan over the whole relevant area of parameter space to identify the pattern.

For the helical skyrmion lattice, we compute the main Chern numbers of the first and third gap, U_1 and U_3 , for φ ranging from 0 to π and m ranging from -2 to 2 with the phase space origin set to $\varphi = (\varphi, 0, 0)$ as presented in Fig. 5.21.

Conversely, for the sinusoidal skyrmion lattice, we choose the gaps U'_1 and U_1 that were already the subject of the line cuts in Fig. 5.20. Now, we compute the Chern numbers for φ between 0 and π and m between $-\frac{2}{\sqrt{3}}$ and $\frac{2}{\sqrt{3}}$ with the phase space origin set to $\varphi = (\varphi, 0, 0)$.

5.3. Topological Phase Transitions following a Change in Real Space Winding

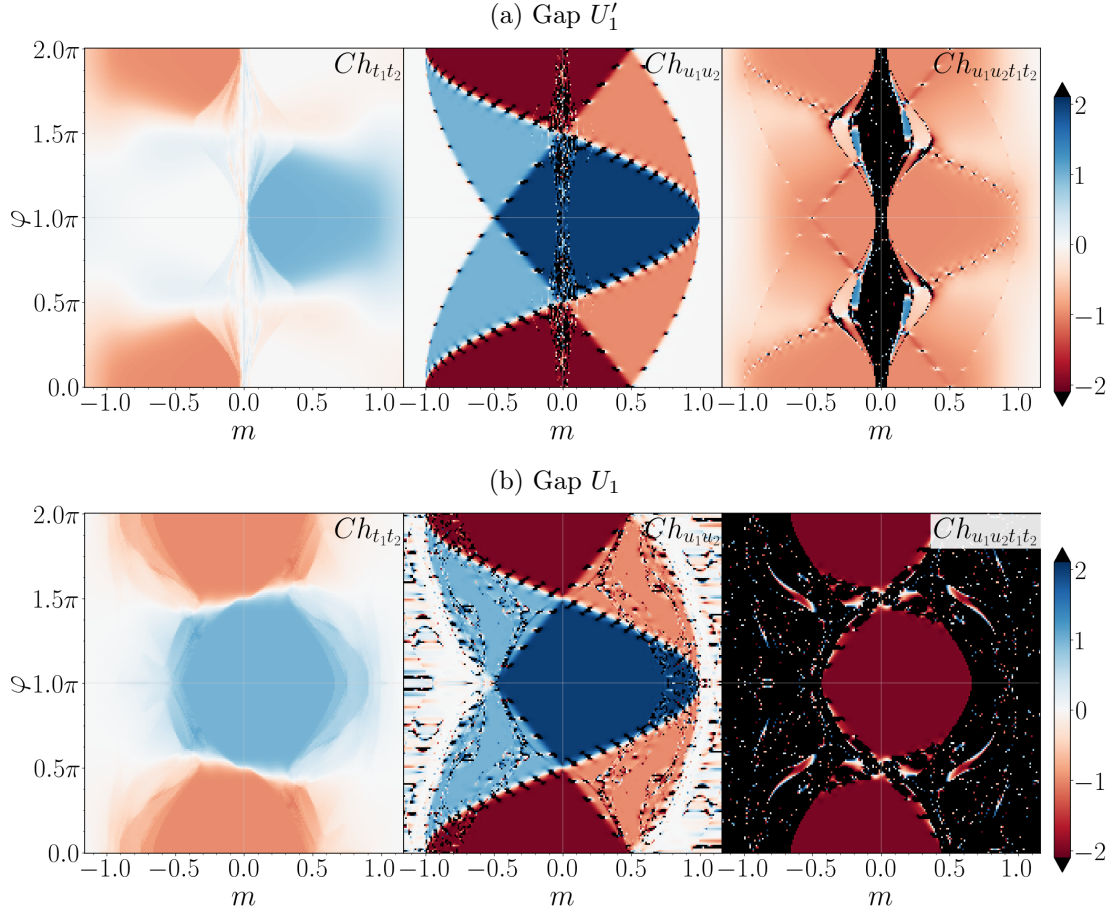


Figure 5.22.: **Topological phase diagrams for the sinusoidal skyrmion lattice.** For constant IDS $1 + 1 \cdot \left(\frac{10}{57}\right)^2$ in Fig. 5.22(a) and $1 + 2 \cdot \left(\frac{10}{57}\right)^2$ in Fig. 5.22(b), these diagrams trace the Chern numbers across the phase space spanned by (m, φ) . We compute them in a system with 57×57 sites at $\vartheta = \frac{10}{57}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$ and numeric parameter $\Delta\varphi = 10^{-5}$.

For the case of helical skyrmions, as shown in Fig. 5.21, it is remarkable how $Ch_{\{u_1, u_2\}}$ of both gaps perfectly reproduces the winding number phase diagram from Fig. 1.4(a). On the borderlines between the different areas, $Ch_{\{u_1, u_2\}}$ of U_1 exhibits singularities at regular distances. They coincide with the points in parameter space for which a discontinuity in the magnetisation texture lies in the immediate vicinity of a lattice site. Due to the different choices of φ these positions do not coincide with the singularities observed along the paths above. Computing the average over the phase space would cause singularities along the whole border. For U_3 there are additional artefacts visible with unclear origin.

Helical skyrmions

For the momentum space Chern number these diagrams show clearly, that $Ch_{\{t_1, t_2\}}$ deviates from the winding number. In particular, around the areas where the winding number changes to ± 2 this Chern number vanishes. Interestingly, the sharp change in $Ch_{\{t_1, t_2\}}$ at which band crossings occur coincides with the parameter line in which the average out-of-plane magnetisation $\langle \hat{n}_z \rangle$ is zero. Precisely at those positions, the system is

5. Chern Hierarchy of Multi-q Textures

time-reversal invariant (modulo lattice symmetry), and thus $Ch_{\{t_1, t_2\}}$ is forced to vanish by symmetry. For U_1 the borders of the areas with $Ch_{\{t_1, t_2\}} = \pm 1$, for $|m| \rightarrow 2$ resemble the borders of the winding number diagram, but are more fuzzy which might be a finite system size effect. For U_3 the borders are similar but significantly sharper.

As for the line cuts, the second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ remains mostly constant at -1 and -3 in the area of non-zero winding number. At the transition borders of the other Chern numbers it is affected by peaks or singularities but does not change, except for the outside border for $|m| \rightarrow 2$ for which it transitions to 0 in U_1 . For U_3 the convergence fails beyond the area where the winding number is non-zero, except for a small strip for which the formula for $Ch_{\{u_1, u_2, t_1, t_2\}}$ briefly converges without any clear reason.

*Sinusoidal
skyrmions*

For the sinusoidal skyrmion system depicted in Fig. 5.22, $Ch_{\{u_1, u_2\}}$ also reproduces the winding number phase diagram from Fig. 1.6(a). For U'_1 , we have artefacts around the borders as before, and along $m = 0$, where U'_1 closes, whereas U_1 is free from artefacts in the area where it is open with a multitude of artefacts outside.

The distribution of $Ch_{\{t_1, t_2\}}$ significantly differs between these two gaps. For both, it takes values of ± 1 , but for U'_1 seemingly only in the areas with $\deg \hat{\mathbf{n}} = -2$ and $m < 0$ and $\deg \hat{\mathbf{n}} = 2$ and $m > 0$. Since the net magnetisation $\langle \hat{n}_z \rangle$ is zero at $m = 0$, this is consistent with the observations for the helical skyrmion lattice. However, for U_1 the situation is different. There, $Ch_{\{t_1, t_2\}}$ is non-zero in the area with $\deg \hat{\mathbf{n}} = \pm 2$, where the gap U_1 is open.

The second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ of U'_1 stays constant at -1 where the gap is open with strong artefacts around $m = 0$. For U_1 the distribution is nearly opposite, but follows the same pattern. Where the gap is open, it is constant at -2 and the formula diverges everywhere else.

5.4. The Existence of Spectral Flow

The gap labels are invariant under continuous deformations of the system that preserve the gap. Nevertheless, in the last section, we had several instances of change in the real space Chern number $Ch_{\{u_1, u_2\}}$ that were seemingly not accompanied by states crossing the spectral gap. We conjecture that the reason for this lies in the singular nature of the winding number transition in real space that is not necessarily captured by the finite, discretised representation of the electronic observables.

In this section, we apply a regularisation to the normalised vector field, such that the singularity becomes continuous and affects the spins at lattice sites in a neighbourhood of the critical parameter point. In the DOS evolution along the line cuts computed with this regularised texture, there are, in fact, states crossing the gaps, especially the zero energy gap. We compute the Chern number transitions to match these gap crossings with the change in gap labels. The analysis for the helical skyrmion system is partially adapted from [Pra+24, Chap. 5.3].

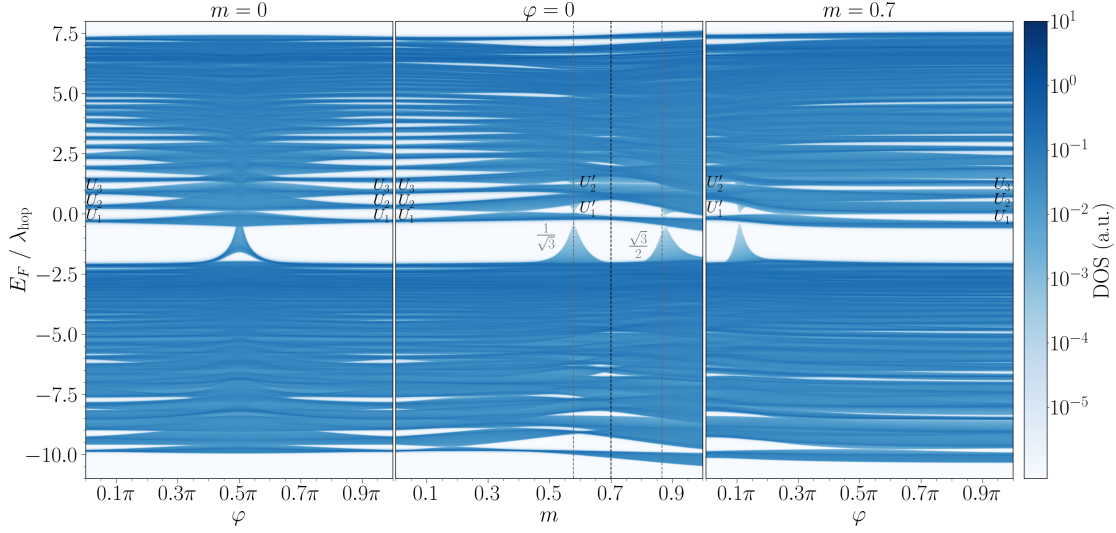


Figure 5.23.: **Density of states evolution across real space phase transitions for the helical skyrmion lattice with regularisation.** We perform three different line cuts through the phase space spanned by the texture parameters (m, φ) and compute the DOS along them using the KPM for a system of size $N = 401$ with $\vartheta = \frac{70}{401}$ with system parameters $\lambda_{\text{xc}}/\lambda_{\text{hop}} = 5$ and texture regularisation $\eta = 0.1$. This figure was adapted from [Pra+24, Fig. 12].

In Chap. 1.3.4, we discussed how the winding number transitions occur and how regularising the normalised vector field makes the transitions continuous. We demonstrated this for the case of an isolated skyrmion seen in Fig. 1.11. Following that procedure, we regularise the $3q$ skyrmion textures with a parameter $\eta = 0.1$, as described in Eq. (1.35):

$$\hat{\mathbf{n}} = \frac{\mathbf{n}}{\|\mathbf{n}\|} \longrightarrow \frac{\mathbf{n}}{\|\mathbf{n}\| + \eta} = \hat{\mathbf{n}}_\eta.$$

This leads to a shift in energy close to the transition, a shift of the critical parameter point (φ_c, m_c) at which the transition occurs, and a crossing of energy eigenstates.

We compute the spectrum of the tight-binding Hamiltonian with regularised magnetic skyrmion texture analogous to Fig. 5.11 and Fig. 5.12 with the KPM on a system of size 401 as displayed in Fig. 5.23 and Fig. 5.24.

Indeed, for the DOS of the helical skyrmion crystal in Fig. 5.23, along the $m = 0$ path, we clearly see the band crossing at $\varphi = \pi$. The bands of the upper block bend downwards and the bands of the lower block bend upwards. At the top of the lower block, a single band bends upwards until it touches the bottom band of the upper block, crossing the zero energy gap. Similarly, we also see band crossings along $\varphi = 0$ at the parameter positions of the winding number jumps, however with a lower density of states. Since, for this computation, the phase space origin φ of the texture was chosen in such a way, that the first singularity along this line cut would sit right on the lattice site with label $\mathbf{0}$, the first band crossing fully closes the gap while the second crossing leaves a small gap open. Further, at $m = 0.7$, we can see how states from the lower block bend upwards and cross the gap around $\varphi = 0.1\pi$, where the winding number transition takes place.

Regularisation

DOS Evolution

Helical skyrmions

5. Chern Hierarchy of Multi-q Textures

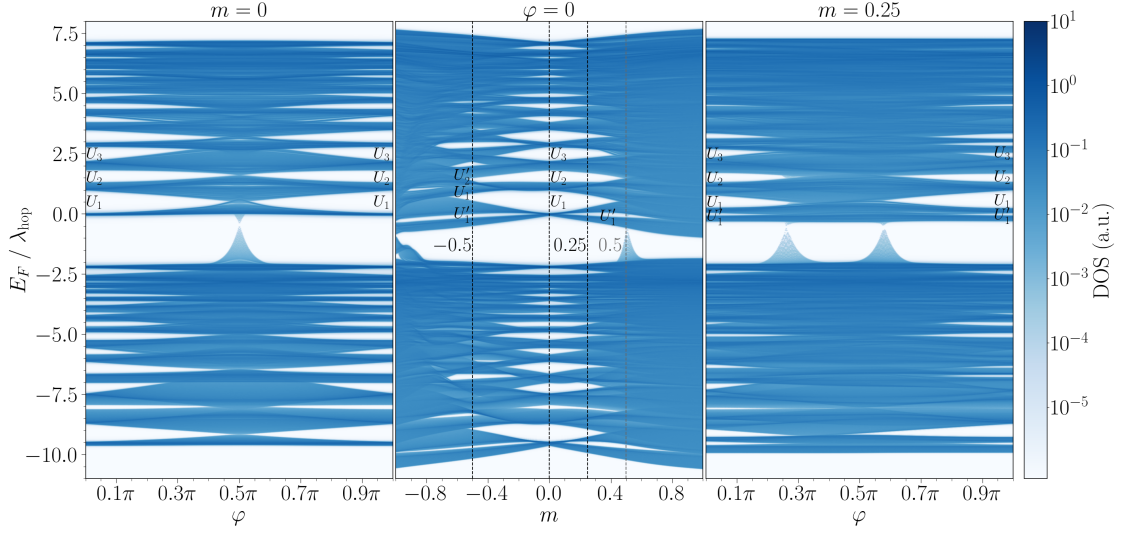


Figure 5.24.: **Density of states evolution across real space phase transitions for the sinusoidal skyrmion lattice with regularisation.** We perform three different line cuts through the phase space spanned by the texture parameters (m, φ) and compute the DOS along them using the KPM for a system of size $N = 401$ with $\vartheta = \frac{70}{401}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$ and texture regularisation $\eta = 0.1$.

Sinusoidal skyrmions

For the sinusoidal skyrmion crystal, band crossings are revealed in the DOS in Fig. 5.24. At the parameter values for which the winding number changes, the gaps close, which is in particular striking for the zero energy gap. In addition, at $\varphi = 0$ the central gap closes fully for $m \rightarrow -1$, where the winding number jumps to zero.

Chern Transitions

Finally, we need to examine the effect of the regularisation on the Chern number transitions, which we do for the helical skyrmions in Fig. 5.25 and for the sinusoidal skyrmions in Fig. 5.26 computed analogously to Fig. 5.19 and Fig. 5.20, but with the regularisation procedure applied. We can observe the behaviour of the individual energy eigenstates of the tight-binding Hamiltonian for system size $N = 57$ and the corresponding main Chern numbers.

Helical skyrmions

Along $m = 0$ in Fig. 5.25, we see how a high number of states is bent upwards, such that several states close the gap. The transition of the Chern numbers is nearly identical to that in Fig. 5.19, except for $Ch_{\{u_1, u_2, t_1, t_2\}}$ which exhibits a broader peak than before. For $\varphi = 0$, we see a single energy state close the gaps for the first transition, due to the choice of the phase space origin, and a few states bend only halfway upwards to close the gaps for the second transition.

The Chern numbers behave very similar to those in Fig. 5.19, except for the position of the $Ch_{\{t_1, t_2\}}$ transition which happens at around $m \approx 0.375$ in comparison to $m \approx 0.275$ for the texture which was not regularised. The regularisation predominantly impacts the magnetisation and therefore also the parameter position for which $\langle \hat{n}_z \rangle$ goes to zero. $Ch_{\{u_1, u_2, t_1, t_2\}}$ exhibits a new dip at the second transition.

5.4. The Existence of Spectral Flow

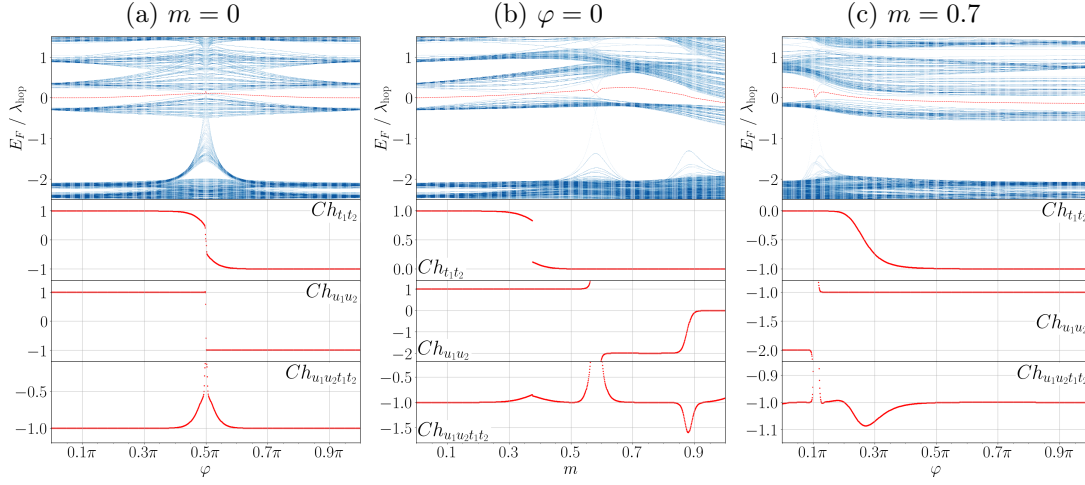


Figure 5.25.: **Chern number evolution across real space phase transitions for the helical skyrmion crystal with regularisation.** We perform three line cuts through the phase space spanned by the texture parameters (m, φ) and fix the IDS to $1 + 1 \cdot \left(\frac{10}{57}\right)^2$ with the red dashed line marking the Fermi energy positioned in the middle of the gap. We compute the main Chern numbers of the first gap in a system with 57×57 sites at $\vartheta = \frac{10}{57}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, numeric parameter $\Delta\varphi = 10^{-8}$, and texture regularisation $\eta = 0.1$. This figure was adapted from [Pra+24, Fig. 13].

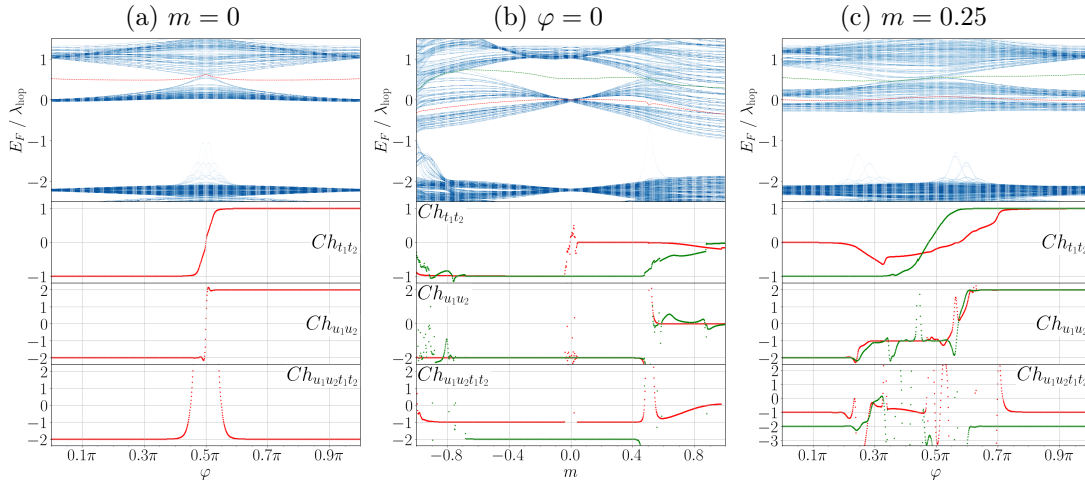


Figure 5.26.: **Chern number evolution across real space phase transitions for the sinusoidal skyrmion crystal with regularisation.** We perform three line cuts through the phase space spanned by the texture parameters (m, φ) and fix the IDS to $1 + 1 \cdot \left(\frac{10}{57}\right)^2$ and $1 + 2 \cdot \left(\frac{10}{57}\right)^2$ with the green and red dashed lines marking the Fermi energy positioned in the middle of the gaps. We compute the main Chern numbers of the first gaps in a system with 57×57 sites at $\vartheta = \frac{10}{57}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, numeric parameter $\Delta\varphi = 10^{-5}$, and texture regularisation $\eta = 0.1$.

5. Chern Hierarchy of Multi-q Textures

For $m = 0.7$, we also only have a single energy state which nearly closes the gap at the position where formerly the singularity occurred. The position of the $Ch_{\{t_1, t_2\}}$ transition is shifted from around $\varphi = 0.4\pi$ to around $\varphi = 0.27\pi$, which is also due to the change in magnetisation.

Sinusoidal skyrmions

For the sinusoidal skyrmion lattice, the regularisation with $\eta = 0.1$ is not strong enough to close the zero energy gap in any instance for this system size. However, the DOS still provides us with some insights: For $m = 0$, the states bending upwards to close the gap form out two peaks, which may explain the peculiar oscillating behaviour of $Ch_{\{u_1, u_2, t_1, t_2\}}$ in Fig. 5.20(a). At $\varphi = 0$ and $m = 0.5$, we see a single energy eigenstate cross the gap, while for the line cut along $m = 0.25$ the states do not cross the gap fully.

Conclusion spectral flow

The reason why the spectral flow over the phase transition does or does not appear in real space can be found in algebraic arguments. For a change to occur in the gap labels, the continuous path of gap projections must exit the K_0 -equivalence class of the projection at the initial parameter point. In the case of a normalised texture undergoing a discontinuous transition, we leave the observable algebra $M_2(\mathbb{C}) \otimes (C(T^2) \rtimes_{\theta}^{\Phi} \mathbb{Z}^2)$, which requires the continuity of the texture functions on the phase space T^2 and, thereby, on the real space $\mathbb{R}^2$. With that, we no longer have a continuous path of Hamilton operators, which at each point are given by the covariant representation of an element from the observable algebra. Consequently, the Fermi projections prior to and following the critical point are no longer homotopic in the space of projections from the observable algebra.

It is important to note that this does not necessitate the closure of the gap in the spectrum of the Hamiltonian. The singularity of the texture is located at a point of zero measure and almost surely occurs between the lattice sites, where it does not affect the computation. Even if it would fall exactly on a lattice site, e.g. by choice of the phase origin φ , the programme would abort due to the undefined behaviour. By regularising the singularities of the texture, the continuous path of Hamilton operators is restored. Now, K -theory needs to enforce the existence of spectral flow. Since the gap labels preceding and following the critical point are distinct, even though the algebra is no longer exited, the homotopy needs to be disrupted otherwise to allow for this alteration: The gap needs to be closed to ensure that the path of operators exits the space of projections.

