Reply to "Comment on 'New physics constraints from atomic parity violation in ^{133}Cs'"

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In B. K. Sahoo, B. P. Das, and H. Spiesberger, Phys. Rev. D **103**, L111303 (2021), we had reported an improved calculation of the nuclear spin-independent parity violating electric dipole transition amplitude ($E1_{\rm PV}$) for the $6s^2S_{1/2} - 7s^2S_{1/2}$ transition in ^{133}Cs by employing a relativistic coupled-cluster theory. In a recent Comment, Roberts and Ginges have raised questions about our calculation of the so-called Core contribution to $E1_{\rm PV}$. Our result for this contribution does not agree with theirs, but is in agreement with results from previous calculations where this contribution is given explicitly. In our Reply, we explain in detail the validity of the evaluation of our core contribution. We emphasize that the Main, Core and Tail contributions have been treated on an equal footing in our work unlike the sum-over-states calculations. We also address their concerns about our approximate treatment of the contributions from the QED corrections, which was not the aim of our work, but was carried out for completeness. Nonetheless, conclusion of our above-mentioned paper is not going to affect if we replace our estimated QED contribution to $E1_{\rm PV}$ by earlier estimation.

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I. BACKGROUND

In order to set the scene for our reply to the Comment by Roberts and Ginges [1] on our paper [2], we would like to mention that the calculation of the parity violating electric dipole transition amplitude of ^{133}Cs has a long history. In particular, there was an unsettled issue about the contributions from the occupied orbitals, referred to as "Core" contribution, to the parity violating electric dipole amplitude ($E1_{\rm PV}$) of the $6s^2S_{1/2} \rightarrow 7s^2S_{1/2}$ transition in the ^{133}Cs atom from the Dirac-Coulomb (DC) Hamiltonian that differed by about 200% between the previous two high-precision calculations reported in Refs. [3,4]. On page 26 of the review article by Safronova, Budker, DeMille, Kimball, Derevianko and Clark [5], it is explicitly mentioned that: "*One of us, A.D., thinks that the correction to the contribution of highly excited states (Dzuba et al., 2012) may have come from the use of many-body intermediate states by Dzuba et al. (2012) that is inconsistent with the one employed by Porsev, Beloy, and Derevianko (2009), as the summation over intermediate states while evaluating $k_{\rm PV}$ must be carried out over a complete set and thereby the results of Dzuba et al. (2012) require revision. This matter remains unresolved at present but new methods are being developed to address it. The ever-increasing power of computation is anticipated to bring further improvements in the atomic-structure analysis.*"

Similar comments were also made in another unpublished article [6] soon after the above review. Our work in Ref. [2] was mainly devoted to addressing the above issue by directly solving the first-order perturbed wave functions due to the weak interaction with reference to the zeroth-order wave functions of the DC Hamiltonian using the relativistic coupled-cluster (RCC) theory. This overcomes the shortcomings of the sum-over-states RCC theory approach of Ref. [3] to include the Core contributions to all-orders in the singles and doubles RCC theory approximation (RCCSD method) and singles, doubles and triples RCC theory approximation (RCCSDT method). In view of

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the practical limitations from a computational point of view, triple excitations were considered only for selected low-lying orbitals. In addition, the corrections due to the exchange of transverse photons between pairs of electrons, known as the Breit interaction, and the quantum electrodynamics (QED) interactions were included to improve the atomic wave function in the RCCSDT method. This method was evaluated to use the Main, Core and Tail contributions on an equal footing. Moreover, the Hamiltonians representing electromagnetic ($H_{\rm em}$) and weak ($H_{\rm weak}$) interactions were treated in a consistent manner. The accuracies of these calculations were estimated by comparing the results of calculated spectroscopic properties with those available from experiments as has been done traditionally, e.g., in Ref. [3]. In fact, well before our results were published in Ref. [2] they were uploaded on arXiv in order to seek responses from others [2,7]. Nonetheless, we are convinced that the arguments presented by Roberts and Ginges leave a lot to be desired and they do not change the conclusions we arrived at in Ref. [2].