6 | Orbital Magnetisation and Finite Magnetic Field

By incorporating an external magnetic field, we can describe the electronic system's response to changes in the magnetic flux in terms of orbital magnetism. Moreover, we can generally consider multi- q textures permeated by a finite magnetic field, as is common in skyrmion experiments.

The helical skyrmion texture breaks time-reversal invariance, which causes the circulation of the electrons in the material to induce an orbital contribution to the magnetisation [San+16; SL17; Lux+18; Göb+19]. This orbital magnetisation can be computed in our framework according to the derivation in Chap. 3.4.3. This enables us to study the Fermi energy dependence of the orbital magnetisation in the helical skyrmion crystal at zero external magnetic field, as well as the texture parameter dependence for a fixed gap.

*Orbital
Magnetism*

The energy spectrum of a non-interacting electron gas on a two-dimensional lattice permeated by a magnetic field splits into Landau levels. Visualising their dependence on the magnetic flux reveals a fractal pattern, known as Hofstadter's butterfly [Hof76], that can be classified by K -theoretic gap labels. This is a similar phenomenon to the one we witness in the presence of a non-collinear spin texture. If both a magnetic field and a helical skyrmion texture are present simultaneously, the number of states per level is determined by the competing influences of the magnetic flux ϕ and the skyrmion density ϑ^2 . This widens the spectral gaps and modifies the respective dependences on the other parameter. The computational programme allows us to evaluate the Chern numbers and orbital magnetisation of the helical skyrmion crystal for a finite magnetic field. This is a common situation in experimental setups where the spin texture is stabilised by an external magnetic field. We further investigate the scaling behaviour of the orbital magnetisation in a fixed gap for varying magnetic flux and texture pitch and reveal a non-linear dependence.

Finite Field

The transitional state with zero winding of the helical skyrmion lattice for the relative phase $\frac{\pi}{2}$ is a so-called meron-antimeron lattice. Meron refers to a spin structure that can be assigned a half-integer winding number, whereas an anti-meron carries the compensating contribution. In the absence of an external magnetic field, all gaps are closed as presented in Chap. 5.3. However, in the presence of finite magnetic flux, gaps are forced to open. Since the winding number transition is characterised by an isolated singularity, the vector field describing the meron-antimeron lattice is discontinuous. This makes the tight-binding Hamiltonian an element outside the observable algebra. Nevertheless, the numerical methods are still applicable, and the implications can be studied.

*Meron-
Antimeron
lattice*

6. Orbital Magnetisation and Finite Magnetic Field

Chapter content

This chapter considers the helical skyrmion texture in zero and finite magnetic fields. We start by evaluating the orbital magnetisation at zero flux over the Fermi energy and in dependence on the texture parameters in Sec. 6.1. Next, we examine the effects of a finite magnetic flux on the DOS with and without the skyrmion texture in Sec. 6.2. Then, we evaluate the orbital magnetisation at finite flux and investigate the scaling behaviour for the orbital magnetisation of a fixed gap in Sec. 6.3. Lastly, we consider the case of the meron-antimeron lattice in a finite field and discuss the findings in Sec. 6.4.

6.1. Orbital Magnetisation of the Skyrmion Lattice at Zero Field

In materials with an internal spin magnetisation, such as the skyrmion lattice, the time-reversal symmetry suppressing orbital magnetisation may be broken. The C^* -algebra description of the electronic system facilitates calculating the derivative of physical observables with respect to the magnetic flux, as introduced in form of the Itô-derivative in Chap. 3.2.3. We can therefore compute the orbital magnetisation as the response of the free energy to changes in the magnetic flux, as outlined in Chap. 3.4.3. In the following, we focus on the helical skyrmion lattice introduced in Chap. 1.2.3.3, which has been the subject of research before [Göb+19; GSM25], and can qualitatively reproduce the literature results. To further investigate the relationship between the real space properties, such as the winding number and the net magnetisation, to the orbital magnetisation, we extend our analysis regarding the topological phase transitions from Chap. 5.3.

In this section, we compute the orbital magnetisation on the helical skyrmion crystal. First, we evaluate the dependence on the Fermi energy, then we consider the first gap along line cuts through parameter space, and finally we generate a diagram for the first gap in the full parameter space. We separate and compare the local and itinerant circulation contributions to the overall orbital magnetisation.

*Energy
dependence*

In Fig. 6.1, we display the orbital magnetisation M_{orb}^z and its local and itinerant circulation components for the helical skyrmion lattice over the full range of Fermi energies, next to the DOS and main Chern numbers, that were already presented in Fig. 5.5. Inside the spectral gaps, the orbital magnetisation has a constant slope of $-2Ch_{\{t_1, t_2\}}$ as ensured by the implemented formula Eq. (4.29). It qualitatively reproduces the findings from literature for the orbital magnetisation in a tight-binding model on a triangular lattice with $N^2 = 49$ sites coupled to a skyrmion lattice [Göb+19, Fig. S5(c)]. It is interesting, that the orbital magnetisation is non-zero in the central zero-energy gap, even though the momentum space Chern number is zero. Above the highest and below the lowest energy state it vanishes as to be expected. The two components to the overall orbital magnetisation are the local and itinerant circulation contributions adjusted to the Fermi energy, which are therefore respectively linear with slope $-Ch_{\{t_1, t_2\}}$. We find them competing and enveloping the total orbital magnetisation. This is consistent with their semi-classical interpretation, as first described in [Tho+05]. Around the VHS we find the two contributions switching signs, which coincides with the change of sign in the momentum space Chern number.

6.1. Orbital Magnetisation of the Skyrmion Lattice at Zero Field

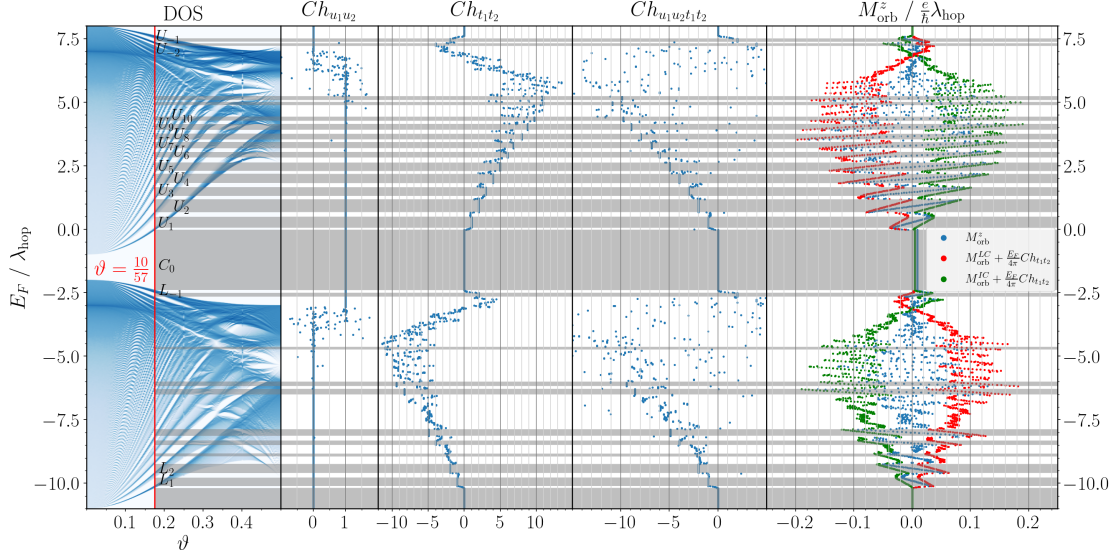


Figure 6.1.: **Orbital Magnetisation in the helical skyrmion crystal at zero shift and net magnetisation at zero magnetic field.** We evaluate the orbital magnetisation and its components in a system of size $N = 57$ at $\vartheta = \frac{10}{57}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = 0$ and $m = 0$, and numeric parameter $\Delta\varphi = 10^{-8}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$, $i \in \{0, \dots, N/2 - 1\}$.

Next, we consider the orbital magnetisation at the Fermi energy pinned to the middle of the gap U_1 . In Fig. 6.2, we follow the line cuts introduced in Chap. 5.3 for the same scenario as in Fig. 5.19.

Orbital magnetisation transitions

For the line cut at $m = 0$ in Fig. 6.2(a), for which the start and end point are related by time reversal, we find the orbital magnetisation and its contributions switch sign after crossing zero at $\varphi = 0.5\pi$. Since the contributions decrease for increasing φ before the momentum space Chern number starts its transition, this cannot be fully attributed to the role of $Ch_{\{t_1, t_2\}}$. Of further significance are the zero transitions of M_{orb}^z at around $\varphi = 0.32\pi$ and $\varphi = 0.68\pi$, which do not match any of the considered texture properties.

For $\varphi = 0$ the situation is more straightforward, as seen in Fig. 6.2(b). The orbital magnetisation stays negative and the two contributions decrease in size for increasing m . They do not seem to depend strongly on $Ch_{\{t_1, t_2\}}$ except for discontinuities at the point of the transition, where the net magnetisation $\langle n_z \rangle$ changes sign. It further seems uncorrelated to the changes in the real space winding number.

Along the $m = 0.7$ line cut in Fig. 6.2(c), we have a similar but opposite development. The two contributions cross at around $\varphi = 0.14\pi$ and then increase in size but level out for $\varphi > 0.5\pi$. This seems similar to the end point of the transition along $m = 0$, however M_{orb}^z is of opposite sign.

6. Orbital Magnetisation and Finite Magnetic Field

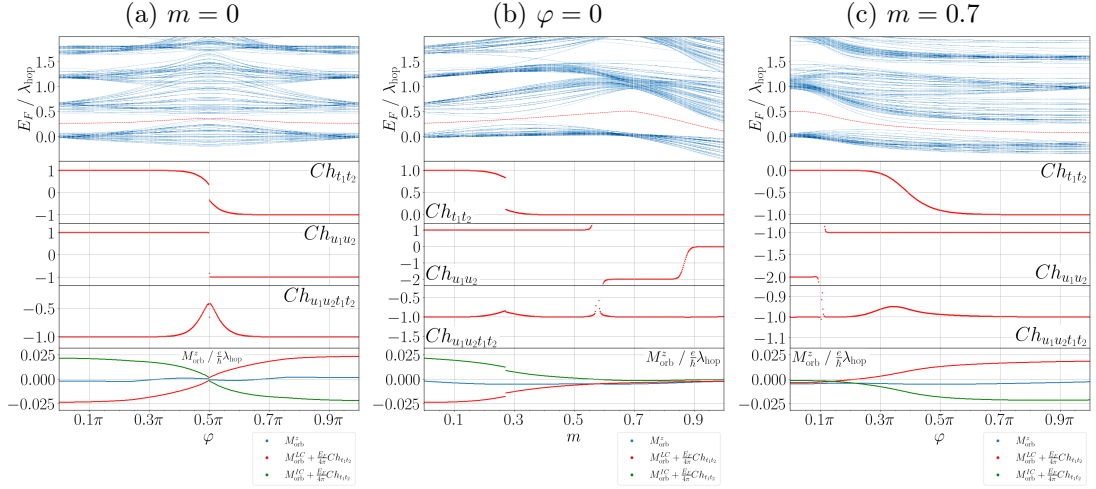


Figure 6.2.: **Orbital magnetisation evolution across real space phase transitions for the helical skyrmion crystal.** We perform three line cuts through the phase space spanned by the texture parameters (m, φ) and fix the IDS to $1 + 1 \cdot \left(\frac{10}{57}\right)^2$ with the red dashed line marking the Fermi energy positioned in the middle of the gap. We compute the orbital magnetisation and its components for the U_1 gap in a system with 57×57 sites at $\vartheta = \frac{10}{57}$.

In conclusion, from the three line cuts there is no obvious relationship between the orbital magnetisation and its contributions, the real space texture properties as displayed in Fig. 1.4, and the gap labels apparent. However, this could be obfuscated by the influence of the Fermi energy that varies over the parameter range and has a linear influence on the orbital magnetisation (in areas of constant $Ch_{\{t_1, t_2\}}$).

*Orbital
magnetisation
diagram*

In order to investigate the overall relationship between the texture properties and the orbital magnetisation, we compute the Fermi energy, the total orbital magnetisation, and both its contributions over the full range of parameters, as presented in Fig. 6.3. We find the orbital magnetisation changes its sign around $m = 0$, but not along the line with $\langle n_z \rangle = 0$. This line feature is also discernible in the first diagram, which depicts the Fermi energy fixed to the middle of the U_1 gap over the texture parameter range. It is important to note that the Fermi energy landscape depends heavily on the chosen location inside the gap, as the gap is neither symmetric nor of equal width over the parameter range, as seen in Fig. 6.2 along the line cuts. Therefore, the line in parameter space of the zero transition might hold no wider significance. The local and itinerant circulation contributions are largest in the areas where the momentum space Chern number is non-zero, as seen when comparing with Fig. 5.21(a). Also, for them, the new line feature is clearly discernible and bounds a region of larger value for the local circulation and lower value for the itinerant circulation contribution.

In conclusion, the orbital magnetisation and its contributions in the U_1 gap vary for different texture parameters. This cannot be purely attributed to the linear influence of the Fermi energy (in the regions with fixed momentum space Chern number). Nevertheless, the sign of the orbital magnetisation seems to correspond loosely to the sign of m .

6.2. The Skyrmion Lattice at Finite Field

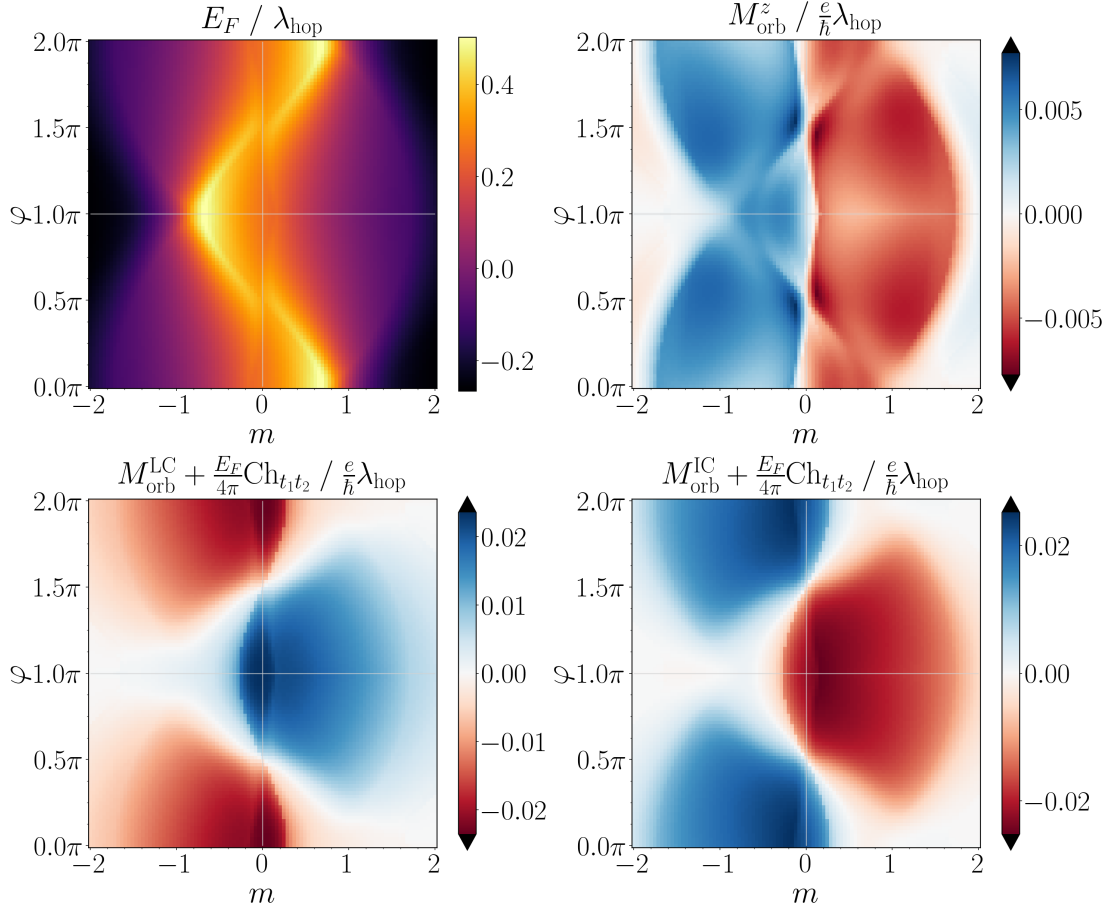


Figure 6.3.: **Orbital magnetisation diagram for the helical skyrmion lattice.** For constant IDS $1 + 1 \cdot \left(\frac{10}{57}\right)^2$, these diagrams trace the orbital magnetisation and its components across the phase space spanned by (m, φ) . We compute them in system with 57×57 sites at $\vartheta = \frac{10}{57}$ with system parameters $\lambda_{xc}/\lambda_{hop} = 5$ and numeric parameter $\Delta\varphi = 10^{-8}$.

6.2. The Skyrmion Lattice at Finite Field

The magnetic field and the skyrmion texture both create spectral gaps by binding states to an energy level. From the decomposition of the IDS we know that the number of states is, respectively, proportional to the magnetic flux ϕ and the skyrmion density ϑ^2 . In case both the non-collinear spin texture and the external magnetic field are present at once, these effects are amplified.

In this section, we consider the density of states over the magnetic flux with no background, ferromagnetic background, and helical skyrmion lattices of different densities. For the cases without the skyrmion texture, we analyse the integrated density of states and compute the gap labels as done in Chap. 5.1-5.2. Finally, we also compare the density of states over the texture's pitch for a variety of magnetic fluxes.

6. Orbital Magnetisation and Finite Magnetic Field

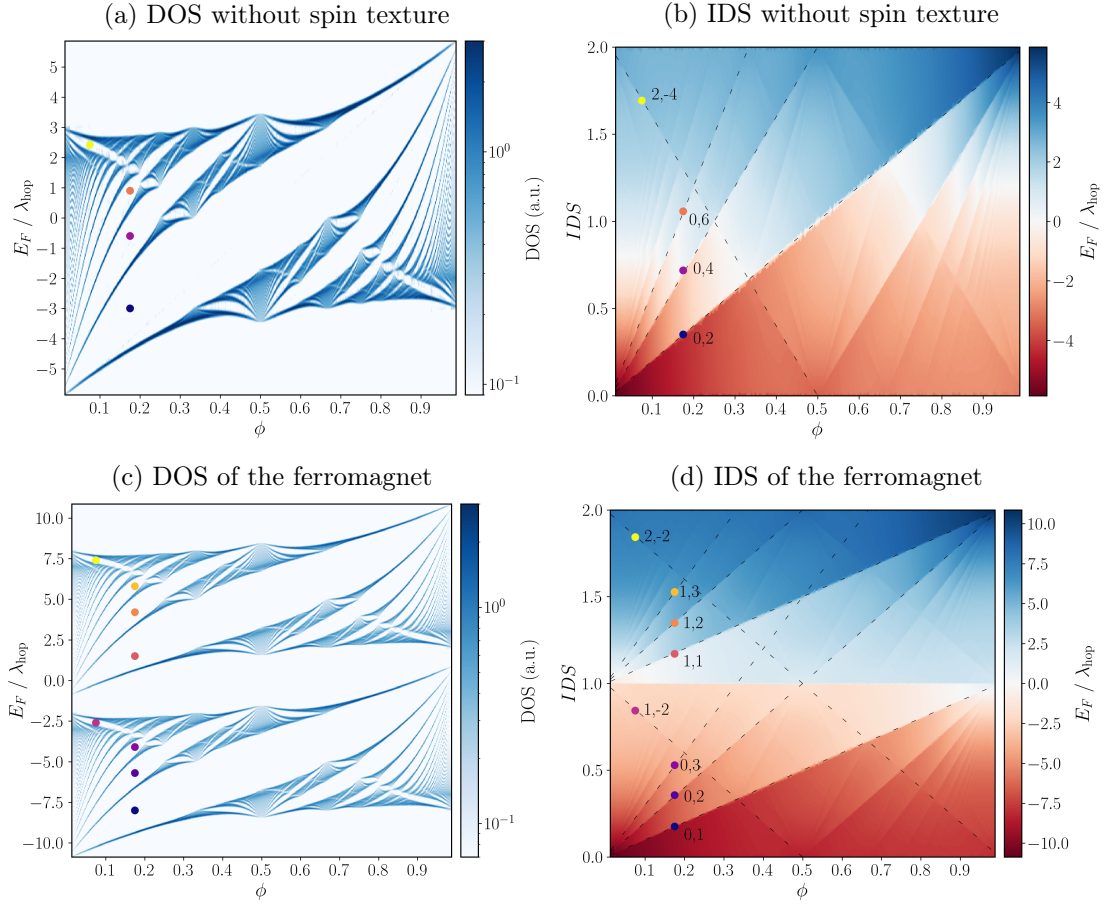


Figure 6.4.: **Hofstadter's butterfly of the triangular lattice.** DOS and IDS for systems at $k_B T = 0.01 \lambda_{\text{hop}}$ with N^2 sites and periodic boundary conditions, where $N \in [19, 79] \cap \mathbb{N}$ and $\phi \in (0, 1)$ such that $N\phi \in \mathbb{N}$ for some N . (a) and (b) without spin texture ($\lambda_{\text{xc}} = 0$), and (c) and (d) coupled to a ferromagnetic background ($\lambda_{\text{xc}}/\lambda_{\text{hop}} = 5$ and $\vartheta = 0$). Coloured bullets are used to match some gaps in the DOS with the corresponding line features in the IDS.

*Hofstadter's
butterfly*

Hofstadter's Butterfly is the colloquial term for the spectrum of a non-interacting two-dimensional electron gas in a lattice permeated by a perpendicular magnetic field of varying flux [Hof76]. The gaps between the Landau levels follow a fractal, self-similar pattern. On a square lattice the graph is symmetric in x - and y -direction and the largest gap therefore resembles the wings of a butterfly. If we set the exchange parameter λ_{xc} from our model to zero, we obtain the well-known variant on the triangular lattice [Oh00; LWG11], as presented in Fig. 6.4(a). Since the observable algebra of this system is generated by just the translation generators t_1, t_2 , the IDS of the gaps follows the linear relation

$$n_\emptyset + \phi n_{\{t_1, t_2\}}, \quad (6.1)$$

which we obtain from the Chern number decomposition in Chap. 3.4.2 with $\vartheta = 0$.