Our arguments are the following:

(i) In Refs. [3,4], the Breit and QED corrections to $E1_{\rm PV}$ and other properties were borrowed from previous calculations, which were reported using lower-order many-body methods and basis functions different from those used in the DC calculations. In our work, the above interactions were included along with the DC Hamiltonian in H_{em} for the determination of atomic wave functions in Ref. [2]. This enabled us to show that the Breit and QED contributions from the RCC theory were different from the earlier values using less rigorous many-body methods. A single rigorous relativistic many-body method, using H_{em} which includes the DC, Breit and QED interactions, serves as a more realistic way of estimating uncertainties in the calculated atomic properties rather than either borrowing corrections from other calculations or by scaling the atomic wave functions to produce the results matching with the experimental values even though small corrections from the QED effects to the property evaluation were neglected. The important point is that the QED effects were included at the same level of approximations as those of the DC and Breit interactions, and the estimated QED contributions matched reasonably well for all the properties with the earlier evaluations. Similar to Ref. [3], the accuracies of the final results of various properties were analyzed by comparing with those of their experimental values in Ref. [2].

(ii) The Core contribution to $E1_{\rm PV}$ [given in units of $-i(Q_W/N)ea_0 \times 10^{-11}$ here onwards with nuclear weak charge Q_W and neutron number N] of the $6s^2S_{1/2} \rightarrow 7s^2S_{1/2}$ transition in ^{133}Cs were evaluated using lower-order methods as -0.0020 while the Hartree-Fock (HF) value is about -0.0017 [1,2,4]. This Core contribution was reported to be about -0.0019 using the RCCSD method [8–10] by us much before $E1_{\rm PV}$ calculations were reported in Refs. [1,3,4]. In Ref. [2], it was investigated using the RCCSDT method to find whether higher-order effects are responsible for the large difference in the results between Refs. [3,4]. It was, however, found that the result changed marginally to -0.0018. Our RCCSD method was also employed earlier to estimate the Core contributions to $E1_{\rm PV}$ of Ba^+ [11] and Ra^+ [12], and Roberts and Ginges have acknowledged saying that they have reproduced our result for Ra^+. The reasons for the disagreement for the Core contribution for Cs between the results referred to by Roberts and Ginges and ours is the difference in the physical effects included in the two works and the improper scaling of the atomic wave functions to compensate for the missing physical effects in the evaluation of $E1_{\rm PV}$. Since a $S \leftrightarrow S$ transition is involved in the Cs atom, there are huge cancellations in the contributions to $E1_{\rm PV}$ from both states. In contrast, contributions to $E1_{\rm PV}$ arise mainly from the S state of a $S \leftrightarrow D_{3/2}$ transition in Ra^+.

II. $E1_{\rm PV}$ EVALUATION PROCEDURE

Using the sum-over-states approach, $E1_{\rm PV}$ is evaluated as [3,13]

$$E1_{\rm PV} \simeq \frac{\lambda}{\mathcal{N}} \sum_{I \neq f} \frac{\langle \Psi_f^{(0)} | H_{\rm weak} | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | D | \Psi_i^{(0)} \rangle}{(E_f^{(0)} - E_I^{(0)})} + \frac{\lambda}{\mathcal{N}} \sum_{I \neq i} \frac{\langle \Psi_f^{(0)} | D | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | H_{\rm weak} | \Psi_i^{(0)} \rangle}{(E_i^{(0)} - E_I^{(0)})}, \quad (1)$$

where $\lambda = \frac{G_F}{2\sqrt{2}} Q_W$, $|\Psi_{k=i,f,I}^{(0)}\rangle$ are the wave functions corresponding to H_{em} with energies $E_k^{(0)}$, D is the electric dipole (E1) operator, I denotes all the intermediate states and $\mathcal{N}$ is the normalization constant. This approach has the limitation that contributions only from a few low-lying bound states can be evaluated through this approach (usually referred as "Main" contribution), whereas contributions from the occupied orbitals (referred as Core contributions) and high-lying bound states including continuum (denoted as "Tail") contributions are challenging to treat accurately for practical reasons. Thus, the Core and Tail are usually estimated by applying either a lower-order theory or mixed many-body methods. The limitations of using a mixed approach to determine $E1_{\rm PV}$ amplitude is that the correlations among the Core, Main and Tail parts (the latter two together referred as "Virtuals" from here onwards) and

corrections due to $\mathcal{N}$ do not lend themselves to being included naturally at the same level of approximation. In particular, the interplay of the correlations among all these contributions cannot be accounted for by the above mentioned many-body methods that have been used in the sum-over-states approach. In addition, the interplay of the correlations among the electromagnetic interactions and weak interactions are also not accounted for properly in such an approach. This clearly suggests that it is imperative to consider the Core, Main and Tail contributions and also the interplay of the correlations between the interactions due to H_{em} and $H_{\rm weak}$ on an equal footing, and estimate corrections due to $\mathcal{N}$ from all these contributions at the same level of approximation.