6.2. The Skyrmion Lattice at Finite Field

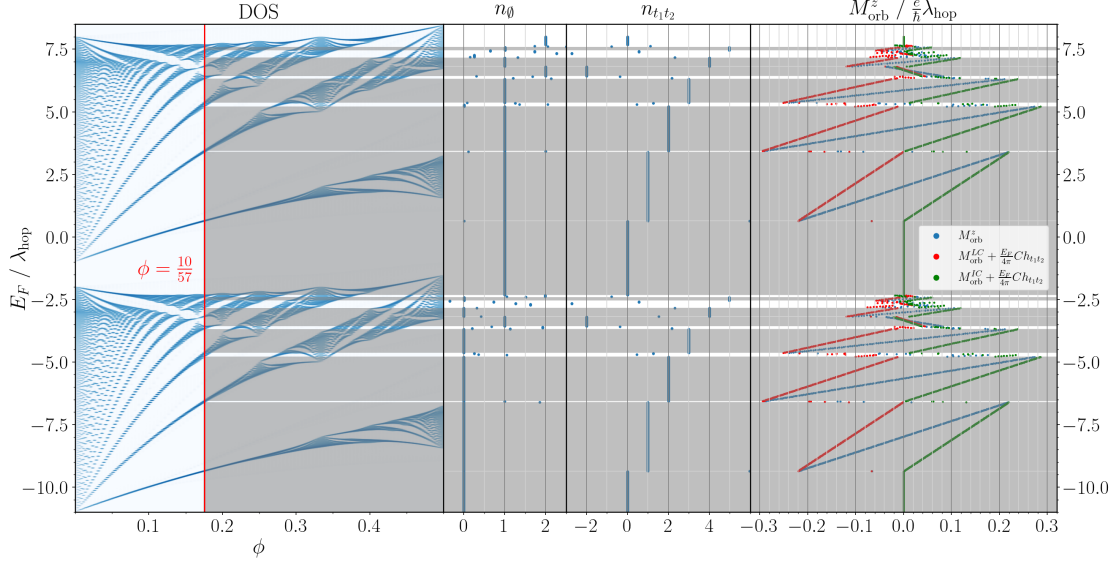


Figure 6.5.: Main gap labels and orbital magnetisation of the Hofstadter butterfly. We evaluate the gap labels and orbital magnetisation in a system of size $N = 57$ at $\phi = \frac{10}{57}$ and $\varphi = 0$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$ and numeric parameter $\Delta\varphi = 10^{-5}$. The DOS is computed via KPM for a system of size $N = 400$ with $\phi = i/N$, $i \in \{0, \dots, N/2 - 1\}$.

With our choice of normalisation, each Landau level carries a momentum space Chern number contribution of 2 as it contains both the states with spin parallel and with spin antiparallel to the magnetic field. The IDS with annotated gap labels is shown in Fig. 6.4(b). This is the case for a low field, whereas for higher fields the levels would split and separate [Dav97, Chap. 6.4.3].

By choosing a ferromagnetic background with $\lambda_{xc} = 5\lambda_{hop}$ and $\varphi = 0$, we can separate the DOS into two blocks of aligned and anti-aligned states (with respect to the magnetic field's direction) with a zero energy gap in between, as in Fig. 6.4(c). By doing this, the states per Landau level in both blocks are halved, as can be detected from the IDS in Fig. 6.4(d).

As a verification, we can also compute the gap labels using our computational programme, as presented in Fig. 6.5. For this computation it is important to disregard any results involving the real space derivations ∂_{u_i} . With the implementation presented in Eq. (4.26), the choice of $\vartheta = 0$ does not affect the computation of the derivations, which leads to non-zero results. For the proper choice of $\hat{\mathbf{n}} \equiv \hat{\mathbf{e}}_z$, these derivations vanish and the gap labels for $\{u_1, u_2\}$ and $\{u_1, u_2, t_1, t_2\}$ are zero. We can further compute the orbital magnetisation caused by the circulation of the electrons [AAM96].

If we consider a system coupled to a multi- q texture, such as the $3q$ helical skyrmion lattice, permeated by a perpendicular external magnetic field, both compete in binding states to the energy levels. For Hofstadter's butterfly the skyrmion lattice binds $-\vartheta^2 Ch_{\{u_1 u_2 t_1 t_2\}}$ additional states to each Landau level. In particular, we find the first gap

Skyrmion lattice

6. Orbital Magnetisation and Finite Magnetic Field

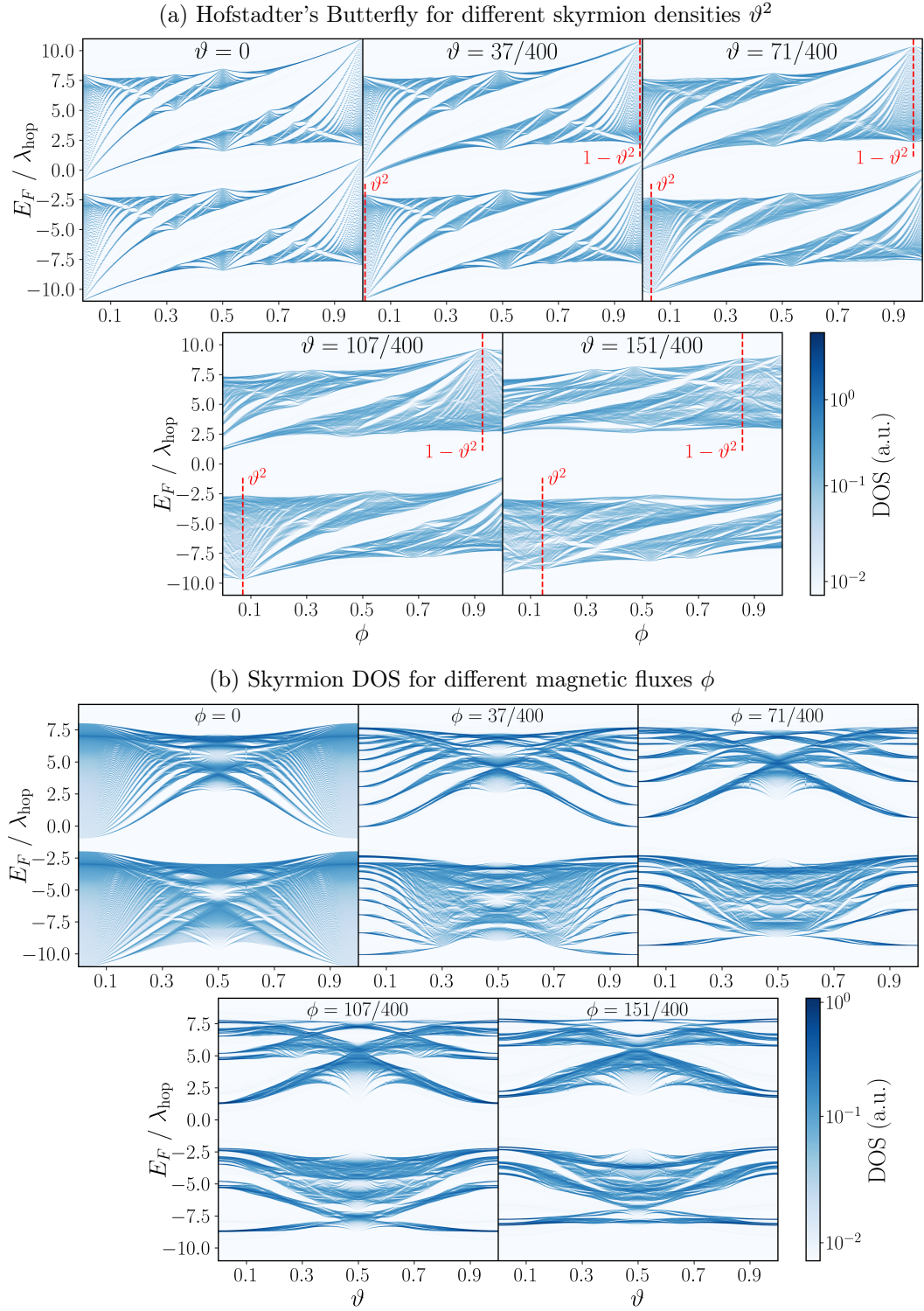


Figure 6.6.: **DOS of the helical skyrmion lattice and magnetic flux.** Electronic spectrum for a helical skyrmion lattice with pitch ϑ permeated by a perpendicular magnetic field with flux ϕ for system parameters $\lambda_{xc}/\lambda_{hop} = 5$ and texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = 0$ and $m = 0$. The DOS is computed via KPM for a system of size $N = 400$ with $\phi = i/N$ for (a) and $\vartheta = i/N$ for (b), $i \in \{0, \dots, N/2 - 1\}$.

6.3. Orbital Magnetisation of the Skyrmion Lattice at Finite Field

of the upper block closes for $\phi = 1 - \vartheta^2$, where the IDS reaches 2. In contradistinction, for the lower block, we find the lowest gap closes and opens at ϑ^2 . The two blocks are shifted by ϑ^2 in opposite directions. This implies, that the mixed space second Chern number $Ch_{\{u_1 u_2 t_1 t_2\}}$ has the opposite sign for the two blocks, which is a striking difference to the situation without the magnetic field, where both blocks exhibited the same sign.

For the DOS over the skyrmion pitch, we find the gaps open wider with increasing flux, especially for small ϑ . Further, the number of gaps decreases, which is the immediate consequence of each level carrying $-\phi Ch_{\{t_1 t_2\}}$ additional states.

6.3. Orbital Magnetisation of the Skyrmion Lattice at Finite Field

Both the skyrmion texture and the finite magnetic field cause the electrons to produce an orbital contribution to the magnetisation. Since the number of states at each energy level in the electronic spectrum depends on the magnetic flux and the skyrmion density, the orbital magnetisation also needs to depend on the flux and pitch parameters.

In this section, we first evaluate the gap labels and orbital magnetisation over the Fermi energies for the helical skyrmion lattice permeated by a finite field. Then, we focus on the orbital magnetisation for the Fermi energy fixed to the first gap and compute its dependence on the magnetic flux and the pitch of the skyrmion texture.

For the helical skyrmion lattice with pitch $\vartheta = 10/57$, as visualised in Fig. 5.7, we compute the Chern numbers and orbital magnetisation in the finite magnetic field with flux $\phi = 10/57$, and present it in Fig. 6.7. The results for this skyrmion lattice at zero field have been shown in Fig. 6.1 and the results for this flux with ferromagnetic background have been shown in Fig. 6.5. The flux and pitch values are close to $71/400$, at which we considered the respective DOS scaling in Fig. 6.6.

Finite pitch and flux

As established in the preceding section, we find both influences competing within the spectrum. However, the gap labels appear to be more aligned with the pattern set out in the Hofstadter butterfly: The momentum space first Chern number $Ch_{\{t_1, t_2\}}$ exhibits the same sign for both blocks of aligned and anti-aligned spin states, whereas the sign of the mixed space second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ differs for them. This is a striking discrepancy from the zero field scenario where it is the opposite case, but it is in line with the ferromagnetic background scenario, where the momentum space Chern number behave the same way.

The real space label $n_{\{u_1, u_2\}}$ is still in agreement with the zero field case, although the van Hove singularity is no longer discernible. However, it no longer is the sole contributor to the real space Chern number $Ch_{\{u_1, u_2\}}$, which receives an additional contribution proportional to the flux ϕ and $n_{\{u_1, u_2, t_1, t_2\}}$:

$$Ch_{\{u_1, u_2\}} = n_{\{u_1, u_2\}} + \phi n_{\{u_1, u_2, t_1, t_2\}}. \quad (6.2)$$

In particular, the real space Chern number is no longer carried in full by the states at

6. Orbital Magnetisation and Finite Magnetic Field

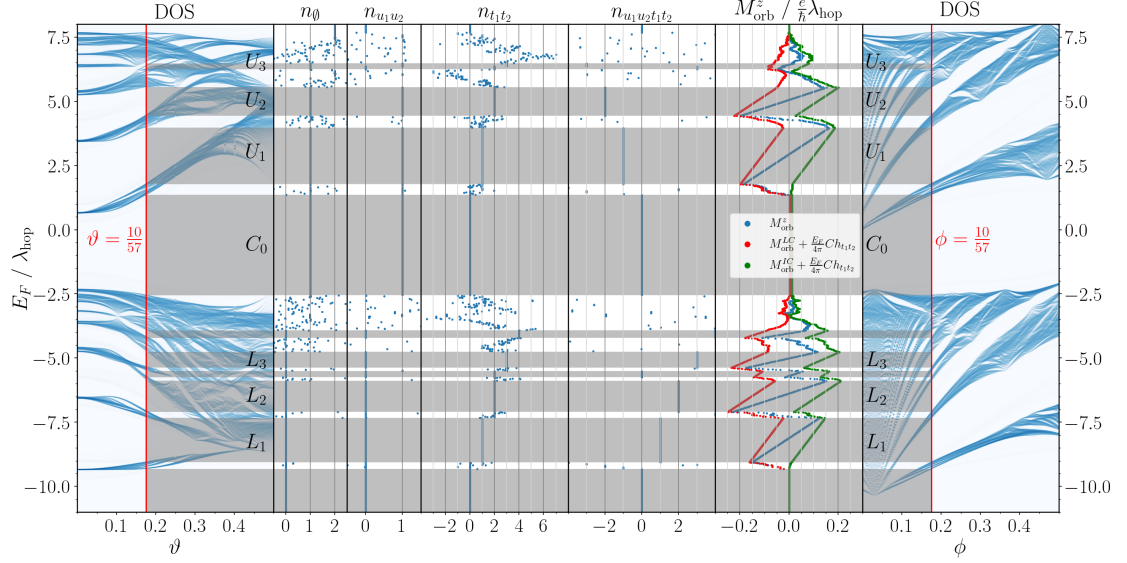


Figure 6.7.: **Orbital magnetisation in the helical skyrmion crystal at zero shift and net magnetisation in a finite magnetic field.** We evaluate the orbital magnetisation and its components in a system of size $N = 57$ at $\vartheta = \frac{10}{57}$ and $\phi = \frac{10}{57}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = 0$ and $m = 0$, and numeric parameter $\Delta\varphi = 10^{-5}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$ and $\phi = 71/400$ (left) and $\vartheta = 71/N$ and $\phi = i/400$ (right), $i \in \{0, \dots, N/2 - 1\}$.

one specific energy level (at the van Hove singularity), but receives contributions from all energy levels. All states exhibit non-trivial real space spin winding.

Conclusion orbital magnetisation

The orbital magnetisation resembles largely that of the ferromagnetic system with finite field from Fig. 6.5. The signs of the contributions are the same for both blocks stemming from the momentum space Chern number. Also, there is no discernible reversal as at the VHS in the zero field scenario.

Orbital magnetisation scaling

In contradistinction to the gap labels which are invariant under changes in pitch and flux that do not close the respective gap, the orbital magnetisation should be sensitive to such changes. To investigate this, we again choose to fix the Fermi energy to the middle of the U_1 gap and vary ϕ and ϑ in the range 0 to 0.5. The resulting orbital magnetisation is presented in Fig. 6.8. Again, this choice affects the behaviour of the Fermi energy and by linearity (since $Ch_{\{t_1t_2\}} = 1$ is constant for this gap) also the orbital magnetisation and its contributions. As seen in Fig. 6.7, the overall orbital magnetisation is around zero in the centre of the gap and both contributions are of equal size.

Flux scaling

In Fig. 6.8(a), we vary the magnetic flux ϕ for six different fixed pitches ϑ . The Fermi energy increases approximately linearly over this flux range, with nearly equal distance between the pitches and larger Fermi energy for larger pitches. The total orbital magnetisation at zero flux is negative and largest for the largest pitch. At around $\phi = 0.3$ the graphs cross each other and following this the orbital magnetisation becomes positive for larger pitches. The change is, however, not linear at all.

6.3. Orbital Magnetisation of the Skyrmion Lattice at Finite Field

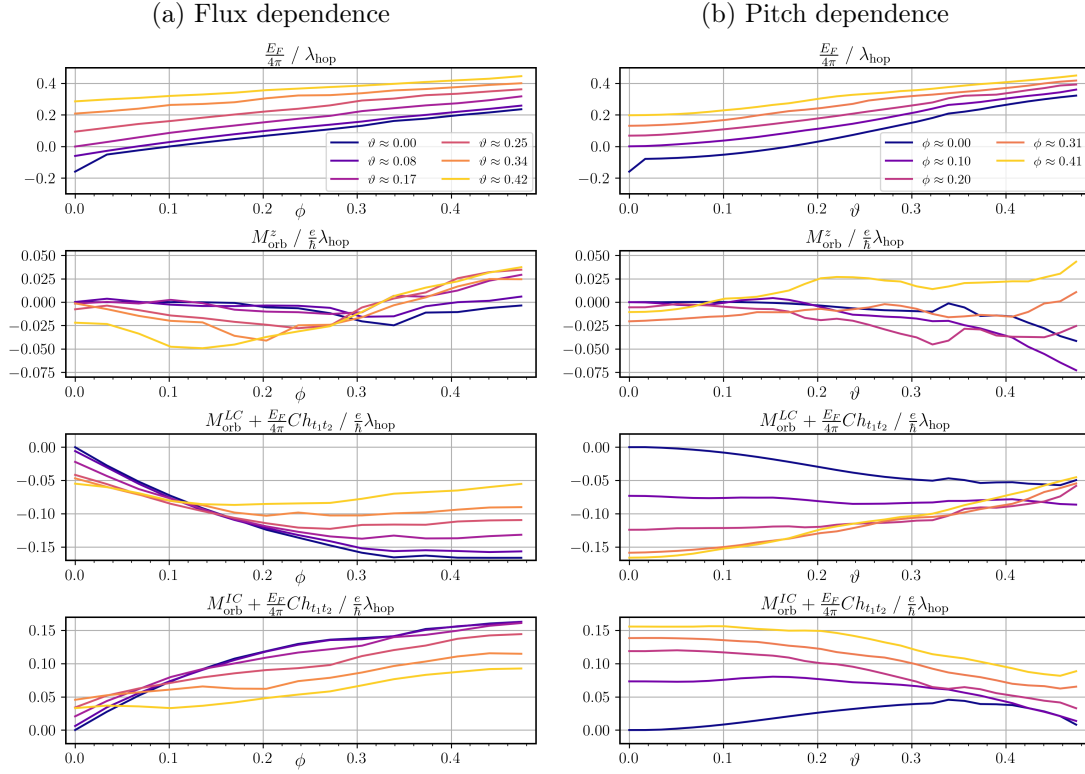


Figure 6.8.: Orbital magnetisation scaling of the helical skyrmion lattice and magnetic flux. Orbital magnetisation for Fermi energy fixed to the middle of the U_1 gap (IDS $1+1\cdot\phi+1\cdot\vartheta^2$) for a helical skyrmion lattice with pitch $\vartheta = \frac{i}{59}$, $i = 0, \dots, 28$ on a triangular lattice with system size $N = 59$ permeated by perpendicular magnetic field with flux $\phi = \frac{2j}{59}$, $j = 0, \dots, 14$, for system parameters $\lambda_{xc}/\lambda_{hop} = 5$, and texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = 0$ and $m = 0$. (a) shows the data over the flux and (b) over the pitch.

The local and itinerant circulation contributions both start with a small spread at zero flux which spreads out for $\varphi \rightarrow 0.5$. The order of the sizes, in dependence on the different pitches, reverses over the range. The orbital magnetisation contributions for the system with zero pitch (the ferromagnet) start at zero and go to the largest for increasing flux. On the contrary, the system with the largest pitch starts with the largest contribution, which changes the least and ends up the lowest for higher fluxes.

The behaviour for varying pitches is presented in Fig. 6.8(b) for five different fixed magnetic flux values ϕ . The Fermi energy behaves overall similarly, albeit less linearly. For lower fluxes and lower pitches it is lower, however the discrepancy at different fluxes decreases for increasing pitch. The total orbital magnetisation displays a surprising behaviour, where it fans out into opposite directions for different flux values. It starts negative for all fluxes and for the system with the largest fluxes $\phi \approx 0.41, 0.31, 0.20$ it increases for larger pitch values, while it decreases for the smaller flux values $\phi \approx 0.0, 0.1$.

Pitch scaling

6. Orbital Magnetisation and Finite Magnetic Field

The overall behaviour of the two contributions on their own does not elucidate this behaviour. The local circulation contributions for the different flux values narrow in their spread for increasing pitch values. In particular, the size for the fluxes $\phi \approx 0.41, 0.31, 0.20$ decreases, while for $\phi \approx 0.0, 0.1$ it increases. In contrast, the itinerant circulation contributions for larger flux values all decrease for increasing pitch values, while the zero flux IC contribution, that starts at zero, increases for increasing pitch up to approximately $\vartheta = 0.3$, and then decreases again.

*Conclusion
scaling*

In conclusion, we find the magnetic flux and skyrmion density to compete with one another in their influence on the orbital magnetisation. Skyrmion textures with a large pitch appear to compensate for the effect of the magnetic flux, resulting in a decrease in the orbital magnetisation for small fluxes and an increase for large ones.

6.4. The Meron-Antimeron Lattice at Finite Field

The meron-antimeron lattice is a spin texture with zero winding that can be subdivided into regions assigned compensating half-integer winding numbers. The helical $3q$ skyrmion lattice with relative phase $\frac{\pi}{2}$ between the superimposed spin waves generates a triangular meron-antimeron lattice as depicted in Fig. 6.9. The meron-antimeron lattice is a common subject in the study of multi- q states [HOM21; HY21], and it is conjectured to arise as the $3q$ near zero field ground state (IC-1) of the geometrically frustrated centrosymmetric triangular-lattice magnet Gd_2PdSi_3 [Kur+19].

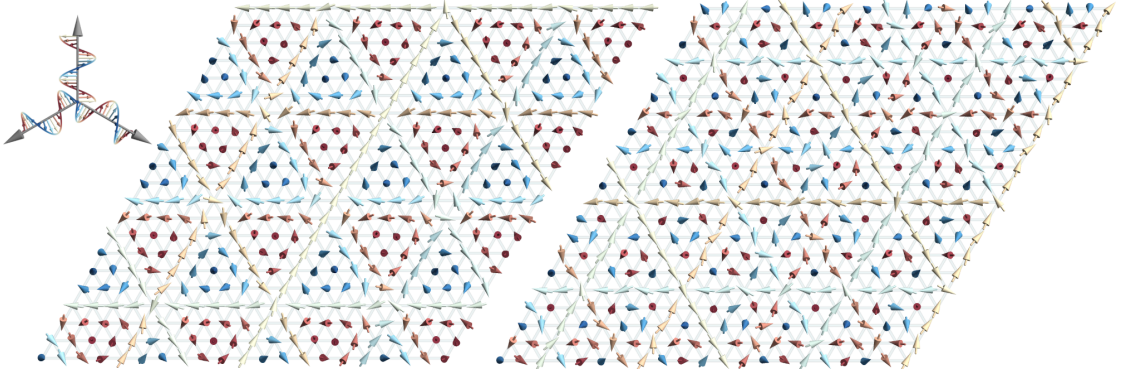


Figure 6.9.: **3q meron-antimeron lattice at $\vartheta = 10/57$ and $\vartheta = 22/57$.** The figure shows 21×21 sites of the helical skyrmionic $3q$ texture with $\deg \hat{\mathbf{n}} = 0$ ($\varphi = \frac{\pi}{2}$, $m = 0$) for $\vartheta = 10/57$ (left), at which the labels were evaluated in Fig. 6.11, and for $\vartheta = 22/57$ (right).

*Beyond
continuity*

In Fig. 5.11 we observed that all gaps in the DOS of the helical skyrmion lattice close at $\varphi = \frac{\pi}{2}$. However, by including an external magnetic field, the spectral gaps can be opened and the effect of the meron-antimeron lattice on the electronic states can be studied. Since the underlying vector field of the meron-antimeron lattice is discontinuous, the tight-binding Hamiltonian coupled to it is not a representation of an element in the observable algebra $\mathcal{A} = M_2(C(T^2) \rtimes_{\theta}^{\Phi} \mathbb{Z}^2)$. Consequently, the Fermi projections do not belong to a K_0 -class of $\mathcal{A}$ and the gap labelling theorem fails. Nevertheless, the

6.4. The Meron-Antimeron Lattice at Finite Field

computational machinery laid out in Chap. 4 can evaluate the formulas, and we obtain results that may be interpretable in a broader framework. This application leaves the established scope of the mathematical framework in this work, but we want to consider it anyway due to its physical relevance.

In this section, we examine the density of states for a meron-antimeron lattice in an external magnetic field in dependence on the magnetic flux and texture pitch. Then, we evaluate the gap label formulas and orbital magnetisation formulas over the Fermi energy and try to interpret the results in relation to the helical skyrmion lattice.

Section content

At first glance, the DOS in dependence on the flux and pitch in Fig. 6.10 seems similar

DOS scaling

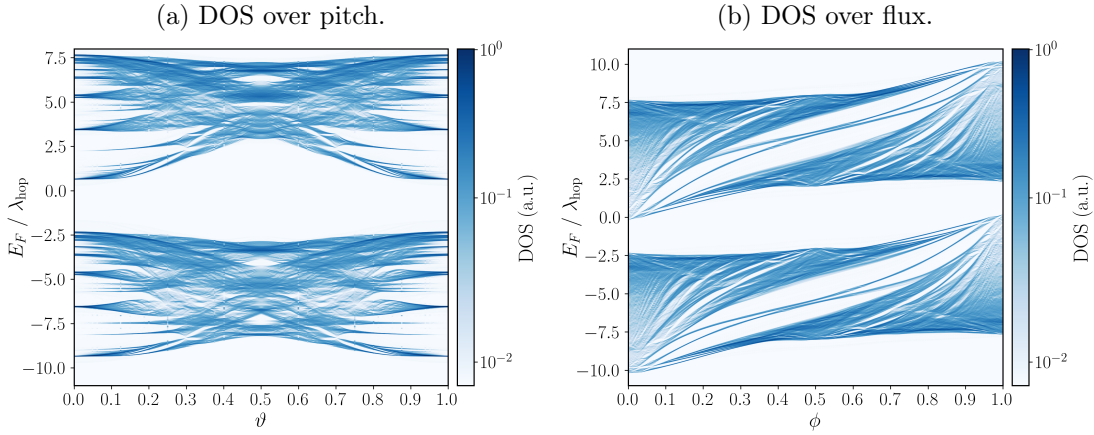


Figure 6.10.: Spectrum of the 3q meron-antimeron lattice. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$ and $\phi = 71/400$ (left) and $\vartheta = 71/400$ and $\phi = i/N$ (right) with $i \in \{0, \dots, N/2 - 1\}$.

to the case of the helical skyrmion lattice with $\varphi = 0$ as depicted in Fig. 6.6. However, a salient difference is apparent in the respective first gaps of both blocks, which are populated by two additional narrow energy levels. In Fig. 6.10(a), we see how these energy levels appear in all gaps of the Hofstadter butterfly at $\vartheta = 0$, and become more substantial for ϑ away from 0. We can therefore attribute them to the influence of the meron-antimeron lattice.

The implications of the discontinuous texture are immediately recognisable by the non-integer values for $n_{\{u_1, u_2\}}$ and $n_{\{u_1, u_2, t_1, t_2\}}$. We recall, that the gap labels are evaluated as

Gap labels

$$n_\emptyset = Ch_\emptyset - \phi Ch_{\{t_1, t_2\}} - \vartheta Ch_{\{u_1, t_1\}} - \vartheta Ch_{\{u_2, t_2\}} - \vartheta^2 Ch_{\{u_1, u_2, t_1, t_2\}}, \quad (6.3)$$

$$n_{\{u_1, u_2\}} = Ch_{\{u_1, u_2\}} - \phi Ch_{\{u_1, u_2, t_1, t_2\}}, \quad (6.4)$$

$$n_{\{t_1, t_2\}} = Ch_{\{t_1, t_2\}}, \quad (6.5)$$

$$n_{\{u_1, u_2, t_1, t_2\}} = Ch_{\{u_1, u_2, t_1, t_2\}}. \quad (6.6)$$

6. Orbital Magnetisation and Finite Magnetic Field

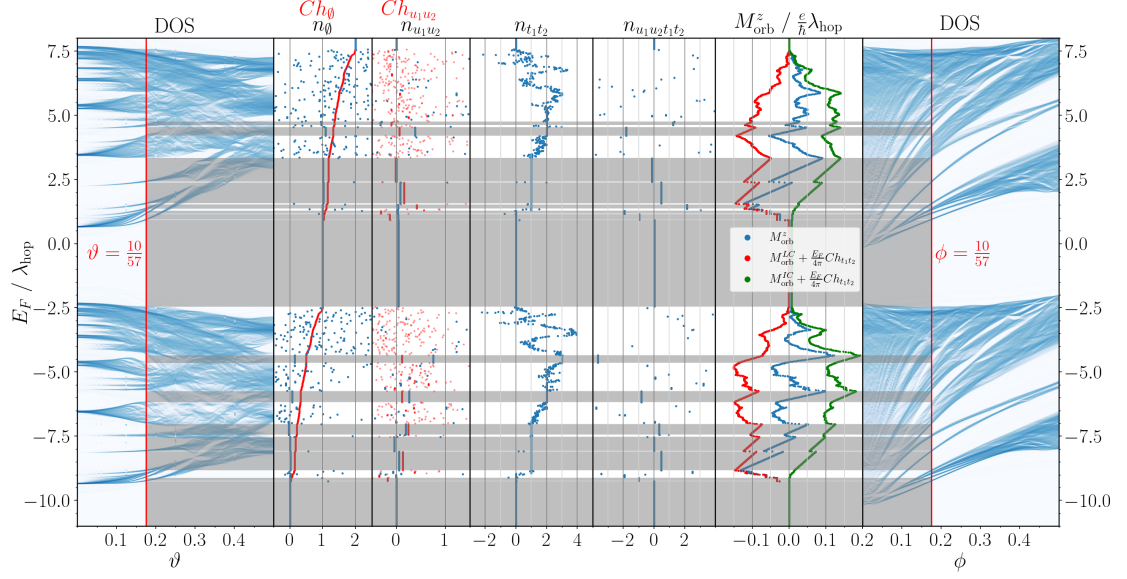


Figure 6.11.: **Gap labels and orbital magnetisation in the helical skyrmion crystal at $\frac{\pi}{2}$ shift and zero magnetisation in finite magnetic field.** We evaluate the main gap labels and the orbital magnetisation and its components in a system of size $N = 57$ at $\vartheta = \frac{10}{57}$ and $\phi = \frac{10}{57}$ for Fermi energies in the full energy range, with system parameters $\lambda_{xc}/\lambda_{hop} = 5$, texture parameters $\varphi = \varphi_1 + \varphi_2 + \varphi_3 = \frac{\pi}{2}$ and $m = 0$, and numeric parameter $\Delta\varphi = 10^{-5}$. The DOS is computed via KPM for a system of size $N = 400$ with $\vartheta = i/N$ and $\phi = 71/400$ (left) and $\vartheta = 71/400$ and $\phi = i/N$ (right), $i \in \{0, \dots, N/2 - 1\}$. For $n_\emptyset$ and $n_{\{u_1, u_2\}}$ we underlay the respective Chern numbers in red.

The momentum space Chern number $Ch_{\{t_1, t_2\}}$ is seemingly unaffected by the states inside the gap and converges still reasonable well to the integers familiar from the Hofstadter butterfly. Also, the number of states $Ch_\emptyset$ at each level seems to still follow the polynomial behaviour, such that the extracted label assumes approximately integer numbers inside the gaps. For the real space Chern number $Ch_{\{u_1, u_2\}}$ this is not the case. It takes values in the vicinity of zero, which is consistent with the zero winding number in the texture. The extracted gap label $n_{\{u_1, u_2\}}$ however deviates, which can be attributed to the influence of $Ch_{\{u_1, u_2, t_1, t_2\}}$.

The behaviour of the mixed space second Chern number $Ch_{\{u_1, u_2, t_1, t_2\}}$ is most peculiar. From the computation of $n_\emptyset$ we inferred that it still describes a contribution to the number of states at each energy level caused by the spin texture reasonable well. However, in the first gap in the lower block we find it subtracting states from the ones added by the flux. It takes approximately the value 0.5 which changes to 0 in between the two energy levels inside the gap and back to ≈ 0.5 above. We find a similar behaviour in the first gap of the upper block, even though at $\phi = 10/57$ there is no gap above the higher level inside the gap.

6.4. The Meron-Antimeron Lattice at Finite Field

We conjecture, that the two energy levels can be attributed to the individual meron and antimeron inside the texture unit cell. We tried to corroborate this hypothesis by depicting the real space distributions of the curvatures

Interpretation

$$\frac{(2\pi i)^n}{n!} \sum_{\sigma \in S_{2n}} (-1)^\sigma \text{tr} \hat{\pi}_\varphi^\times(p) \hat{\pi}_\varphi^\times(\hat{\partial}_{\sigma_1} p) \dots \hat{\pi}_\varphi^\times(\hat{\partial}_{\sigma_{2n}} p) \quad (6.7)$$

that are summed up to the respective Chern numbers in Eq. (4.20), but to no avail. Also, the separation of spin-up and spin-down states did not prove fruitful.

The computation of the orbital magnetisation for the meron-antimeron lattice in the external magnetic field, is conceptually less affected by the discontinuous texture. It is qualitatively similar to the one in the helical skyrmion crystal, but exhibits additional jumps for the energy levels inside the gap that are independent of the momentum space Chern number.

*Orbital
magnetisation*

In conclusion, the merit of applying our computational programme to the fascinating case of the meron-antimeron lattice is, at the current stage, only of speculative nature. However, this departure from the algebra involving continuous textures might be worth pursuing for future research.

*Conclusion
meron-
antimerons*

Conclusion

In the course of the doctoral project, we demonstrated the validity and utility of the C^* -algebraic framework for the study of the electronic properties of nanometric multi- q magnets in the presence of magnetic fields. We further demonstrated the viability of the non-commutative computational programme for the evaluation of systems with extensive supercell sizes and achieved a high accuracy through rapid convergence in one and two dimensions.

*Main objectives
and
achievements*

With the application to skyrmion textures, we were able to substantiate the unconventional behaviour of the Chern numbers caused by the topology of the structural lattice by extending it to all admissible Chern numbers. Our primary motivation was the elucidation of the relationship between the real space properties of the skyrmion textures, such as the winding number, and the topological properties of the electronic spectrum. By juxtaposing them, we unveiled a mismatch between the parameter dependence of the momentum space Chern number determining the anomalous Hall conductivity and the texture winding number, which is consequential for the study of the quantised topological Hall effect.

The framework further facilitates the evaluation of any correlation function, including the orbital magnetisation. This allowed us to corroborate the existence of orbital magnetisation in non-collinear magnets devoid of spin-orbit coupling, to compute the orbital magnetisation in the presence of external magnetic fields, and to investigate its dependence on texture parameters, skyrmion density, and magnetic flux.

In the diligent construction of the C^* -algebraic framework, we demonstrated that the translation behaviour of the multi- q system can be encoded into the crossed product structure of the non-commutative torus algebra. We extended the usual differential calculus by derivations with respect to the phases of the texture, and constructed the Itô derivatives that facilitate the derivation with respect to the texture pitch. Using them, we were able to prove an extension of the generalised Středa formula to the pitch parameters, which, in turn, allowed us to obtain a suitable gap labelling formula to extract all K -theoretic integer labels from the Chern numbers.

C^ -algebraic
framework*

For the computational programme, we adapted the finite volume approximating algebras and the approximate differential calculus to include the continuous phase functions, and found the proper finite representations. We proved that the upper bounds on the error introduced by this approximation prescription fall faster than any inverse power of the system size, and we presented the convergence of the numerical implementation for a selected example.

Conclusion

Chern numbers

The study of the Chern numbers and gap labels for various multi- q textures in one and two dimensions validated our efforts and unearthed some novel findings. As a first result, we were able to substantiate the gap labels obtained from the analysis of the integrated density of states by evaluating them numerically.

By computing the Chern numbers for Fermi energies in the full range of the spectrum, we further identified the individual contributions at different energy levels. Thereby, we substantiated the unconventional behaviour of the momentum space Chern number, which receives a large contribution from the states at the van Hove singularity of the triangular atomic lattice [Göb+17b]. We observed the same behaviour for all main Chern numbers. In particular, we identified the full contribution to the real space Chern number describing the winding of the electron spin to be carried exclusively by the states at the van Hove singularity.

By tuning the texture parameter, we were able to observe the behaviour of the Chern number during the topological transitions of the texture winding number. We found the real space Chern number coinciding with the winding number, whereas the momentum space Chern number exhibits a significant discrepancy, especially in the areas of parameter space where the texture winding number changes magnitude. We identified one of the parameter lines along which the momentum space transitions take place to coincide with the textures for which the average out-of-plane magnetisation vanishes.

The texture winding number transitions did generally not coincide with gap crossings of states, also known as spectral flow. We attributed this to the singular nature of the winding number transition and were able to enforce spectral flow by regularising the spin texture at the transition into a continuous vector field.

Orbital magnetisation

The computational program further enabled us to compute the orbital magnetisation for the $3q$ skyrmion crystal in the absence and presence of a finite external magnetic field. We were able to qualitatively reproduce the zero field results from [Göb+19] in dependence on the Fermi energy and to investigate the texture parameter dependence, although without finding a clear correlation.

In the simultaneous presence of both the skyrmion texture and the magnetic flux, we found both binding states to energy levels, which leads to shifts in the respective density of states dependence diagrams. For the orbital magnetisation in a selected gap, the two influences seem to compete with each other, leading to non-linear scaling in the texture pitch and the magnetic flux.

Open problems and future directions

The C^* -algebraic framework can be used for the evaluation of any correlation function constructed from the Hamiltonian and can be applied to a wide range of systems. These include multi- q textures in arbitrary dimensions, electronic systems including higher orbital complexity, and further energy terms (as long as those satisfy the translation covariance property). The downside of higher-dimensional textures lies in the increasing system size that quickly leads to issues with the available computational resources. This could be mended by extending an approximation algorithm, such as the Kernel polynomial method [Wei+06], to the computation of Fermi projections.

Extending the framework to driven systems, for instance, through an applied electric field, could enable the computation of magneto-electric transport effects [ST13]. This could be done in a straightforward fashion by including the electric field strength as a parameter. Another extension could include arbitrary non-constant magnetic fields. However, this would require a significant change in the construction of the representation.

We already touched on the issue of non-continuous textures such as the meron-antimeron lattices. Although we can evaluate them in the current framework, the mathematical predictions, like the integer gap labels that depend on the affiliation with the non-commutative torus, fail. It might be possible to treat such texture in a wider context or by applying mathematical tricks such as regularisation. Due to their appearance in physical systems, this appears to be a relevant endeavour.

A Calculations

The ensuing paragraphs comprise comprehensive calculations and proofs of identities, formulas, and theorems featured in the main body of the dissertation. Each paragraph is referenced in the text and references back to the equations, definitions, and theorems for which they provide their systematic derivations.

A1. Hall conductivity with Fermi projections Eq. (2.3.1)

We want to verify that

$$\sigma_H = \frac{e^2}{h} \sum_n^{\text{occ}} \int_{\text{B}^A} \frac{d^2 \mathbf{k}}{2\pi} (-2 \text{Im} \langle \partial_{k_1} u_{n\mathbf{k}} | \partial_{k_2} u_{n\mathbf{k}} \rangle) = \frac{e^2}{h} \int_{\text{B}^A} \frac{d^2 \mathbf{k}}{2\pi} i \text{tr}(P_{\mathbf{k}} [\partial_{k_1} P_{\mathbf{k}}, \partial_{k_2} P_{\mathbf{k}}]).$$

Let $P = \sum_j^{\text{occ}} |u_j\rangle \langle u_j|$ denote the projection to the occupied bands with energy below the Fermi level μ , and let $\partial_i = \partial_{k_i}$, $i = 1, 2$, denote the derivative with respect to the Brillouin zone momenta. Then, it is

$$\text{tr}(P [\partial_1 P, \partial_2 P]) \quad (\text{A.1})$$

$$= \sum_i \langle u_i | \sum_j^{\text{occ}} |u_j\rangle \langle u_j| \left[\sum_k^{\text{occ}} |\partial_1 u_k\rangle \langle u_k| + |u_k\rangle \langle \partial_1 u_k|, \sum_l^{\text{occ}} |\partial_2 u_l\rangle \langle u_l| + |u_l\rangle \langle \partial_2 u_l| \right] |u_i\rangle \quad (\text{A.2})$$

$$= \sum_{i,k}^{\text{occ}} \langle u_i | \partial_1 u_k \rangle \langle u_k | \partial_2 u_i \rangle + \sum_i^{\text{occ}} \langle \partial_1 u_i | \partial_2 u_i \rangle + \sum_{i,k}^{\text{occ}} \langle u_i | \partial_1 u_k \rangle \langle \partial_2 u_k | u_i \rangle \quad (\text{A.3})$$

$$+ \sum_{i,l}^{\text{occ}} \langle \partial_1 u_i | u_l \rangle \langle \partial_2 u_l | u_i \rangle - \sum_{i,k}^{\text{occ}} \langle u_i | \partial_2 u_k \rangle \langle u_k | \partial_1 u_i \rangle - \sum_i^{\text{occ}} \langle \partial_2 u_i | \partial_1 u_i \rangle \quad (\text{A.4})$$

$$- \sum_{i,k}^{\text{occ}} \langle u_i | \partial_2 u_k \rangle \langle \partial_1 u_k | u_i \rangle - \sum_{i,l}^{\text{occ}} \langle \partial_2 u_i | u_l \rangle \langle \partial_1 u_l | u_i \rangle \quad (\text{A.5})$$

$$= \sum_{i,k}^{\text{occ}} \langle u_i | \partial_1 u_k \rangle \langle u_k | \partial_2 u_i \rangle + \sum_i^{\text{occ}} \langle \partial_1 u_i | \partial_2 u_i \rangle - \sum_{i,k}^{\text{occ}} \langle u_i | \partial_1 u_k \rangle \langle u_k | \partial_2 u_i \rangle \quad (\text{A.6})$$

$$+ \sum_{i,l}^{\text{occ}} \langle \partial_1 u_i | u_l \rangle \langle \partial_2 u_l | u_i \rangle - \sum_{i,k}^{\text{occ}} \langle u_i | \partial_2 u_k \rangle \langle u_k | \partial_1 u_i \rangle - \sum_i^{\text{occ}} \langle \partial_1 u_i | \partial_2 u_i \rangle^* \quad (\text{A.7})$$

$$+ \sum_{i,k}^{\text{occ}} \langle u_i | \partial_2 u_k \rangle \langle u_k | \partial_1 u_i \rangle - \sum_{l,i}^{\text{occ}} \langle \partial_2 u_l | u_i \rangle \langle \partial_1 u_i | u_l \rangle = 2i \sum_i^{\text{occ}} \text{Im} \langle \partial_1 u_i | \partial_2 u_i \rangle. \quad (\text{A.8})$$

A. Calculations

A useful relation in this calculation is $\langle \partial_i u_j | u_k \rangle = -\langle u_j | \partial_i u_k \rangle \quad \forall i = 1, 2 \quad \forall j, k$ which follows from $0 = \partial_i \delta_{jk} = \partial_i \langle u_j | u_k \rangle = \langle \partial_i u_j | u_k \rangle + \langle u_j | \partial_i u_k \rangle \quad \forall i = 1, 2 \quad \forall j, k$.

A2. Orbital magnetisation with Fermi projections Eq. (2.4.1)

The z -component of the orbital magnetisation in Eq. (2.8) is given by

$$\mathbf{M}_{\text{orb}}^z = \frac{e}{\hbar} \text{Im} \sum_n^{\text{occ}} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \langle \partial_{k_1} u_{n\mathbf{k}} | H_{\mathbf{k}} + E_{n\mathbf{k}} - 2\mu | \partial_{k_2} u_{n\mathbf{k}} \rangle. \quad (\text{A.9})$$

From the calculation in App. A1 follows analogously

$$\text{Im} \sum_i^{\text{occ}} \langle \partial_1 u_i | H | \partial_2 u_i \rangle = -\frac{i}{2} \text{Tr}(P \partial_1 P H \partial_2 P - P \partial_2 P H \partial_1 P) = \text{Im} \text{Tr}(P \partial_1 P H \partial_2 P), \quad (\text{A.10})$$

$$\text{Im} \sum_i^{\text{occ}} \langle \partial_1 u_i | E_i | \partial_2 u_i \rangle = -\frac{i}{2} \text{Tr}(H P [\partial_1 P, \partial_2 P]) = \text{Im} \text{Tr}(H P \partial_1 P \partial_2 P), \quad (\text{A.11})$$

$$\text{Im} \sum_i^{\text{occ}} \langle \partial_1 u_i | -2\mu | \partial_2 u_i \rangle = 2\mu \frac{i}{2} \text{Tr}(P [\partial_1 P, \partial_2 P]) = -2\mu \text{Im} \text{Tr}(P \partial_1 P \partial_2 P), \quad (\text{A.12})$$

where we additionally used the relations

$$\begin{aligned} \text{Tr}((P \partial_1 P H \partial_2 P)^\dagger) &= (-1)^2 \text{Tr}(P \partial_2 P H \partial_1 P), \\ \text{Tr}((H P \partial_1 P \partial_2 P)^\dagger) &= (-1)^2 \text{Tr}(H P \partial_2 P \partial_1 P), \\ \text{and } \text{Tr}((P \partial_1 P \partial_2 P)^\dagger) &= (-1)^2 \text{Tr}(P \partial_2 P \partial_1 P), \end{aligned}$$

together with $a - a^* = 2i \text{Im } a$. Consequently, we obtain

$$M_{\text{orb}}^z = \frac{e}{\hbar} \text{Im} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \text{Tr}(P \partial_1 P H \partial_2 P + H P \partial_1 P \partial_2 P - 2\mu P \partial_1 P \partial_2 P). \quad (\text{A.13})$$

A3. Multiplication relation of the magnetic translation operator Eq. (3.15)

$$\hat{U}_{\mathbf{m}}^A \hat{U}_{\mathbf{n}}^A = \pi \left(e^{i\Gamma_A([\bullet, \bullet - \mathbf{m}])} \right) \hat{T}_{\mathbf{m}} \pi \left(e^{i\Gamma_A([\bullet, \bullet - \mathbf{n}])} \right) \hat{T}_{\mathbf{n}} \quad (\text{A.14})$$

$$= \pi \left(e^{i\Gamma_A([\bullet, \bullet - \mathbf{m}])} \right) \pi \left(e^{i\Gamma_A([\bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n}])} \right) \hat{T}_{\mathbf{m}} \hat{T}_{\mathbf{n}} \quad (\text{A.15})$$

$$= \pi \left(e^{i\Gamma_A([\bullet, \bullet - \mathbf{m}])} \right) \pi \left(e^{i\Gamma_A([\bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n}])} \right) \pi \left(e^{-i\Gamma_A([\bullet, \bullet - (\mathbf{m} + \mathbf{n})])} \right) \hat{U}_{\mathbf{m} + \mathbf{n}}^A \quad (\text{A.16})$$

$$= \pi \left(e^{i\Gamma_B(\langle \bullet, \bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n} \rangle)} \right) \hat{U}_{\mathbf{m} + \mathbf{n}}^A \quad (\text{A.17})$$

The last equality contains the application of Stokes Theorem:

$$\Gamma_A([\bullet, \bullet - \mathbf{m}]) + \Gamma_A([\bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n}]) - \Gamma_A([\bullet, \bullet - (\mathbf{m} + \mathbf{n})]) \quad (\text{A.18})$$

$$= \frac{e}{\hbar} \int_{\partial \langle \bullet, \bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n} \rangle} A \stackrel{dA=B}{=} \frac{e}{\hbar} \int_{\langle \bullet, \bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n} \rangle} B \quad (\text{A.19})$$

$$= \Gamma_B(\langle \bullet, \bullet - \mathbf{m}, \bullet - \mathbf{m} - \mathbf{n} \rangle). \quad (\text{A.20})$$

This calculation has been presented in [Pra20, App. A.4].

A4. 2-cocycle condition and normalisation of the magnetic cocycle Eq. (3.17)

First, the left-hand side of the 2-cocycle condition Eq. (3.4):

$$\gamma_B(\bullet; \mathbf{l} + \mathbf{m}, \mathbf{n}) \gamma_B(\bullet; \mathbf{l}, \mathbf{m}) = e^{i\Gamma_B(\langle \bullet, \bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n} \rangle)} e^{i\Gamma_B(\langle \bullet, \bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m} \rangle)}. \quad (\text{A.21})$$

From App. A3, we know

$$\Gamma_B(\langle \bullet, \bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n} \rangle) + \Gamma_B(\langle \bullet, \bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m} \rangle) \quad (\text{A.22})$$

$$= \Gamma_A([\bullet, \bullet - \mathbf{l} - \mathbf{m}]) + \Gamma_A([\bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) - \Gamma_A([\bullet, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) \quad (\text{A.23})$$

$$+ \Gamma_A([\bullet, \bullet - \mathbf{l}]) + \Gamma_A([\bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m}]) - \Gamma_A([\bullet, \bullet - \mathbf{l} - \mathbf{m}]) \quad (\text{A.24})$$

$$= \Gamma_A([\bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) - \Gamma_A([\bullet, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) + \Gamma_A([\bullet, \bullet - \mathbf{l}]) \quad (\text{A.25})$$

$$+ \Gamma_A([\bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m}]) \quad (\text{A.26})$$

$$= \Gamma_B(\langle \bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}, \bullet, \bullet - \mathbf{l} \rangle), \quad (\text{A.27})$$

which is the magnetic flux through the tetragon $\langle \bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}, \bullet, \bullet - \mathbf{l} \rangle$. We can split it again into two triangles along the diagonal:

$$\Gamma_B(\langle \bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}, \bullet, \bullet - \mathbf{l} \rangle) \quad (\text{A.28})$$

$$= \Gamma_A([\bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) - \Gamma_A([\bullet, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) + \Gamma_A([\bullet, \bullet - \mathbf{l}]) \quad (\text{A.29})$$

$$+ \Gamma_A([\bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m}]) \quad (\text{A.30})$$

$$= \Gamma_A([\bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) + \Gamma_A([\bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) \quad (\text{A.31})$$

$$- \Gamma_A([\bullet, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) + \Gamma_A([\bullet, \bullet - \mathbf{l}]) \quad (\text{A.32})$$

$$+ \Gamma_A([\bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m}]) - \Gamma_A([\bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n}]) \quad (\text{A.33})$$

$$= \Gamma_B(\langle \bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n} \rangle) + \Gamma_B(\langle \bullet, \bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n} \rangle). \quad (\text{A.34})$$

Thus, we arrive at the right-hand side of Eq. (3.4):

$$e^{i\Gamma_B(\langle \bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n} \rangle)} e^{i\Gamma_B(\langle \bullet, \bullet - \mathbf{l}, \bullet - \mathbf{l} - \mathbf{m} - \mathbf{n} \rangle)} \quad (\text{A.35})$$

$$= \gamma_B(\bullet - \mathbf{l}; \mathbf{m}, \mathbf{n}) \gamma_B(\bullet; \mathbf{l}, \mathbf{m} + \mathbf{n}) = \theta_1[\gamma_B(\bullet; \mathbf{m}, \mathbf{n})] \gamma_B(\bullet; \mathbf{l}, \mathbf{m} + \mathbf{n}). \quad (\text{A.36})$$

The normalisation of the cocycle is given by

$$\gamma_B(\bullet; \mathbf{0}, \mathbf{l}) = e^{i\Gamma_B(\langle \bullet, \bullet, \bullet - \mathbf{l} \rangle)} = 1 = e^{i\Gamma_B(\langle \bullet, \bullet - \mathbf{l}, \bullet - \mathbf{l} \rangle)} = \gamma_B(\bullet; \mathbf{l}, \mathbf{0}), \quad (\text{A.37})$$

since the area of the triangles is 0 and, thus, the integral Γ_B over it vanishes. This calculation has been presented in [Pra20, App. A.6].

A. Calculations

A5. *-homomorphism properties of the integrated representation Eq. (3.10)

$\pi_\varphi^\times$ is a *-homomorphism:

(i) $\pi_\varphi^\times$ is linear. For any $a, b \in C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ and $\lambda \in \mathbb{C}$ it is

$$\pi_\varphi^\times(a + \lambda b) = \pi_\varphi^\times \left(\sum_{\mathbf{m} \in \mathbb{Z}^d} (a_{\mathbf{m}} + \lambda b_{\mathbf{m}}) \otimes t^{\mathbf{m}} \right) \quad (\text{A.38})$$

$$= \sum_{\mathbf{n}, \mathbf{m} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n}}(a_{\mathbf{m}} + \lambda b_{\mathbf{m}}))(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \quad (\text{A.39})$$

$$= \sum_{\mathbf{n}, \mathbf{m} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n}} a_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A + \lambda (\alpha_{-\mathbf{n}} b_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \quad (\text{A.40})$$

$$= \pi_\varphi^\times(a) + \lambda \pi_\varphi^\times(b). \quad (\text{A.41})$$

(ii) $\pi_\varphi^\times$ is multiplicative with respect of the multiplication defined in Eq. (3.6). For $a, b \in C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ it is

$$\pi_\varphi^\times(ab) = \pi_\varphi^\times \left(\sum_{\mathbf{l}, \mathbf{m} \in \mathbb{Z}^d} e^{2\pi i \mathbf{l} \wedge_\Phi \mathbf{m}} a_{\mathbf{l}} \alpha_{\mathbf{l}}(b_{\mathbf{m}-\mathbf{l}}) \otimes t^{\mathbf{m}} \right) \quad (\text{A.42})$$

$$= \sum_{\mathbf{l}, \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} \left(\alpha_{-\mathbf{n}} \left(e^{2\pi i \mathbf{l} \wedge_\Phi \mathbf{m}} a_{\mathbf{l}} \alpha_{\mathbf{l}}(b_{\mathbf{m}-\mathbf{l}}) \right) \right) (\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \quad (\text{A.43})$$

$$= \sum_{\mathbf{l}, \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{l} \wedge_\Phi \mathbf{m}} (\alpha_{-\mathbf{n}} a_{\mathbf{l}})(\varphi) (\alpha_{\mathbf{l}-\mathbf{n}} b_{\mathbf{m}-\mathbf{l}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \quad (\text{A.44})$$

$$= \sum_{\mathbf{l}, \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{l} \wedge_\Phi \mathbf{m}} (\alpha_{-\mathbf{n}} a_{\mathbf{l}})(\varphi) (\alpha_{\mathbf{l}-\mathbf{n}} b_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{l}+\mathbf{m}}^A \quad (\text{A.45})$$

$$= \sum_{\mathbf{l}, \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{l} \wedge_\Phi \mathbf{m}} (\alpha_{-\mathbf{n}} a_{\mathbf{l}})(\varphi) (\alpha_{\mathbf{l}-\mathbf{n}} b_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| e^{2\pi i \mathbf{m} \wedge_\Phi \mathbf{l}} \hat{U}_{\mathbf{l}}^A \hat{U}_{\mathbf{m}}^A \quad (\text{A.46})$$

$$= \sum_{\mathbf{l}, \mathbf{k}, \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} (\alpha_{-\mathbf{k}} a_{\mathbf{l}})(\varphi) (\alpha_{\mathbf{l}-\mathbf{n}} b_{\mathbf{m}})(\varphi) |\mathbf{k}\rangle \langle \mathbf{k}| \mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{l}}^A \hat{U}_{\mathbf{m}}^A \quad (\text{A.47})$$

$$= \sum_{\mathbf{l}, \mathbf{k}, \mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} (\alpha_{-\mathbf{k}} a_{\mathbf{l}})(\varphi) |\mathbf{k}\rangle \langle \mathbf{k}| \hat{U}_{\mathbf{l}}^A (\alpha_{\mathbf{l}-\mathbf{n}} b_{\mathbf{m}})(\varphi) |\mathbf{n}-\mathbf{l}\rangle \langle \mathbf{n}-\mathbf{l}| \hat{U}_{\mathbf{m}}^A \quad (\text{A.48})$$

$$= \sum_{\mathbf{l}, \mathbf{k} \in \mathbb{Z}^d} (\alpha_{-\mathbf{k}} a_{\mathbf{l}})(\varphi) |\mathbf{k}\rangle \langle \mathbf{k}| \hat{U}_{\mathbf{l}}^A \sum_{\mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n}} b_{\mathbf{m}})(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \quad (\text{A.49})$$

$$= \pi_\varphi^\times(a) \pi_\varphi^\times(b). \quad (\text{A.50})$$

(iii) $\pi_\varphi^\times$ preserves the involution defined in Eq. (3.7). For $a \in C_c(\mathbb{Z}^d, C(T^r), \alpha, \gamma)$ it is

$$\pi_\varphi^\times(a^*) = \pi_\varphi^\times \left(\sum_{\mathbf{m} \in \mathbb{Z}^d} (\alpha_{\mathbf{m}} a_{-\mathbf{m}}^*) \otimes t^{\mathbf{m}} \right) \quad (\text{A.51})$$

$$= \sum_{\mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} (\alpha_{\mathbf{m}-\mathbf{n}} a_{-\mathbf{m}}^*)(\varphi) |\mathbf{n}\rangle \langle \mathbf{n}| \hat{U}_{\mathbf{m}}^A \quad (\text{A.52})$$

$$= \sum_{\mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n}} a_{\mathbf{m}}^*)(\varphi) |\mathbf{n}-\mathbf{m}\rangle \langle \mathbf{n}-\mathbf{m}| \hat{U}_{-\mathbf{m}}^A \quad (\text{A.53})$$

$$= \sum_{\mathbf{m}, \mathbf{n} \in \mathbb{Z}^d} (\alpha_{-\mathbf{n}} a_{\mathbf{m}}^*)(\varphi) \hat{U}_{\mathbf{m}}^{A*} |\mathbf{n}\rangle \langle \mathbf{n}| \quad (\text{A.54})$$

$$= \pi_\varphi^\times(a)^*. \quad (\text{A.55})$$

A6. *-derivation conditions Def. 3.7

(1) *-derivations defined in Eq. (3.33)

$$\partial_i^u a = \sum_{\mathbf{m} \in \mathbb{Z}^d} \partial_{\varphi_i} a_{\mathbf{m}} \otimes t^{\mathbf{m}} \quad (\text{A.56})$$

Condition (i):

$$\partial_i^u(ab) = \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} \partial_{\varphi_i} (a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}})) \otimes t^{\mathbf{m}} \quad (\text{A.57})$$

$$= \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} ((\partial_{\varphi_i} a_{\mathbf{n}}) \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) + a_{\mathbf{n}} (\partial_{\varphi_i} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}))) \otimes t^{\mathbf{m}} \quad (\text{A.58})$$

$$= \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} (\partial_{\varphi_i} a_{\mathbf{n}}) \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.59})$$

$$+ \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}(\partial_{\varphi_i} b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.60})$$

$$= (\partial_i^u a) b + a (\partial_i^u b) \quad (\text{A.61})$$

Condition (ii):

$$\partial_i^u(a^*) = \sum_{\mathbf{m} \in \mathbb{Z}^d} \partial_{\varphi_i} \alpha_{\mathbf{m}}(a_{-\mathbf{m}}^*) \otimes t^{\mathbf{m}} = \sum_{\mathbf{m} \in \mathbb{Z}^d} \alpha_{-\mathbf{m}}((\partial_{\varphi_i} a_{\mathbf{m}})^*) \otimes t^{-\mathbf{m}} \quad (\text{A.62})$$

$$= \sum_{\mathbf{m} \in \mathbb{Z}^d} (\partial_{\varphi_i} a_{\mathbf{m}} \otimes t^{\mathbf{m}})^* = (\partial_i^u a)^* \quad (\text{A.63})$$

A. Calculations

(2) $*$ -derivations defined in Eq. (3.34)

$$\partial_i^t a = i \sum_{\mathbf{m} \in \mathbb{Z}^d} m_i a_{\mathbf{m}} \otimes t^{\mathbf{m}} \quad (\text{A.64})$$

Condition (i):

$$\partial_i^t(ab) = i \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge_{\Phi} \mathbf{m}} m_i a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.65})$$

$$= i \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge_{\Phi} \mathbf{m}} (n_i + m_i) a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}}) \otimes t^{\mathbf{m}+\mathbf{n}} \quad (\text{A.66})$$

$$= i \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge_{\Phi} \mathbf{m}} n_i a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}}) \otimes t^{\mathbf{m}+\mathbf{n}} \quad (\text{A.67})$$

$$+ i \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge_{\Phi} \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}(m_i b_{\mathbf{m}}) \otimes t^{\mathbf{m}+\mathbf{n}} \quad (\text{A.68})$$

$$= i \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge_{\Phi} \mathbf{m}} n_i a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.69})$$

$$+ i \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge_{\Phi} \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}((m_i - n_i) b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.70})$$

$$= (\partial_i^t a) b + a (\partial_i^t b) \quad (\text{A.71})$$

Here, we used several times that $\mathbf{n} \wedge_{\Phi} \mathbf{m} = \mathbf{n} \wedge_{\Phi} (\mathbf{m} + \mathbf{n}) = \mathbf{n} \wedge_{\Phi} (\mathbf{m} - \mathbf{n})$ since Φ is antisymmetric.

Condition (ii):

$$\partial_i^t(a^*) = i \sum_{\mathbf{m} \in \mathbb{Z}^d} m_i \alpha_{\mathbf{m}}(a_{-\mathbf{m}}^*) \otimes t^{\mathbf{m}} = \sum_{\mathbf{m} \in \mathbb{Z}^d} \alpha_{-\mathbf{m}}((im_i a_{\mathbf{m}})^*) \otimes t^{-\mathbf{m}} \quad (\text{A.72})$$

$$= \sum_{\mathbf{m} \in \mathbb{Z}^d} (im_i a_{\mathbf{m}} \otimes t^{\mathbf{m}})^* = (\partial_i^t a)^* \quad (\text{A.73})$$

A7. Fast decay property Eq. (3.38)

We need to verify the inequality $|(1, \mathbf{m})^{\nu} \Phi_{1\mathbf{m}}(a)| \leq \|\partial^{\nu} a\|$ with $\mathbf{l} \in \mathbb{Z}^r$, $\mathbf{m} \in \mathbb{Z}^d$, and $\nu = (\nu_1, \nu_2) \in \mathbb{N}_0^{r+d}$.

$$|(1, \mathbf{m})^{\nu} \Phi_{1\mathbf{m}}(a)| = \left| \mathbf{l}^{\nu_1} \mathbf{m}^{\nu_2} \int_{T^r} \frac{d\varphi}{(2\pi)^r} e^{-i\mathbf{l} \cdot \varphi} \Phi_{\mathbf{m}}(a)(\varphi) \right| \quad (\text{A.74})$$

$$= \left| \mathbf{m}^{\nu_2} \int_{T^r} \frac{d\varphi}{(2\pi)^r} \left((-i\partial_{\varphi})^{\nu_1} e^{-i\mathbf{l} \cdot \varphi} \right) \Phi_{\mathbf{m}}(a)(\varphi) \right| \quad (\text{A.75})$$

$$= \left| \mathbf{m}^{\nu_2} \int_{T^r} \frac{d\varphi}{(2\pi)^r} e^{-i\mathbf{l} \cdot \varphi} ((i\partial_{\varphi})^{\nu_1} \Phi_{\mathbf{m}}(a))(\varphi) \right| \quad (\text{A.76})$$

$$\leq \sup_{\varphi \in T^r} \left| \mathbf{m}^{\nu_2} e^{-i\mathbf{l} \cdot \varphi} (i)^{\nu_1} \Phi_{\mathbf{m}}(\partial_u^{\nu_1} a)(\varphi) \right| \quad (\text{A.77})$$

$$= \sup_{\varphi \in T^r} |\mathbf{m}^{\nu_2} \Phi_{\mathbf{m}}(\partial_u^{\nu_1} a)(\varphi)| \quad (\text{A.78})$$

$$= \sup_{\varphi \in T^r} \left| \langle 0 | \sum_{\mathbf{n}, \mathbf{k} \in \mathbb{Z}^d} \mathbf{k}^{\nu_2} (\alpha_{-\mathbf{n}} \Phi_{\mathbf{k}}(\partial_u^{\nu_1} a))(\varphi) | \mathbf{n} \rangle \langle \mathbf{n} | \hat{U}_{\mathbf{k}}^A | -\mathbf{m} \rangle \right| \quad (\text{A.79})$$

$$= \sup_{\varphi \in T^r} |(-i)^{\nu_2} \langle 0 | \pi_{\varphi}^{\times} (\partial_t^{\nu_2} \partial_u^{\nu_1} a) | -\mathbf{m} \rangle| \quad (\text{A.80})$$

$$\leq \| \partial^{\nu} a \|_r \quad (\text{A.81})$$

A8. Itô derivative rules Relations (iv)

First, we consider the magnetic flux parameters $\Theta_{(r+i)(r+j)} = \Theta_{t_i t_j} = \Phi_{ij}$, $1 \leq i, j \leq d$, for which we have

$$\delta_{\Theta_{t_i t_j}}(ss') = \delta_{\Phi_{ij}}(ss') \quad (\text{A.82})$$

$$= \sum_{\mathbf{m} \in \mathbb{Z}^d} \delta_{\Phi_{ij}} \left(\sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \right) \otimes t^{\mathbf{m}} \quad (\text{A.83})$$

$$= \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} (\partial_{\Phi_{ij}} a_{\mathbf{n}}) \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.84})$$

$$+ \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}((\partial_{\Phi_{ij}} b_{\mathbf{m}-\mathbf{n}})) \otimes t^{\mathbf{m}} \quad (\text{A.85})$$

$$+ \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} \left(\partial_{\Phi_{ij}} e^{2\pi i \frac{1}{2} \sum_{i', j'}^d \Phi_{i' j'} n_{i'} m_{j'}} \right) a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.86})$$

$$= (\delta_{\Phi_{ij}} s) s' + s (\delta_{\Phi_{ij}} s') - \frac{2\pi i}{2} (\partial_i^t s \partial_j^t s' - \partial_j^t s \partial_i^t s'). \quad (\text{A.87})$$

The last equality follows with

$$\sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} \left(\partial_{\Phi_{ij}} e^{2\pi i \frac{1}{2} \sum_{i', j'}^d \Phi_{i' j'} n_{i'} m_{j'}} \right) a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.88})$$

$$= \frac{2\pi i}{2} \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} (n_i m_j - n_j m_i) e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.89})$$

$$= \frac{2\pi i}{2} \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} n_i a_{\mathbf{n}} \alpha_{\mathbf{n}}((m_j - n_j) b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.90})$$

$$- \frac{2\pi i}{2} \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} n_j a_{\mathbf{n}} \alpha_{\mathbf{n}}((m_i - n_i) b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.91})$$

$$= (-i)^2 \frac{2\pi i}{2} (\partial_i^t s \partial_j^t s' - \partial_j^t s \partial_i^t s'). \quad (\text{A.92})$$

Here, we used $n_i m_j - n_j m_i = n_i(m_j - n_j) - n_j(m_i - n_i)$ for the second equality.

A. Calculations

Next, we consider the spin wave pitch parameters $\Theta_{(i)(r+j)} = \Theta_{u_i t_j} = \theta_{ij}$, $1 \leq i \leq r$ and $1 \leq j \leq d$, for which we have

$$\delta_{\Theta_{u_i t_j}}(ss') = \delta_{\theta_{ij}}(ss') \quad (\text{A.93})$$

$$= \sum_{\mathbf{m} \in \mathbb{Z}^d} \partial_{\theta_{ij}} \left(\sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} a_{\mathbf{n}} \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \right) \otimes t^{\mathbf{m}} \quad (\text{A.94})$$

$$= \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} (\partial_{\theta_{ij}} a_{\mathbf{n}}) \alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} \quad (\text{A.95})$$

$$+ \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} a_{\mathbf{n}} (\partial_{\theta_{ij}} (\alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}))) \otimes t^{\mathbf{m}} \quad (\text{A.96})$$

$$= (\delta_{\theta_{ij}} s) s' + s (\delta_{\theta_{ij}} s') + 2\pi i \partial_j^t s \partial_i^u s'. \quad (\text{A.97})$$

For the last equality we use $\alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}})(\varphi) = (b_{\mathbf{m}-\mathbf{n}})(\varphi_i - 2\pi \sum_{j=1}^d \theta_{ij} n_j)$ and, thus,

$$\partial_{\theta_{ij}} (\alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}})) = -2\pi n_j \alpha_{\mathbf{n}}(\partial_{\varphi_i} b_{\mathbf{m}-\mathbf{n}}) + \alpha_{\mathbf{n}}(\partial_{\theta_{ij}} b_{\mathbf{m}-\mathbf{n}}). \quad (\text{A.98})$$

From this follows further

$$\sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} a_{\mathbf{n}} (\partial_{\theta_{ij}} (\alpha_{\mathbf{n}}(b_{\mathbf{m}-\mathbf{n}}))) \otimes t^{\mathbf{m}} \quad (\text{A.99})$$

$$= -2\pi \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{\mathbf{n} \in \mathbb{Z}^d} e^{2\pi i \mathbf{n} \wedge \Phi \mathbf{m}} n_j a_{\mathbf{n}} \alpha_{\mathbf{n}}(\partial_{\varphi_i} b_{\mathbf{m}-\mathbf{n}}) \otimes t^{\mathbf{m}} + s (\delta_{\theta_{ij}} s') \quad (\text{A.100})$$

$$= 2\pi i \partial_j^t s \partial_i^u s' + s (\delta_{\theta_{ij}} s'). \quad (\text{A.101})$$

A9. Classical Středa formulas Eq. (3.52) and Eq. (3.53)

From the Itô-like product rules Eq. (3.40) and (3.41), it follows for an Itô-differentiable smooth projection p that

$$0 = \delta_{\Phi_{ij}}(p(1-p)) = (\delta_{\Phi_{ij}} p)(1-p) - p(\delta_{\Phi_{ij}} p) + \frac{2\pi i}{2} [\partial_i^t p, \partial_j^t p] \quad \text{and} \quad (\text{A.102})$$

$$0 = \delta_{\theta_{ij}}(p(1-p)) = (\delta_{\theta_{ij}} p)(1-p) - p(\delta_{\theta_{ij}} p) - 2\pi i \partial_j^t p \partial_i^u p. \quad (\text{A.103})$$

By multiplication with p from the right-hand side or $(1-p)$ from the left-hand side the following expression for the diagonal parts of the Itô derivatives of p is obtained

$$p(\delta_{\Phi_{ij}} p)p = \frac{2\pi i}{2} [\partial_i^t p, \partial_j^t p]p, \quad (\text{A.104})$$

$$(1-p)(\delta_{\Phi_{ij}} p)(1-p) = -\frac{2\pi i}{2} (1-p)[\partial_i^t p, \partial_j^t p], \quad (\text{A.105})$$

$$p(\delta_{\theta_{ij}} p)p = -2\pi i \partial_j^t p \partial_i^u p \quad \text{and} \quad (\text{A.106})$$

$$(1-p)(\delta_{\theta_{ij}} p)(1-p) = 2\pi i (1-p) \partial_j^t p \partial_i^u p. \quad (\text{A.107})$$

The Středa formula for the magnetic flux parameters follows from the application of these rules

$$\partial_{\Phi_{ij}} \text{Ch}_\emptyset([p]_0) = \partial_{\Phi_{ij}} \mathcal{T}(p) = \mathcal{T}(\delta_{\Phi_{ij}} p) \quad (\text{A.108})$$

$$= \mathcal{T}(p(\delta_{\Phi_{ij}} p) + (1-p)(\delta_{\Phi_{ij}} p)(1-p)) \quad (\text{A.109})$$

$$= \frac{2\pi i}{2} \mathcal{T}([\partial_i^t p, \partial_j^t p]) - \frac{2\pi i}{2} \mathcal{T}((1-p)[\partial_i^t p, \partial_j^t p]) \quad (\text{A.110})$$

$$= 2\pi i \mathcal{T}(p[\partial_i^t p, \partial_j^t p]) \quad (\text{A.111})$$

$$= \text{Ch}_{\{t_i, t_j\}}([p]_0). \quad (\text{A.112})$$

In the second to last equality $\mathcal{T}([\partial_i^t p, \partial_j^t p])$ vanishes due to partial integration. Since it is $\mathcal{T}(\partial A) = 0$ for any of the $*$ -derivations, it follows

$$\mathcal{T}(\partial_i A \partial_j B) = -\mathcal{T}(A \partial_i \partial_j B) = -\mathcal{T}(A \partial_j \partial_i B) = \mathcal{T}(\partial_j A \partial_i B). \quad (\text{A.113})$$

For the pitch parameter, we have analogously

$$\partial_{\theta_{ij}} \text{Ch}_\emptyset([p]_0) = \partial_{\theta_{ij}} \mathcal{T}(p) = \mathcal{T}(\delta_{\theta_{ij}} p) \quad (\text{A.114})$$

$$= \mathcal{T}(p(\delta_{\theta_{ij}} p) + (1-p)(\delta_{\theta_{ij}} p)(1-p)) \quad (\text{A.115})$$

$$= -2\pi i \mathcal{T}(p \partial_j^t p \partial_i^u p) + 2\pi i \mathcal{T}((1-p) \partial_j^t p \partial_i^u p) \quad (\text{A.116})$$

$$= -2\pi i \mathcal{T}(p \partial_j^t p \partial_i^u p) + 2\pi i \mathcal{T}(\partial_j^t p p \partial_i^u p) \quad (\text{A.117})$$

$$= 2\pi i \mathcal{T}(p[\partial_i^u p, \partial_j^t p]) \quad (\text{A.118})$$

$$= \text{Ch}_{\{u_i, t_j\}}([p]_0). \quad (\text{A.119})$$

In line (A.117), we used the following off-diagonal property of $*$ -derivations of a projection p : $(1-p)\partial p = (\partial p)p$, which can be derived from $0 = \partial((1-p)p) = -(\partial p)p + (1-p)\partial p$.

A10. Generalised Středa formulas Thm. 3.8

We want to show

$$\partial_{\Theta_{ab}} \text{Ch}_I([p]_0) = \text{Ch}_{\{\mu_a, \mu_b\} \cup I}([p]_0) \quad (\text{A.120})$$

for an ordered set $I \subset \{\mu_1, \dots, \mu_{r+d}\}$ of even cardinality $|I| = n$, indices $a, b = 1, \dots, r+d$ (but not $a, b = 1, \dots, r$) with $\mu_a, \mu_b \notin I$, and $p \in \mathcal{P}(\mathcal{A}_\Theta)$ Itô-differentiable.

The case for $a, b = r+1, \dots, r+d$ has already been derived in [PS16, Thm. 5.6.3 (i)] and we modify this derivation to verify also the case for $a = 1, \dots, r$ and $b = r+1, \dots, r+d$. Let now $i = 1, \dots, r$ and $j = 1, \dots, d$, then this case can be expressed as the derivative with respect to the pitch parameters $\Theta_{ab} = \Theta_{u_i t_j} = \theta_{ij}$:

$$\partial_{\Theta_{u_i t_j}} \text{Ch}_I([p]_0) = \text{Ch}_{\{u_i, t_j\} \cup I}([p]_0). \quad (\text{A.121})$$

A. Calculations

The derivative of the n -cocycle can be evaluated by the Itô derivative acting on the content of the trace:

$$\partial_{\Theta_{u_i t_j}} \text{Ch}_I([p]_0) = \partial_{\theta_{ij}} \text{Ch}_I([p]_0) = \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}(\delta_{\theta_{ij}}(p \partial_{\sigma_1} p \dots \partial_{\sigma_n} p)) \quad (\text{A.122})$$

$$= \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}((\delta_{\theta_{ij}} p) \partial_{\sigma_1} p \dots \partial_{\sigma_n} p) \quad (\text{A.123})$$

$$+ \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}(p \delta_{\theta_{ij}}(\partial_{\sigma_1} p \dots \partial_{\sigma_n} p)) \quad (\text{A.124})$$

$$+ 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}(\partial_j^t p \partial_i^u(\partial_{\sigma_1} p \dots \partial_{\sigma_n} p)) \quad (\text{A.125})$$

$$= \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}((\delta_{\theta_{ij}} p) \partial_{\sigma_1} p \dots \partial_{\sigma_n} p) \quad (\text{A.126})$$

$$+ \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{k=1}^n \mathcal{T}(p \partial_{\sigma_1} p \dots (\delta_{\theta_{ij}} \partial_{\sigma_k} p) \dots \partial_{\sigma_n} p) \quad (\text{A.127})$$

$$+ 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{1 \leq k < l \leq n} \mathcal{T}(p \partial_{\sigma_1} p \dots \partial_j^t \partial_{\sigma_k} p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p) \quad (\text{A.128})$$

$$+ 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{l=1}^n \mathcal{T}(\partial_j^t p \partial_{\sigma_1} p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p) \quad (\text{A.129})$$

$$= (n+1) \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}((\delta_{\theta_{ij}} p) \partial_{\sigma_1} p \dots \partial_{\sigma_n} p) \quad (\text{A.130})$$

$$+ 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{l=1}^n \mathcal{T}(\partial_j^t p \partial_{\sigma_1} p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p) \quad (\text{A.131})$$

$$+ 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{1 \leq k < l \leq n} \mathcal{T}(p \partial_{\sigma_1} p \dots \partial_j^t \partial_{\sigma_k} p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p). \quad (\text{A.132})$$

Here, we iteratively applied the Itô product rule from Eq. (3.41) and the ordinary product rule for the $*$ -derivative ∂_i^u to the content of the trace. We then collected the terms with the Itô derivative $\delta_{\theta_{ij}} p$ in the first sum and used the cyclicity of the cyclic cocycle to bring them to the front of the trace, while we collected the terms with the $*$ -derivations in the second and third sums. Let us refer to these sums in the following as T_1 , T_2 and T_3 .

The first sum T_1 can also be rewritten in terms of $*$ -derivations by replacing $\delta_{\theta_{ij}} p$ with its diagonal part $p(\delta_{\theta_{ij}} p) + (1-p)\delta_{\theta_{ij}} p(1-p)$. This can be done by using $(1-p)\partial p = (\partial p)p$ since we have an even number n derivations of p in the product under the trace. For the diagonal part follows from Eq. (A.106) and Eq. (A.107), that

$$p(\delta_{\theta_{ij}} p)p + (1-p)\delta_{\theta_{ij}} p(1-p) = -2\pi i \partial_j^t p \partial_i^u p + 2\pi i (1-p) \partial_j^t p \partial_i^u p \quad (\text{A.133})$$

$$= 2\pi i (1-2p) \partial_j^t p \partial_i^u p, \quad (\text{A.134})$$

and therefore, we obtain

$$T_1 = 2\pi i (n+1) \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}((1-2p)\partial_j^t p \partial_i^u p \partial_{\sigma_1} p \dots \partial_{\sigma_n} p) \quad (\text{A.135})$$

$$= 2\pi i (n+1) \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \mathcal{T}((1-2p)\partial_{\sigma_1} p \dots \partial_{\sigma_n} p \partial_j^t p \partial_i^u p). \quad (\text{A.136})$$

In the last step we used the handy relation $(1-2p)\partial p = -\partial p(1-2p)$, which can be derived by $(1-2p)\partial p = (1-p)\partial p - p\partial p = \partial p p - \partial p(1-p) = -\partial p(1-2p)$, and will be used a lot in the following.

Next, we rewrite T_2 . For that, we replace $\partial_i^u \partial_{\sigma_l} p$ by its diagonal part (which again requires n even) and separate the second derivations into products of derivations

$$p(\partial_i^u \partial_{\sigma_l} p)p + (1-p)(\partial_i^u \partial_{\sigma_l} p)(1-p) \quad (\text{A.137})$$

$$= -\{\partial_i^u p, \partial_{\sigma_l} p\}p + (1-p)\{\partial_i^u p, \partial_{\sigma_l} p\} = (1-2p)\{\partial_i^u p, \partial_{\sigma_l} p\}. \quad (\text{A.138})$$

The latter part uses a relation valid for any second $*$ -derivation of a projection p .

$$0 = \partial_1 \partial_2 (p(1-p)) = \partial_1 (\partial_2 p(1-p) - p\partial_2 p) \quad (\text{A.139})$$

$$= \partial_1 \partial_2 p(1-p) - \partial_2 p \partial_1 p - \partial_1 p \partial_2 p - p \partial_1 \partial_2 p, \quad (\text{A.140})$$

and thus, by multiplication with p from the right-hand side or $(1-p)$ from the left-hand side, one obtains

$$p(\partial_1 \partial_2 p)p = -\{\partial_1 p, \partial_2 p\}p \quad (\text{A.141})$$

$$(1-p)(\partial_1 \partial_2 p)(1-p) = (1-p)\{\partial_1 p, \partial_2 p\}. \quad (\text{A.142})$$

With this T_2 takes the form

$$T_2 = 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{l=1}^n \mathcal{T}(\partial_j^t p \partial_{\sigma_1} p \dots (1-2p)\{\partial_i^u p, \partial_{\sigma_l} p\} \dots \partial_{\sigma_n} p) \quad (\text{A.143})$$

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{l=1}^n (-1)^l \mathcal{T}((1-2p)\partial_j^t p \partial_{\sigma_1} p \dots \{\partial_i^u p, \partial_{\sigma_l} p\} \dots \partial_{\sigma_n} p) \quad (\text{A.144})$$

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{l=1}^n (-1)^l \left(\mathcal{T}((1-2p)\partial_j^t p \partial_{\sigma_1} p \dots \partial_i^u p \partial_{\sigma_l} p \dots \partial_{\sigma_n} p) \right. \quad (\text{A.145})$$

$$\left. + \mathcal{T}((1-2p)\partial_j^t p \partial_{\sigma_1} p \dots \partial_{\sigma_l} p \partial_i^u p \dots \partial_{\sigma_n} p) \right). \quad (\text{A.146})$$

This is a telescope sum, since the second term for any $l < n$ cancels with the first term for $l+1$. It remains only the first term for $l=1$ and the second term for $l=n$.

A. Calculations

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \left(-\mathcal{T}((1-2p)\partial_j^t p \partial_i^u p \partial_{\sigma_1} p \dots \partial_{\sigma_n} p) \right. \quad (\text{A.147})$$

$$\left. + \mathcal{T}((1-2p)\partial_j^t p \partial_{\sigma_1} p \dots \partial_{\sigma_n} p \partial_i^u p) \right) \quad (\text{A.148})$$

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \left(-\mathcal{T}((1-2p)\partial_{\sigma_1} p \dots \partial_{\sigma_n} p \partial_j^t p \partial_i^u p) \right. \quad (\text{A.149})$$

$$\left. + \mathcal{T}((1-2p)\partial_j^t p \partial_{\sigma_1} p \dots \partial_{\sigma_n} p \partial_i^u p) \right) \quad (\text{A.150})$$

For the computation of T_3 , we perform a partial integration with respect to ∂_{σ_k} for $k = 1, \dots, n$

$$\mathcal{T}(p \partial_{\sigma_1} p \dots \partial_j^t \partial_{\sigma_k} p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p) \quad (\text{A.151})$$

$$= \mathcal{T}(\partial_{\sigma_k}(p \partial_{\sigma_1} p \dots \partial_j^t p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p)) \quad (\text{A.152})$$

$$- \mathcal{T}(\partial_{\sigma_k} p \partial_{\sigma_1} p \dots \partial_j^t p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p) \quad (\text{A.153})$$

$$- \sum_{\substack{m=1 \\ m \neq k}}^n \mathcal{T}(p \partial_{\sigma_1} p \dots \partial_{\sigma_k} \partial_{\sigma_m} p \dots \partial_j^t p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p). \quad (\text{A.154})$$

The first term vanishes since the trace of any total $*$ -derivation vanishes and the last term cancels in T_3 since it is symmetric under exchanging m and k , while the signum $(-1)^\sigma$ is odd under any transposition. We arrive at

$$T_3 = -2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{1 \leq k < l \leq n} \mathcal{T}(\partial_{\sigma_k} p \partial_{\sigma_1} p \dots \partial_j^t p \dots \partial_i^u \partial_{\sigma_l} p \dots \partial_{\sigma_n} p). \quad (\text{A.155})$$

We can reorder $\partial_{\sigma_k} p \partial_{\sigma_1} p \dots \partial_{\sigma_{k-1}} p$ to $\partial_{\sigma_1} p \dots \partial_{\sigma_k} p$, which introduces the sign $(-1)^{k-1}$ to every term. Next, we replace $\partial_i^u \partial_{\sigma_l} p$ by its diagonal part as already done in T_2 .

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{1 \leq k < l \leq n} (-1)^k \quad (\text{A.156})$$

$$\mathcal{T}(\partial_{\sigma_1} p \dots \partial_{\sigma_k} p \partial_j^t p \dots (1-2p)\{\partial_i^u p, \partial_{\sigma_l} p\} \dots \partial_{\sigma_n} p) \quad (\text{A.157})$$

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{k=1}^{n-1} \sum_{l=k+1}^n (-1)^{k+l} \quad (\text{A.158})$$

$$\mathcal{T}((1-2p)\partial_{\sigma_1} p \dots \partial_{\sigma_k} p \partial_j^t p \dots \{\partial_i^u p, \partial_{\sigma_l} p\} \dots \partial_{\sigma_n} p) \quad (\text{A.159})$$

Here, we have again a telescope sum in which the second term for any $k+1 \leq l < n$ cancels with the first term for $l+1$. It remains only the first term of $l = k+1$ and the second term of $l = n$.

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{k=1}^{n-1} \left((-1)^{2k+1} \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p \partial_i^u p \dots \partial_{\sigma_n}p) \right. \quad (\text{A.160})$$

$$\left. + (-1)^{k+n} \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p \dots \partial_{\sigma_n}p \partial_i^u p) \right) \quad (\text{A.161})$$

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{k=1}^{n-1} \left(-\mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_n}p \partial_j^t p \partial_i^u p) \right. \quad (\text{A.162})$$

$$\left. + (-1)^k \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p \dots \partial_{\sigma_n}p \partial_i^u p) \right) \quad (\text{A.163})$$

In the last step, we moved $(1-2p)$ behind $\partial_i^u p$ in the first term, which introduced $(-1)^{k+2}$, brought $(1-2p)\partial_{\sigma_{k+1}}p \dots \partial_{\sigma_n}p$ to the front, and reordered $\partial_{\sigma_{k+1}}p \dots \partial_{\sigma_n}\partial_{\sigma_1}p \dots \partial_{\sigma_k}p$ to $\partial_{\sigma_1}p \dots \partial_{\sigma_n}p$ introducing $(-1)^{k(n-k)}$. With n even, this combines to $(-1)^{k-k^2} = -1^{-(k-1)k} = 1$, since the product of any whole number and its predecessor needs to be even. We obtain

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \left(-(n-1) \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_n}p \partial_j^t p \partial_i^u p) \right. \quad (\text{A.164})$$

$$\left. + \sum_{k=1}^{n-1} (-1)^k \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p \dots \partial_{\sigma_n}p \partial_i^u p) \right). \quad (\text{A.165})$$

Now, we can recombine the sums T_1 , T_2 , and T_3 to obtain

$$\partial_{\Theta_{u_i t_j}} \text{Ch}_I(p) = T_1 + T_2 + T_3 \quad (\text{A.166})$$

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \left((n+1) \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_n}p \partial_j^t p \partial_i^u p) \right. \quad (\text{A.167})$$

$$\left. - \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_n}p \partial_j^t p \partial_i^u p) \right. \quad (\text{A.168})$$

$$+ \mathcal{T}((1-2p)\partial_j^t p \partial_{\sigma_1}p \dots \partial_{\sigma_n}p \partial_i^u p) \quad (\text{A.169})$$

$$\left. - (n-1) \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_n}p \partial_j^t p \partial_i^u p) \right. \quad (\text{A.170})$$

$$\left. + \sum_{k=1}^{n-1} (-1)^k \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p \dots \partial_{\sigma_n}p \partial_i^u p) \right) \quad (\text{A.171})$$

$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \left(\mathcal{T}((1-2p)\partial_j^t p \partial_{\sigma_1}p \dots \partial_{\sigma_n}p \partial_i^u p) \right. \quad (\text{A.172})$$

$$\left. + \sum_{k=1}^{n-1} (-1)^k \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p \dots \partial_{\sigma_n}p \partial_i^u p) \right. \quad (\text{A.173})$$

$$\left. + \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_n}p \partial_j^t p \partial_i^u p) \right) \quad (\text{A.174})$$

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$$= 2\pi i \Lambda_n \sum_{\sigma \in S_n} (-1)^\sigma \sum_{k=0}^n (-1)^k \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p \dots \partial_{\sigma_n}p \partial_i^u p). \quad (\text{A.175})$$

Now, we can rearrange the order of one half of each term to introduce the permutations of $\partial_j^t p$ and $\partial_i^u p$, that we need for the Chern character expression which sums over all possible permutations of the derivations. It is

$$\mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p \dots \partial_{\sigma_n}p \partial_i^u p) \quad (\text{A.176})$$

$$= (-1)^{k+1} \mathcal{T}((1-2p)\partial_{\sigma_{k+1}}p \dots \partial_{\sigma_n}p \partial_i^u p \partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_j^t p) \quad (\text{A.177})$$

$$= -\mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_i^u p \dots \partial_{\sigma_n}p \partial_j^t p). \quad (\text{A.178})$$

In the second line, we moved $(1-2p)$ before $\partial_{\sigma_{k+1}}p$ generating $(-1)^{k+1}$ and cycled everything in front of it to the back. Then, we reordered the indices (implicitly replacing σ by a composition with the reordering permutation) generating the additional sign $(-1)^{k(n-k)}$. Since $k-k^2$ is even, only (-1) remains, and we obtained a term with switched $\partial_j^t p$ and $\partial_i^u p$ and opposite sign. Let ρ be the bijection between $(1, 2)$ and (u_i, t_j) , then we get

$$= -2\pi i \Lambda_n \sum_{\substack{\sigma \in S_n \\ \rho \in S_2}} (-1)^{\sigma+\rho} \sum_{k=0}^n (-1)^k \frac{1}{2} \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\rho_1}p \dots \partial_{\sigma_n}p \partial_{\rho_2}p). \quad (\text{A.179})$$

To end up with the expression of an $(n+2)$ -cocycle, we need $(n+2)!$ terms for all permutations of the $n+2$ derivations. Right now, we have only $n!2!(n+1)$ terms with a fixed position of $\partial_{\rho_2}p$. Therefore, we take each of these terms $(n+2)$ times and rearrange them into all possible permutations, thereby obtaining $n!2!(n+2)(n+1) = n!2! \frac{(n+2)!}{n!2!} 2$ terms, where each permutation occurs twice.

$$= -\frac{2\pi i \Lambda_n}{2(n+2)} \sum_{\substack{\sigma \in S_n \\ \rho \in S_2}} (-1)^{\sigma+\rho} \quad (\text{A.180})$$

$$\sum_{k=0}^n (-1)^k \left(\sum_{l=0}^n \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_{\rho_1}p \dots \partial_{\sigma_n}p \partial_{\rho_2}p) \right. \quad (\text{A.181})$$

$$\left. + \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_{\rho_1}p \dots \partial_{\sigma_n}p \partial_{\rho_2}p) \right) \quad (\text{A.182})$$

$$= -\frac{2\pi i \Lambda_n}{n+2} \sum_{\substack{\sigma \in S_n \\ \rho \in S_2}} (-1)^{\sigma+\rho} \quad (\text{A.183})$$

$$\sum_{0 \leq l \leq k \leq n} (-1)^{k+l} \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_l}p \partial_{\rho_1}p \dots \partial_{\sigma_k}p \partial_{\rho_2}p \dots \partial_{\sigma_n}p). \quad (\text{A.184})$$

This rearrangement is done the following way: First, we rewrite the terms with $l \leq k$ by bringing the first $k-l$ derivations to the back passing $(1-2p)$.

$$\mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_{\rho_1}p \dots \partial_{\sigma_n}p \partial_{\rho_2}p) \quad (\text{A.185})$$

$$= (-1)^{k-l} \mathcal{T}((1-2p)\partial_{\sigma_{k-l+1}}p \dots \partial_{\sigma_k}p \partial_{\rho_1}p \dots \partial_{\sigma_n}p \partial_{\rho_2}p \partial_{\sigma_1}p \dots \partial_{\sigma_{k-l}}p) \quad (\text{A.186})$$

$$= \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_l}p \partial_{\rho_1}p \dots \partial_{\sigma_{n-k+l}}p \partial_{\rho_2}p \dots \partial_{\sigma_n}p) \quad (\text{A.187})$$

Now let us consider the sum over all terms with $l \leq k \leq n$. For any fixed l the index $n-k+l$ runs from n to l . We can reverse this by substituting $n-k+l$ with k running from l to n . This changes the sign from $(-1)^k$ to $(-1)^{n-k+l} = (-1)^{k+l}$.

$$\sum_{l=0}^n \sum_{k=l}^n (-1)^{k+l} \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_l}p \partial_{\rho_1}p \dots \partial_{\sigma_k}p \partial_{\rho_2}p \dots \partial_{\sigma_n}p) \quad (\text{A.188})$$

Next, we do the opposite with the terms with $l \geq k$ (here comes the extra term into play for $l = k$) and bring the last $n-l+1$ derivations to the front passing $(1-2p)$.

$$\mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_{\rho_1}p \dots \partial_{\sigma_n}p \partial_{\rho_2}p) \quad (\text{A.189})$$

$$= (-1)^{n-l+1} \mathcal{T}((1-2p)\partial_{\sigma_{l+1}}p \dots \partial_{\sigma_n}p \partial_{\rho_2}p \partial_{\sigma_1}p \dots \partial_{\sigma_k}p \partial_{\rho_1}p \dots \partial_{\sigma_l}p) \quad (\text{A.190})$$

$$= -\mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_{n-l}}p \partial_{\rho_2}p \dots \partial_{\sigma_{n-l+k}}p \partial_{\rho_1}p \dots \partial_{\sigma_n}p). \quad (\text{A.191})$$

Here, we consider the sum over all terms with $k \leq l$. The index $n-l$ runs from n to 0, and we reverse this by substituting $n-l$ for l thereby running from 0 to n . This changes $k \leq l$ to $k \leq n-l$, and the index $n-l+k$ to $l+k$ running for any fixed l from l to n . We substitute therefore $l+k$ for k with $k \geq l$, which changes the sign $(-1)^k$ to $(-1)^{k-l} = (-1)^{k+l}$, and switch ρ_2 and ρ_1 introducing (-1) to obtain for a second time

$$\sum_{l=0}^n \sum_{k=l}^n (-1)^{k+l} \mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_l}p \partial_{\rho_1}p \dots \partial_{\sigma_k}p \partial_{\rho_2}p \dots \partial_{\sigma_n}p). \quad (\text{A.192})$$

Now, we can replace the prefactor $2\frac{2\pi i}{n+2}\Lambda_n = \frac{2\pi i}{\frac{n+2}{2}} \frac{(2\pi i)^{\frac{n}{2}}}{(\frac{n}{2})!} = \frac{(2\pi i)^{\frac{n+2}{2}}}{(\frac{n+2}{2})!}$ by Λ_{n+2} and introduce the bijection ω between $(1, \dots, n+2)$ and $\{u_i, t_j\} \cup I$.

$$\partial_{\Theta_{u_i t_j}} \text{Ch}_I(p) = -\frac{2\pi i}{n+2} \Lambda_n \sum_{\substack{\sigma \in S_n \\ \rho \in S_2}} (-1)^{\sigma+\rho} \sum_{0 \leq l \leq k \leq n} (-1)^{k+l} \quad (\text{A.193})$$

$$\mathcal{T}((1-2p)\partial_{\sigma_1}p \dots \partial_{\sigma_l}p \partial_{\rho_1}p \dots \partial_{\sigma_k}p \partial_{\rho_2}p \dots \partial_{\sigma_n}p) \quad (\text{A.194})$$

$$= -\frac{\Lambda_{n+2}}{2} \sum_{\omega \in S_{n+2}} (-1)^\omega \mathcal{T}((1-2p)\partial_{\omega_1}p \dots \partial_{\omega_{n+2}}p) \quad (\text{A.195})$$

$$= \Lambda_{n+2} \sum_{\omega \in S_{n+2}} (-1)^\omega \mathcal{T}(p \partial_{\omega_1}p \dots \partial_{\omega_{n+2}}p) \quad (\text{A.196})$$

$$= \text{Ch}_{\{u_i, t_j\} \cup I}([p]_0). \quad (\text{A.197})$$

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The term with $\mathcal{T}(\partial_{\omega_1} p \dots \partial_{\omega_{n+2}} p)$ vanishes by symmetry in the third equality. It is

$$\mathcal{T}(\partial_{\omega_1} p \dots \partial_{\omega_{n+2}} p) = \mathcal{T}(\partial_{\omega_1} (p \dots \partial_{\omega_{n+2}} p)) - \sum_{i=2}^{n+2} \mathcal{T}(p \partial_{\omega_2} \dots \partial_{\omega_1} \partial_{\omega_i} p \dots \partial_{\omega_{n+2}} p). \quad (\text{A.198})$$

The first term is zero since it is the trace of a total derivation and all terms in the sum are even under exchanging ω_1 and ω_i , whereas the signum $(-1)^\omega$ is odd under any transposition.

A11. Orbital magnetisation Eq. (3.67)

We use the Itô-like calculus to derive the magnetic flux derivative of the free energy density at zero temperature given by the trace of the smooth and Itô-differentiable algebra element $(\mu - h)p$:

$$\begin{aligned} \partial_\phi \mathcal{T}((\mu - h)p) &= \mathcal{T}(\delta_{\Phi_{12}}((\mu - h)p)) \\ &= \mathcal{T}((\mu - h)\delta_{\Phi_{12}} p) - \frac{2\pi i}{2} \mathcal{T}(\partial_1^t(\mu - h)\partial_2^t p - \partial_2^t(\mu - h)\partial_1^t p) \\ &= \mathcal{T}((\mu - h)\delta_{\Phi_{12}} p) \\ &= \mathcal{T}((\mu - h)p(\delta_{\Phi_{12}} p)p + (\mu - h)(1 - p)(\delta_{\Phi_{12}} p)(1 - p)) \\ &= \frac{2\pi i}{2} \mathcal{T}((\mu - h)(p[\partial_1^t p, \partial_2^t p] - (1 - p)[\partial_1^t p, \partial_2^t p])) \\ &= -\frac{2\pi i}{2} \mathcal{T}((\mu - h)(1 - 2p)[\partial_1^t p, \partial_2^t p]) \\ &= \frac{2\pi i}{2} \mathcal{T}(|\mu - h|[\partial_1^t p, \partial_2^t p]), \end{aligned}$$

where we used $\delta_{\Phi_{12}} h = 0$ for the third equality. The last equality follows from the eigenvalues of $(1 - 2p)$

$$\begin{cases} -1 & \text{for } E_i \leq \mu \\ +1 & \text{for } E_i > \mu \end{cases}, \quad (\text{A.199})$$

where the E_i denote the corresponding energy eigenvalues of h . It follows for the product of with the shifted Hamiltonian: $(\mu - h)(1 - 2p) = -|\mu - h|$.

The decomposition of the formula into contributions corresponding to those from modern theory is performed the following way:

$$\begin{aligned} &\mathcal{T}((\mu - h)(1 - 2p)[\partial_1^t p, \partial_2^t p]) \\ &= \mathcal{T}((\mu - h)[\partial_1^t p, \partial_2^t p] - 2(\mu - h)p[\partial_1^t p, \partial_2^t p]) \\ &= \mathcal{T}(-h[\partial_1^t p, \partial_2^t p] + 2hp[\partial_1^t p, \partial_2^t p] - 2\mu p[\partial_1^t p, \partial_2^t p]) \\ &= \mathcal{T}(-h[\partial_1^t p, \partial_2^t p] + hp[\partial_1^t p, \partial_2^t p] + hp[\partial_1^t p, \partial_2^t p] - 2\mu p[\partial_1^t p, \partial_2^t p]). \end{aligned}$$

The last two terms already occur in the modern theory formula, and the first two terms can be rewritten further using $p(\partial_k^t p) = (\partial_k^t p)(1 - p)$ as

$$\begin{aligned}
& \mathcal{T}(-h[\partial_1^t p, \partial_2^t p] + hp[\partial_1^t p, \partial_2^t p]) \\
&= \mathcal{T}(-\partial_2^t p h \partial_1^t p + \partial_1^t p h \partial_2^t p + h \partial_1^t p (1 - p) \partial_2^t p - h \partial_2^t p (1 - p) \partial_1^t p) \\
&= \mathcal{T}(\partial_1^t p h \partial_2^t p - \partial_2^t p h \partial_1^t p - (1 - p) \partial_1^t p h \partial_2^t p + (1 - p) \partial_2^t p h \partial_1^t p) \\
&= \mathcal{T}(p \partial_1^t p h \partial_2^t p - p \partial_2^t p h \partial_1^t p),
\end{aligned}$$

which is then equal to the remaining part of the modern theory expression.

A12. Discrete Fourier transformation identity Eq. (4.1.2)

We want to verify the identity

$$s(\hat{n}) = \sum_{\lambda^{2L+1}=1} c_\lambda \lambda^n, \quad n \in \mathbb{Z} \quad c_\lambda = \begin{cases} \frac{\lambda^{L+1}}{1-\lambda}, & \text{if } \lambda \neq 1 \\ 0, & \text{if } \lambda = 1 \end{cases}.$$

The sum condition $\lambda^{2L+1} = 1$ implies $\lambda \in \left\{ e^{-\frac{2\pi i k}{2L+1}} \mid -L \leq k \leq L \right\}$ and the right hand-side does only depend on $\hat{n}$, since $\lambda^{n+(2L+1)j} = \lambda^n$, for all $j \in \mathbb{Z}$. Thus, we only need to verify that

$$n = \sum_{k=-L}^L c_k e^{-\frac{2\pi i}{2L+1} kn}, \quad n \in \{-L, \dots, L\}. \quad (\text{A.200})$$

This is the discrete Fourier transformation (DFT) of the sequence of $2L + 1$ complex numbers $c_{-L}, \dots, c_L$ into the sequence $-L, \dots, L$. Thus, we can calculate the coefficients c_k using the inverse discrete Fourier transform:

$$c_k = \frac{1}{2L+1} \sum_{n=-L}^L n e^{\frac{2\pi i}{2L+1} kn}, \quad k \in \{-L, \dots, L\}. \quad (\text{A.201})$$

For $k = 0$ this evaluates to $c_k = 0$ and $k \neq 0$ we find

$$c_k = -\frac{1}{2L+1} \sum_{n=-L}^L n e^{-\frac{2\pi i}{2L+1} kn} \quad (\text{A.202})$$

$$= \frac{1}{2\pi i k} \sum_{n=-L}^L \frac{d}{dt} \Big|_{t=1} e^{-\frac{2\pi i}{2L+1} knt} \quad (\text{A.203})$$

$$= \frac{1}{2\pi i k} \frac{d}{dt} \Big|_{t=1} \sum_{n=0}^{2L} e^{-\frac{2\pi i}{2L+1} k(n-L)t} \quad (\text{A.204})$$

$$= \frac{1}{2\pi i k} \frac{d}{dt} \Big|_{t=1} e^{\frac{2\pi i}{2L+1} kLt} \sum_{n=0}^{2L} \left(e^{-\frac{2\pi i}{2L+1} kt} \right)^n \quad (\text{A.205})$$

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$$= \frac{1}{2\pi i k} \frac{d}{dt} \Big|_{t=1} e^{\frac{2\pi i}{2L+1} k L t} \frac{1 - e^{-2\pi i k t}}{1 - e^{-\frac{2\pi i}{2L+1} k t}} \quad (\text{A.206})$$

$$= \frac{L}{2L+1} e^{\frac{2\pi i}{2L+1} k L} \overbrace{\frac{1 - e^{-2\pi i k}}{1 - e^{-\frac{2\pi i}{2L+1} k}}}^{=0 \text{ for } k \in \mathbb{Z}} + e^{\frac{2\pi i}{2L+1} k L} \frac{e^{-2\pi i k}}{1 - e^{-\frac{2\pi i}{2L+1} k}} \quad (\text{A.207})$$

$$- e^{\frac{2\pi i}{2L+1} k L} \overbrace{\frac{1 - e^{-2\pi i k}}{\left(1 - e^{-\frac{2\pi i}{2L+1} k}\right)^2}}^{=0 \text{ for } k \in \mathbb{Z}} \frac{1}{2L+1} e^{-\frac{2\pi i}{2L+1} k} \quad (\text{A.208})$$

$$= \frac{e^{\frac{2\pi i}{2L+1} k L}}{1 - e^{-\frac{2\pi i}{2L+1} k}} \quad (\text{A.209})$$

Due to the $2L+1$ periodicity, we have $e^{\frac{2\pi i}{2L+1} k L} = e^{-\frac{2\pi i}{2L+1} k(L+1)}$

$$c_k = \begin{cases} \frac{\left(e^{-\frac{2\pi i}{2L+1} k}\right)^{L+1}}{1 - e^{-\frac{2\pi i}{2L+1} k}}, & \text{if } 1 \leq |k| \leq L \\ 0, & \text{if } k = 0 \end{cases} \quad (\text{A.210})$$

These are precisely the coefficients from the identity.

A13. Error bounds Thm. 4.1

Let $h \in \mathcal{A}$ and $\hat{h} = \hat{p}(h) \in \mathcal{A}^L$. We want to show, that for any $K \in \mathbb{N}$ there exists a finite positive constant A_K such that:

$$\left| \mathcal{T}(\partial^{\alpha_1} G_1(h) \dots \partial^{\alpha_n} G_n(h)) - \hat{\mathcal{T}}(\hat{\partial}^{\alpha_1} G_1(\hat{h}) \dots \hat{\partial}^{\alpha_n} G_n(\hat{h})) \right| \leq \frac{A_K}{(1 + |V_L|)^K}, \quad (\text{A.211})$$

where $G_i : \mathbb{R} \rightarrow \mathbb{C}$ are smooth functions over $\sigma(h)$ and the α_i 's are multi-indices.

First we derive two upper bounds for the decay of the coefficients, which we require for the proof down the way. The fast decay property was presented in Chap. 3.2.2 and verified in App. A7. From line (A.78) in its proof we know that for $a \in \mathcal{A}_\Theta$ and any multi-index $\alpha \in \mathbb{N}_0^d$ there exists a finite positive constant A_α such that for any $\mathbf{n} \in \mathbb{Z}^d$:

$$\|\mathbf{n}^\alpha a_{\mathbf{n}}\|_{T^r} \leq \|\partial_t^\alpha a\|_r =: A_\alpha < \infty. \quad (\text{A.212})$$

From this we can infer, that for all $J, K \in \mathbb{N}_0$ there exist finite positive constants A_J, A_K such that:

$$(1 + |\mathbf{n}|)^J \|a_{\mathbf{n}}\|_{T^r} \leq A_J \quad \text{and} \quad (1 + \bar{n}^d)^{2K} \|a_{\mathbf{n}}\|_{T^r} \leq A_K, \quad (\text{A.213})$$

where $\bar{n} = \max_{i=1, \dots, d} |n_i|$.

For the first inequality, we consider $(1 + \mathbf{n}^2)^J \|a_{\mathbf{n}}\|_{T^r} \geq (1 + \sqrt{\mathbf{n}^2})^J \|a_{\mathbf{n}}\|_{T^r}$, $\forall \mathbf{n} \in \mathbb{Z}^d$, which can be expanded to a polynomial of which each monomial is of the form $cn_i^{\alpha_i} \|a_{\mathbf{n}}\|_{T^r}$, with $c \in \mathbb{N}$ and $\alpha_i \in 2\mathbb{N}$ for some $i = 1, \dots, d$, and can therefore be bounded by a cA_α . Thus, the whole expression has an upper bound A_J . For the second inequality, we proceed the same way to find an upper bound for $(1 + |n_i|^d)^{2K} \|a_{\mathbf{n}}\|_{T^r}$. We then take the maximum of these upper bounds as the upper bound A_K .

Now, we come to the proof itself, which follows [Pro17, Chap. 6.3]. There are two disparities for which we need to find an upper bound: The one caused by the $*$ -epimorphism $\hat{p}$ onto the finite volume approximating algebra and the one caused by the approximate translation derivations $\hat{\partial}^t$.

The $*$ -epimorphism $\hat{p}$ is a homomorphism and thus commutes with the functional calculus, such that $G_j(\hat{h}) = \hat{p}(G_j(h))$. As presented in Eq. (4.10), a generic element $a \in \mathcal{A}$ with coefficients $a_{\mathbf{m}}$ is mapped to $\hat{p}(a) \in \mathcal{A}^L$ with coefficients

$$\hat{a}_{\mathbf{m}} = \sum_{\substack{\mathbf{n} \in \mathbb{Z}^d \\ \hat{\mathbf{n}} = \mathbf{m}}} a_{\mathbf{n}}. \quad (\text{A.214})$$

Unfortunately, since the translation derivations are approximated, it is in general $\hat{\partial}^{\alpha_j} G_j(\hat{h}) \neq \hat{p}(\partial^{\alpha_j} G_j(h))$. However, we can define $\hat{\partial}_t^\alpha$ on $\mathcal{A}$ by

$$(\hat{\partial}_t^\alpha a)_{\mathbf{m}} = i^{|\alpha|} s(\hat{\mathbf{m}})^\alpha a_{\mathbf{m}}, \quad \mathbf{m} \in \mathbb{Z}^d, \quad (\text{A.215})$$

which maps $\mathcal{A}$ into itself. With this, we have

$$\hat{\partial}^{\alpha_j} G_j(\hat{h}) = \hat{p}(\hat{\partial}^{\alpha_j} G_j(h)), \quad (\text{A.216})$$

since the phase derivations $\hat{\partial}_u^\alpha$ are already the same on both algebras.

Using this identity, we can rewrite Eq. (A.211) to

$$\left| \mathcal{T}(\partial^{\alpha_1} G_1(h) \dots \partial^{\alpha_n} G_n(h)) - \hat{\mathcal{T}}(\hat{p}(\hat{\partial}^{\alpha_1} G_1(h) \dots \hat{\partial}^{\alpha_n} G_n(h))) \right|. \quad (\text{A.217})$$

A difference of the form $|\mathcal{T}(a) - \mathcal{T}(\hat{p}(a))|$ can be expressed the following way:

$$\left| \mathcal{T}(a) - \hat{\mathcal{T}}(\hat{p}(a)) \right| = \left| \int_{T^r} \frac{d\varphi}{(2\pi)^r} \text{tr}(a_0 - \hat{p}(a)_0) \right| = \left| \sum_{\substack{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\} \\ \hat{\mathbf{n}} = \mathbf{0}}} \int_{T^r} \frac{d\varphi}{(2\pi)^r} \text{tr}(a_{\mathbf{n}}) \right|, \quad (\text{A.218})$$

where we sum over all terms of the 0-coefficient of $\hat{p}(a)$ in accordance with Eq. (A.214) without the 0-coefficient of a .

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Now, we can find an upper bound using the second inequality of Eq. (A.213):

$$\left| \mathcal{T}(a) - \hat{\mathcal{T}}(\hat{p}(a)) \right| \leq \sum_{\substack{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\} \\ \hat{\mathbf{n}} = \hat{\mathbf{0}}}} \|a_{\mathbf{n}}^{11}\|_{T^r} + \|a_{\mathbf{n}}^{22}\|_{T^r} \quad (\text{A.219})$$

$$\leq \sum_{\substack{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\} \\ \hat{\mathbf{n}} = \hat{\mathbf{0}}}} \frac{A_K^{11} + A_K^{22}}{(1 + \bar{n}^d)^{2K}} = \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}} \frac{A'_K}{(1 + |V_L| \bar{n}^d)^{2K}} \quad (\text{A.220})$$

$$\leq \frac{A'_K}{(1 + |V_L|)^K} \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}} \frac{1}{(1 + \bar{n}^d)^K} \stackrel{K \geq 1}{\leq} \frac{A_K}{(1 + |V_L|)^K}. \quad (\text{A.221})$$

For the equality in line (A.220) we used that for the permitted $\mathbf{n}$ with $\hat{\mathbf{n}} = \hat{\mathbf{0}}$ it is $n_i = (2L + 1)j$, $j \in \mathbb{Z}$, for all $i = 1, \dots, d$, and thus they correspond to all sites besides the origin of a lattice with lattice constant $2L + 1$. For the last equality we could include the sum over $\mathbf{n}$ in A_K , as it is convergent for $K > 1$:

$$\sum_{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}} \frac{1}{(1 + |\bar{n}|^d)^K} = \sum_{l=1}^{\infty} \sum_{\substack{\mathbf{n} \in \mathbb{Z}^d \\ |\bar{\mathbf{n}}|=l}} \frac{1}{(1 + l^d)^K} = \sum_{l=1}^{\infty} \frac{(2l + 1)^d - (2l - 1)^d}{(1 + l^d)^K} < \infty. \quad (\text{A.222})$$

The polynomial in the numerator is of order $d - 1$ and the polynomial in the denominator of order Kd , therefore the series converges for $K > 1$. Since we confirmed the existence of a suitable constant for $K > 1$, this also implies the existence of one for $K = 1$.

Now, that we found an upper bound for the differences caused by the restriction to the finite-volume approximating algebra, we can rewrite Eq. (A.211) up to these corrections to

$$\left| \mathcal{T}\left(\partial^{\alpha_1} G_1(h) \dots \partial^{\alpha_n} G_n(h)\right) - \mathcal{T}\left(\hat{\partial}^{\alpha_1} G_1(h) \dots \hat{\partial}^{\alpha_n} G_n(h)\right) \right|. \quad (\text{A.223})$$

We are only left to consider the differences caused by the approximated translation derivations. For this, we can extend the difference to a telescope sum

$$\left| \sum_{j=1}^n \mathcal{T}\left(\partial^{\alpha_1} G_1(h) \dots \left(\partial^{\alpha_j} G_j(h) - \hat{\partial}^{\alpha_j} G_j(h)\right) \dots \hat{\partial}^{\alpha_n} G_n(h)\right) \right|, \quad (\text{A.224})$$

where each term is proportional to the difference in derivations. Since the phase derivations are the same in both cases, only the terms involving the translation derivations are non-zero. Using the cyclicity of the trace, its arguments in the individual terms can be expressed as

$$\left(\partial_t^{\alpha^t} \partial_u^{\alpha^u} G(h) - \hat{\partial}_t^{\alpha^t} \hat{\partial}_u^{\alpha^u} G(h)\right) b \quad (\text{A.225})$$

with $b \in \mathcal{A}$. By Eq. (A.215) the difference is of the form

$$\partial_t^{\alpha^t} \partial_u^{\alpha^u} G(h)_{\mathbf{m}} - \hat{\partial}_t^{\alpha^t} \hat{\partial}_u^{\alpha^u} G(h)_{\mathbf{m}} = \begin{cases} 0, & \mathbf{m} \in V_L \\ (i)^{|\alpha^t|} \left(\mathbf{m}^{\alpha^t} - s(\hat{\mathbf{m}})^{\alpha^t}\right) \partial_u^{\alpha^u} G(h)_{\mathbf{m}}, & \mathbf{m} \in \mathbb{Z}^d \setminus V_L \end{cases} \quad (\text{A.226})$$

Any expression $|\mathcal{T}(ab)|$ with $a, b \in \mathcal{A}$ and a , such that $a_{\mathbf{m}} = 0$ for $\mathbf{m} \in V_L$, has an upper bound of the following form:

$$|\mathcal{T}(ab)| = \left| \int_{T^r} \frac{d\varphi}{(2\pi)^r} \text{tr}((ab)_0) \right| \leq \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus V_L} \left| \int_{T^r} \frac{d\varphi}{(2\pi)^r} \text{tr}(a_{\mathbf{n}}(\varphi) \alpha_{\mathbf{n}} b_{-\mathbf{n}}(\varphi)) \right| \quad (\text{A.227})$$

$$\leq \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus V_L} \sup_{\varphi \in T^r} |\text{tr}(a_{\mathbf{n}}(\varphi) \alpha_{\mathbf{n}} b_{-\mathbf{n}}(\varphi))| \leq \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus V_L} \sum_{i,j=1}^2 \|a_{\mathbf{n}}^{ij}\|_{T^r} \|b_{-\mathbf{n}}^{ji}\|_{T^r} \quad (\text{A.228})$$

$$\leq \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus V_L} \sum_{i,j=1}^2 \frac{A_J^{ij} B_J^{ij}}{(1 + |\mathbf{n}|)^{2J}} = \sum_{\mathbf{m} \in V_L} \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}} \frac{A_J}{(1 + |\mathbf{m} + (2L + 1)\mathbf{n}|)^{2J}} \quad (\text{A.229})$$

$$\leq \sum_{\mathbf{m} \in V_L} \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}} \frac{A_J}{(1 + (2L + 1)|\mathbf{n}|)^{2J}} \quad (\text{A.230})$$

$$\leq |V_L| \frac{A_J}{(1 + (2L + 1))^J} \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}} \frac{1}{(1 + |\mathbf{n}|)^J} \quad (\text{A.231})$$

$$\stackrel{J=d(K+1) \geq 2d}{\leq} \frac{A_K}{(1 + |V_L|)^K}. \quad (\text{A.232})$$

From the second to the third line, we used the first inequality of Eq. (A.213). For the last line, we absorbed the sum over $\mathbf{n}$ into the constant, since it is convergent for $K \geq 1$:

$$\sum_{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}} \frac{1}{(1 + |\mathbf{n}|)^{d(K+1)}} \leq \sum_{\mathbf{n} \in \mathbb{Z}^d \setminus \{0\}} \frac{1}{(1 + \hat{n}^d)^{(K+1)}} < \infty. \quad (\text{A.233})$$

With that, we verified that for all $K \in \mathbb{N}$ there exists a finite positive A_K , such that all discrepancies in $\left| \mathcal{T}(\partial^{\alpha_1} G_1(h) \dots \partial^{\alpha_n} G_n(h)) - \hat{\mathcal{T}}(\hat{\partial}^{\alpha_1} G_1(\hat{h}) \dots \hat{\partial}^{\alpha_n} G_n(\hat{h})) \right|$ posses an upper bound $\frac{A_K}{(1 + |V_L|)^K}$.

B | Implementation

The implementation of the computational programme in Python utilises the NumPy package [Har+20] for its linear algebra objects and methods, and the just-in-time compiler Numba [LPS15] to accelerate Python and NumPy functions by translating them into optimised machine code.

```
1 import numpy as np
2 from numba import jit
```

The following paragraphs present the implementation of the components discussed in Sec. 4.2.2 for a 2-dimensional triangular lattice as used to obtain numerical results in this work. The functions only require the above Python packages, the priorly defined functions, and the objects and functions defined in paragraphs B8 Tools, B9 Constants, and B10 Lattice. The full code base can be found in GitHub [prasspascal/chern_numbers_in_multi-q_systems](#).

The implementation of the Hilbert space, the Hamiltonian, and the spectrum were first written by Fabian Lux for [Lux+24] in the version found on GitHub [luxfabian/ncg_spin_systems](#). They were later modified and extended by the functions for the differential calculus and the Chern numbers by the author for [Pra+24] in the version found on GitHub [prasspascal/chern_numbers_in_skyrmion_crystals](#). The function for the Orbital Magnetisation evaluation has not been published so far.

B1. Hilbert space Eq. (4.22)

```
1 @jit(nopython=True)
2 def construct_hilbert_space(n_x, n_y):
3     """
4     systematic labeling of quantum states
5     """
6
7     labels = np.zeros((n_x * n_y * 2, 3), dtype=np.integer)
8     states = np.zeros((n_x, n_y, 2), dtype=np.integer)
9
10    # construct hilbert space
11    ii = 0
12    for i in range(n_x):
```

B. Implementation

```
13     for j in range(n_y):
14         for s in range(2): # spin
15             labels[ii] = np.array([i, j, s])
16             states[i, j, s] = ii
17             ii += 1
18
19     return labels, states
```

B2. Hamiltonian Eq. (4.23)

```
1  @jit(nopython=True)
2  def set_hamiltonian(hamiltonian, states, n_x, n_y, theta, alpha, phi, shift, mag, t, m, texture,
3  boundary_conditions, regularization = 0.0, flux = 0.0):
4      """
5      nearest neighbor hopping on the triangular lattice plus exchange
6      """
7
8      for i in range(n_x):
9          for j in range(n_y):
10
11              # hopping
12              nn = nearest_neighbors(i, j, n_x, n_y, boundary_conditions)
13              hopp = [ t* np.exp(1j* pi* flux * -j), t* np.exp(1j* pi* flux * +i), t*
14                  ↪ np.exp(1j* pi* flux * -(i+j))]
15              for s in range(2):
16                  ii = states[i, j, s]
17                  for site, h in zip(nn, hopp):
18                      jj = states[site[0], site[1], s]
19
20                      hamiltonian[ii, jj] = h
21                      hamiltonian[jj, ii] = np.conjugate(h)
22
23              # onsite term
24              nvec = magnetization(i, j, theta, alpha, phi, shift, mag, texture,
25                  ↪ regularization)
26              onsite = m * (nvec[0] * sx + nvec[1] * sy + nvec[2] * sz)
27              for a in range(2):
28                  for b in range(2):
29                      ii = states[i, j, a]
30                      jj = states[i, j, b]
31                      hamiltonian[ii, jj] = onsite[a, b]
```

```

1 @jit(nopython=True)
2 def nearest_neighbors(i, j, n_x, n_y, boundary_conditions):
3     """
4     Returns a list of nearest neighbors to to the site i,j.
5     The last number in each entry specify which translation was performed
6     """
7
8     if boundary_conditions == "periodic":
9
10         nn = [(i + 1) % n_x, j], [i, (j + 1) % n_y], [(i + 1) % n_x, (j - 1) % n_y]]
11
12     elif boundary_conditions == "open":
13
14         nn = []
15
16         # check if neighbors exist
17         ni = i + 1
18         if ni < n_x:
19             nn.append([ni, j])
20
21         nj = j + 1
22         if nj < n_y:
23             nn.append([i, nj])
24
25         nj2 = j - 1
26         if 0 <= nj2 < n_y and ni < n_x:
27             nn.append([ni, nj2])
28
29     else:
30         raise ValueError(
31             "nearest_neighbors: unkown boundary condition( choose either 'periodic' or
32             ↪ 'open')")
33
34     return nn

```

```

1 @jit(nopython=True)
2 def magnetization(i, j, theta, alpha=0.0, phi=np.array([0.0,0.0]), shift=0.0, mag=0.0,
↪ texture="skx", eta=0.0):
3     """
4     Unraveling of the non-commutative torus onto the skyrmion lattice
5

```

B. Implementation

```

6     theta: wavenumber
7     alpha: twist angle
8     phi : origin in phase torus (used for phase derivatives)
9     shift: phase shift (applied to phase 1), relative phase degree of freedom moving the
    ↪ origin
10    mag: parameter to tune net magnetization (proportional up to normalization)
11    eta: regularization parameter
12    """
13
14    # real space position
15    x = R(i, j)
16
17    # magnetization vector
18    n = np.zeros(3, dtype=np.float64)
19
20    # rotation of magnetic lattice w.r.t atomic lattice
21    twist = Twist(alpha)
22    twist3D = Twist3D(alpha)
23
24    # phase factors
25    phase_1 = theta * np.dot(x, np.dot(twist, G( 1, 0))) + phi[0] + shift
26    phase_2 = theta * np.dot(x, np.dot(twist, G( 0, 1))) + phi[1]
27    phase_3 = theta * np.dot(x, np.dot(twist, G(-1, -1))) - phi[0] - phi[1]
28
29    if texture == "skx":
30        # 'skyrmion' helical triple-Q phase
31
32        n1 = np.dot(rot240, np.array([np.sin(phase_1), 0, np.cos(phase_1)]))
33        n2 = np.array([np.sin(phase_2), 0, np.cos(phase_2)])
34        n3 = np.dot(rot120, np.array([np.sin(phase_3), 0, np.cos(phase_3)]))
35
36        n = np.dot(twist3D, n1 + n2 + n3) + np.array([0, 0, np.sqrt(3) * mag])
37        n = n * 1 / (np.linalg.norm(n) + eta)
38
39    elif texture == "sin":
40        # sinusoidal triple-Q phase
41
42        # Gamma = 0 and theta = arccos( 1/sqrt(3) )
43        n1 = np.dot(rot240, np.array([-np.sqrt(2/3)*np.cos(phase_1), 0,
    ↪ np.sqrt(1/3)*np.cos(phase_1)]))
44        n2 = np.array([-np.sqrt(2/3)*np.cos(phase_2), 0, np.sqrt(1/3)*np.cos(phase_2)])
45        n3 = np.dot(rot120, np.array([-np.sqrt(2/3)*np.cos(phase_3), 0,
    ↪ np.sqrt(1/3)*np.cos(phase_3)]))
46

```

```

47     n = np.dot(twist3D, n1 + n2 + n3) + np.array([0, 0, np.sqrt(3) * mag])
48     n = n / (np.linalg.norm(n) + eta)
49
50     elif texture == "sdw":
51         # spin-density wave triple-Q phase
52
53         n1 = np.dot(rot240, np.array([0, np.sin(phase_1), 0]))
54         n2 = np.array([0, np.sin(phase_2), 0])
55         n3 = np.dot(rot120, np.array([0, np.sin(phase_3), 0]))
56
57         n = np.dot(twist3D, n1 + n2 + n3) / 3.0
58
59     elif texture == "fm":
60         # ferromagnet
61
62         n = np.array([0, 0, 1], dtype=np.float64)
63
64     return n

```

B3. Spectral projection Eq. (4.24)

```

1  def spectrum(
2      states, n_x, n_y, theta, alpha, phi, shift, mag, t, m, texture,
3      ↪ boundary_conditions, regularization = 0.0, flux = 0.0
4  ):
5      """
6      calculate the spectrum by exact diagonalization, return hamiltonian, eigenvalues,
7      ↪ and eigenvectors
8      """
9
10     dim = 2 * n_x * n_y
11     H = np.zeros((dim, dim), dtype=np.complex128)
12     set_hamiltonian(
13         H, states, n_x, n_y, theta, alpha, phi, shift, mag, t, m, texture,
14         ↪ boundary_conditions, regularization, flux
15     )
16
17     eigvals, eigvecs = np.linalg.eigh(H, UPLO="U")
18
19     return H, eigvals, eigvecs

```

B. Implementation

```
1 @jit(nopython=True)
2 def fermi_projection(
3     eigvals, eigvecs, fermi, kbT=0
4 ):
5     """
6     Create a projection D_P onto the occupied subspace in eigenvector basis and switch
7     ↪ to standard basis
8     P = V D_P V^H
9     with V = (v1, ..., vN) matrix with normalized eigenvectors in columns
10    D_P = Diag(1, ..., 1, 0, ..., 0) diagonal projection of rank equal to number of
11    ↪ eigenvalues below fermi
12    ^H hermitian conjugate i.e. transpose and complex conjugate
13    P projection onto eigenspaces with eigenvalues below fermi
14    """
15
16    # array with 1 for each occupied state (energy less or equal fermi energy) and 0 for
17    ↪ each unoccupied state (energy greater fermi energy)
18    if kbT==0:
19        occ = np.array([1 if eigval<= fermi else 0 for eigval in
20        ↪ eigvals],dtype=np.complex128)
21    else:
22        occ = np.array([fermi_distribution(eigval,fermi,kbT) for eigval in
23        ↪ eigvals],dtype=np.complex128)
24
25    # projection onto occupied subspace of states (eigenbasis)
26    eig_projection = np.diag(occ)
27
28    # return projection onto occupied subspace of states (statebasis)
29    return eigvecs.dot(eig_projection.dot(eigvecs.transpose().conj()))
```

```
1 @jit(nopython=True)
2 def spec_projection(
3     n_x, n_y, eigvecs, ids
4 ):
5     """
6     Create a projection D_P onto the occupied subspace in eigenvector basis and switch
7     ↪ to standard basis
8     P = V D_P V^H
9     with V = (v1, ..., vN) matrix with normalized eigenvectors in columns
10    D_P = Diag(1, ..., 1, 0, ..., 0) diagonal projection of rank equal to number of
11    ↪ occupied
12    ^H hermitian conjugate i.e. transpose and complex conjugate
```



```

11         P    projection onto occupied states in eigenbasis
12         """
13
14         # number of occupied states
15         n_occ = int(ids*n_x*n_y)
16         n_unocc = 2*n_x*n_y - n_occ
17
18         # array with 1 for each occupied state and 0 for each unoccupied state
19         occ = np.concatenate(
20             ↪ (np.ones(n_occ,dtype=np.complex128),np.zeros(n_unocc,dtype=np.complex128)) )
21
22         # projection onto occupied subspace of states (eigenbasis)
23         eig_projection = np.diag(occ)
24
25         # return projection onto occupied subspace of states (statebasis)
26         return eigvecs.dot(eig_projection.dot(eigvecs.transpose().conj()))

```

```

1 @jit(nopython=True)
2 def fermi_distribution(E,mu,kbT):
3     return 1.0 / ( np.exp( (E-mu) / kbT) + 1)

```

B4. Derivations Eq. (4.25) and Eq. (4.26)

```

1 @jit(nopython=True)
2 def translation_derivative(
3     P, index, states, n_x, n_y
4 ):
5     """
6     Calculate the translation derivation of the spectral projection
7
8     P: spectral projection
9     index: index of partial derivative
10    states: returns the index of the state with a specific label
11    n_x, n_y: size of the unit cell
12    """
13
14    dP=np.zeros_like(P)
15
16    for i in range(n_x):
17        for j in range(n_y):
18            for s in range(2):
19                for k in range(n_x):

```

B. Implementation

```

20         for m in range(n_y):
21             for t in range(2):
22
23                 row = states[i, j, s]
24                 col = states[k, m, t]
25
26                 if index==0:
27                     dP[row, col] = P[row, col] *
28                     ↪ ((i-k)-int((i-k)/(0.5*n_x))*n_x)
29                 elif index==1:
30                     dP[row, col] = P[row, col] *
31                     ↪ ((j-m)-int((j-m)/(0.5*n_y))*n_y)
32
33     return 1j*dP

```

```

1 def phason_derivative_DQ_fermi(
2     P_phi, dphi, states, n_x, n_y, theta, alpha, phi, shift, mag, t, m, texture,
3     ↪ boundary_conditions, fermi, kbT=0, regularization=0.0, flux = 0.0
4 ):
5     """
6     Return the difference quotient of the fermi projection at phi and phi+dphi
7     IMPORTANT (at zero temperature):
8     The fermi energy for a fixed filling is possibly not the same between the fermi
9     ↪ projection at phi and phi+dphi and needs to be reevaluated accordingly to get
10    ↪ projectors of the same rank
11
12    P_phi    : fermi projection at phi
13    dphi     : array of step width for directional derivative
14    others   : parameters of spectrum of P_phi
15    """
16
17    # diagonalise displaced hamiltonian
18    _, eigvals, eigvecs = spectrum(states, n_x, n_y, theta, alpha, phi+dphi, shift,
19    ↪ mag, t, m, texture, boundary_conditions, regularization, flux)
20
21    if kbT==0:
22        # fermi energy of occupied states with filling as in P_phi (this ensures the
23        ↪ same rank between P_phi and P_phidphi)
24        filling = np.trace(P_phi)
25        fermi = eigvals[int(filling)-1]
26
27    # compute displaced projection
28    P_phidphi = fermi_projection(eigvals, eigvecs, fermi, kbT)

```

```

24
25     return ( P_phidphi - P_phi )/np.linalg.norm(np.array(dphi))

```

```

1  def phason_derivative_DQ_IDS(
2      P_phi, dphi, states, n_x, n_y, theta, alpha, phi, shift, mag, t, m, texture,
3      ↪ boundary_conditions, ids, regularization=0.0, flux = 0.0
4  ):
5      """
6      Return the difference quotient of the spectral projection at phi and phi+dphi
7
8      P_ph      : spectral projection at phi
9      dphi      : array of step width for directional derivative
10     ids       : integrated density of states the spectral projection projects to
11     others    : parameters of spectrum of P_phi
12     """
13     # diagonalise displaced hamiltonian
14     _, _, eigvecs = spectrum(states, n_x, n_y, theta, alpha, phi+dphi, shift, mag, t,
15     ↪ m, texture, boundary_conditions, regularization, flux)
16
17     P_phidphi = spec_projection(n_x, n_y, eigvecs, ids)
18
19     return ( P_phidphi - P_phi )/np.linalg.norm(np.array(dphi))

```

B5. Trace Eq. (4.27)

```

1  @jit(nopython=True)
2  def trace(V,A):
3      """
4      Compute trace per unit volume V of A
5      """
6
7      return 1/V * np.trace(A)

```

B. Implementation

B6. Chern number Eq. (4.28)

```
1 @jit(nopython=True)
2 def chern_number(J,P,dP_J, n_x, n_y):
3     """
4     Compute the chern number for all subsets of even cardinality of the set of labels
5     ↪ True in J
6     """
7
8     # names of the labels
9     labels = ["t1","t2","u1","u2","u3"]
10
11     # dictionary for chern numbers
12     chern_numbers = {}
13
14     # always calculate the 0th chern number
15     chern_numbers[""] = trace(n_x*n_y,P)
16
17     # if there are at least 2 labels True in J, calculate all corresponding 1st Chern
18     ↪ numbers
19     if np.sum(J,dtype=np.int16)>=2:
20         # for all combinations of 2 elements from the list of labels
21         for a,b in comb([0,1,2,3,4],2):
22             # check if both labels are True
23             if J[a] and J[b]:
24                 # compute the chern number by computing the trace of all permutations of
25                 ↪ derivations corresponding to two True labels
26                 chern_numbers[labels[a]+labels[b]] = (2*pi*1j) *
27                 ↪ cyclic_cocycle(n_x*n_y,P,dP_J,[a,b])
28
29     # if there are at least 4 labels True in J, calculate all corresponding 2nd Chern
30     ↪ numbers
31     if np.sum(J,dtype=np.int16)>=4:
32         # for all combinations of 4 elements from the list of labels
33         for a,b,c,d in comb([0,1,2,3,4],4):
34             # check if both labels are True
35             if J[a] and J[b] and J[c] and J[d]:
36                 # compute the chern number by computing the trace of all permutations of
37                 ↪ derivations corresponding to four True labels
38                 chern_numbers[labels[a]+labels[b]+labels[c]+labels[d]] = (2*pi*1j)**2 /
39                 ↪ 2 * cyclic_cocycle(n_x*n_y,P,dP_J,[a,b,c,d])
40
41     return chern_numbers
```

```

1 @jit(nopython=True)
2 def cyclic_cocycle(V,P,dP,J):
3     """
4     Compute the cyclic cocycle as the trace of the product of the spectral projection
5     ↪ and the sum over the product of the permutations of its derivatives (listed in
6     ↪ label set J)
7     """
8
9     # variable for the product of the spectral projection and the sum over the product
10    ↪ of the permutations of its derivatives (listed in label set J)
11    A = np.zeros_like(P)
12
13    # generate array of all permutations of labels in J
14    permutations = [p for p in perm(J)]
15
16    # remove tuples which are the reverse of another tuple in the list
17    # the reverse permutation corresponds to the complex conjugate
18    # if the sign of the reverse permutation is equal we take twice the real part as
19    ↪ result
20    # if the sign of the reverse permutation is switched we take twice the imaginary
21    ↪ part as result
22    permutations = remove_reverse_arrays(permutations)
23
24    # iterate over permutations of labels in J (up to reverse order)
25    for p in permutations:
26
27        # variable for product of the derivatives (in order of one permutation p of
28        ↪ labels in J)
29        temp = np.zeros_like(dP[p[0]])
30        temp += dP[p[0]]
31
32        # compute product of the derivatives
33        for i in range(1,len(p)):
34            temp = temp.dot(dP[p[i]])
35
36        temp *= perm_sign(p)
37
38        # add the product to the sum
39        A += temp
40
41    # product with the spectral projection
42    A = P.dot(A)

```

B. Implementation

```
38     # return twice the real or imaginary part of the trace (depending in the sign of the
    ↪ reverse permutation)
39     if perm_sign(np.array(J)[:,-1])==1:
40         return 2*trace(V,A).real
41     elif perm_sign(np.array(J)[:,-1])==-1:
42         return 2*1j*trace(V,A).imag
```

B7. Orbital Magnetisation Eq. (4.29)

```
1  @jit(nopython=True)
2  def orbital_magnetisation(H, P, dP, fermi, n_x, n_y):
3      """
4      Compute the z-component of the orbital magnetisation contributions
5      (up to prefactor e/(\hbar c) ) from modern theory
6
7      return tuple: Morb, MorbLC, MorbIC, Ch_t1t2
8
9      Morb: orbital magnetisation = MorbLC + MorbIC - 2 * fermi * Ch_t1t2
10     MorbLC: local circulation contribution
11     MorbIC: itinerant current contribution
12     Ch_t1t2: momentum space Chern number
13     """
14
15     # compute products
16     dP1dP2 = dP[0].dot(dP[1])
17     PdP1dP2 = P.dot(dP1dP2)
18
19     # compute Chern number (2 pi i) (2i) Im Tr(P dP1 dP2)
20     Ch_t1t2 = (-4*pi) * trace(n_x*n_y, PdP1dP2).imag
21
22     # compute itinerant current contribution Im Tr(H P dP1 dP2)
23     MorbIC = trace(n_x*n_y, H.dot(PdP1dP2)).imag
24
25     # compute local circulation contribution Im Tr(P dP1 H dP2) = Im Tr(H P dP1 dP2 - H
    ↪ dP1 dP2)
26     MorbLC = MorbIC-trace(n_x*n_y, H.dot(dP1dP2)).imag
27
28     # compute orbital magnetisation (z-component)
29     Morb = MorbLC + MorbIC - 2 * fermi * Ch_t1t2/(-4*pi)
30
31     return (Morb,MorbLC,MorbIC,Ch_t1t2)
```

B8. Tools

```
1 @jit(nopython=True)
2 def comb(pool, r):
3     '''
4     from https://docs.python.org/3/library/itertools.html#itertools.combinations
5     modified for compatibility with numba
6     '''
7
8     n = len(pool)
9     if r > n:
10         return
11     indices = list(range(r))
12     yield [pool[i] for i in indices]
13     while True:
14         for i in range(r-1,-1,-1):
15             if indices[i] != i + n - r:
16                 break
17         else:
18             return
19         indices[i] += 1
20         for j in range(i+1, r):
21             indices[j] = indices[j-1] + 1
22     yield [pool[i] for i in indices]
```

```
1 @jit(nopython=True)
2 def perm(pool, r=None):
3     '''
4     https://docs.python.org/3/library/itertools.html#itertools.permutations
5     modified for compatibility with numba
6     '''
7
8     n = len(pool)
9     r = n if r is None else r
10    if r > n:
11        return
12    indices = list(range(n))
13    cycles = list(range(n, n-r, -1))
14    yield [pool[i] for i in indices[:r]]
15    while n:
16        for i in range(r-1,-1,-1):
17            cycles[i] -= 1
18            if cycles[i] == 0:
```

B. Implementation

```
19         indices[i:] = indices[i+1:] + indices[i:i+1]
20         cycles[i] = n - i
21     else:
22         j = cycles[i]
23         indices[i], indices[-j] = indices[-j], indices[i]
24         yield [pool[i] for i in indices[:r]]
25         break
26     else:
27         return
```

```
1 @jit(nopython=True)
2 def remove_reverse_arrays(array_list):
3     """
4     Remove arrays which are the reverse of another array already in the list
5     """
6     array_list = np.array(array_list)
7     result = []
8     for i in range(len(array_list)):
9         is_reverse = False
10        for j in range(0, i):
11            if np.all(array_list[i] == array_list[j][::-1]):
12                is_reverse = True
13                break
14        if not is_reverse:
15            result.append(array_list[i])
16    return result
```

```
1 @jit(nopython=True)
2 def perm_sign(perm):
3     """
4     Written by OpenAI:
5     The idea is that if the permutation is already sorted, then no swaps are needed and
6     ↪ the sign is 1.
7     If a swap is needed to sort the permutation, the sign will be -1. If two or more
8     ↪ swaps are needed, the sign will be 1 again, and so on.
9
10    This implementation has time complexity of  $O(n \log n)$  in average and worst case,
11    ↪ because it uses bubble sort internally.
12    """
13    sign = 1
14    n = len(perm)
15    for i in range(n-1):
```



```

13         for j in range(i+1, n):
14             if perm[i] > perm[j]:
15                 perm[i], perm[j] = perm[j], perm[i]
16                 sign *= -1
17     return sign

```

```

1 @jit(nopython=True)
2 def mysum(xs):
3     """
4     Sum function for numpy arrays compatible with numba
5     """
6     tmp = np.zeros_like(xs[0])
7     for x in xs:
8         tmp += x
9
10    return tmp

```

B9. Constants

```

1 # -- math constants -----
2
3 pi = np.pi
4 deg = pi / 180
5
6 # -- pauli matrices -----
7
8 s0 = np.array([[1, 0], [0, 1]])
9 sx = np.array([[0, 1], [1, 0]])
10 sy = np.array([[0, -1j], [1j, 0]])
11 sz = np.array([[1, 0], [0, -1]])
12
13 # -- vector operations -----
14
15 # rotation by 120 degrees around z
16 rot120 = np.array(
17     [[-1 / 2.0, -np.sqrt(3) / 2.0, 0], [np.sqrt(3) / 2.0, -1 / 2.0, 0], [0, 0, 1]]
18 )
19
20 # rotation by 240 degrees around z
21 rot240 = np.array(

```

B. Implementation

```
22     [[-1 / 2.0, +np.sqrt(3) / 2.0, 0], [-np.sqrt(3) / 2.0, -1 / 2.0, 0], [0, 0, 1]]
23 )
```

B10. Lattice

```
1  # triangular lattice
2  a = np.array([[1.0, 0], [1 / 2.0, np.sqrt(3) / 2.0]], dtype=np.float64)
3
4  # triangular reciprocal lattice
5  b = np.array(
6      [[2 * pi, -2 * pi / np.sqrt(3)], [0, 4 * pi / np.sqrt(3)]], dtype=np.float64
7  )
8
9  @jit(nopython=True)
10 def R(i, j):
11     """
12     Real space lattice
13     """
14
15     return i * a[0] + j * a[1]
16
17 @jit(nopython=True)
18 def G(i, j):
19     """
20     Reciprocal space lattice
21     """
22
23     return i * b[0] + j * b[1]
24
25 @jit(nopython=True)
26 def Twist(alpha):
27     """
28     Rotation by alpha [rad] around z-axis
29     """
30
31     c = np.cos(alpha)
32     s = np.sin(alpha)
33
34     return np.array([[c, -s], [s, c]], dtype=np.float64)
35
36 @jit(nopython=True)
37 def Twist3D(alpha):
38     """
```

```
39     Rotation by alpha [rad] around z-axis
40     """
41
42     c = np.cos(alpha)
43     s = np.sin(alpha)
44
45     return np.array([[c, -s, 0.0], [s, c, 0.0], [0.0, 0.0, 1.0]], dtype=np.float64)
```

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