The shortcomings of the sum-over-states approach are circumvented in Ref. [2] by calculating $E1_{\rm PV}$ as

$$E1_{\rm PV} \simeq \lambda \frac{\langle \Psi_f^{(1)}|D|\Psi_i^{(0)}\rangle + \langle \Psi_f^{(0)}|D|\Psi_i^{(1)}\rangle}{\sqrt{\langle \Psi_f^{(0)}|\Psi_f^{(0)}\rangle \langle \Psi_i^{(0)}|\Psi_i^{(0)}\rangle}} = \frac{\lambda}{\mathcal{N}}[\langle \Psi_f^{(1)}|D|\Psi_i^{(0)}\rangle + \langle \Psi_f^{(0)}|D|\Psi_i^{(1)}\rangle], \quad (2)$$

where $|\Psi_{k=i,f}^{(1)}\rangle$ denotes the first-order perturbed wave functions due to $H_{\rm weak}$, respectively, which are obtained by solving the following inhomogeneous equations in the RCC theory framework:

$$(H_{em} - E_k^{(0)})|\Psi_k^{(1)}\rangle = -H_{\rm weak}|\Psi_k^{(0)}\rangle. \quad (3)$$

Since both $|\Psi_k^{(0)}\rangle$ and $|\Psi_k^{(1)}\rangle$ wave functions are obtained using the same RCC theory, contributions from the Core and Virtual orbitals are embedded in the evaluation of Eq. (2). In Ref. [2], we had made a special effort to present results in terms of the Core, Main and Tail contributions to facilitate understanding of these contributions to address the unsettled issues raised in Refs. [5,6].

III. RESPONSES TO COMMENTS

Roberts and Ginges start their Comment by referring to the estimated corrections due to the QED interactions in Ref. [2]. As we have mentioned earlier, there have not been significant differences between the estimated QED corrections to $E1_{\rm PV}$ in Cs, though they vary slightly between the different calculations, the major disagreement between Refs. [3,4] was on the Core contribution to $E1_{\rm PV}$ where there was a sign difference. The difference in the Tail contributions among these works was also quite large. Since it is not possible to consider the covariant form of H_{em} for an atomic system for the determination of atomic wave functions, the dominant DC Hamiltonian is usually considered as its first approximation. When necessary, contributions from the Breit and QED interactions are estimated as corrections. Thus, it is imperative to include contributions from the DC Hamiltonian as accurately as possible. However, sometimes a less accurate many-body method is employed to include its contributions, and the calculated properties are rescaled to obtain the final results. Such a procedure cannot always give reliable results. In Ref. [2], we considered the Breit interaction potential and a model QED potential along with the DC Hamiltonian to include its contributions to all-orders in the residual interaction using the RCC theory. The authors of Ref. [4] used the Main contribution from Ref. [3] in their final result, but they had attempted to improve the Core and Tail contributions using the BO + RPA mixed many-body method. Since we evaluated $E1_{\rm PV}$ of Cs in Ref. [2] from first principles treating the Main, Core and Tail contributions on an equal footing using the RCC theory, all of the above contributions were embedded and they were interrelated. It is evident from this that the results in Ref. [2] were obtained in a more natural manner than those compared to other calculations. It does not extrapolate the results by scaling wave functions or using experimental data.

To understand the possible reasons for the difference in the Core contribution to $E1_{\rm PV}$ of Cs reported in Ref. [4] from our RCC calculations [2], we present the Core and Virtual contributions to $E1_{\rm PV}$ of Cs from Refs. [1–4] in Table I. As can be seen from this table the HF value to the Core contribution is about −0.0017. This is different than what is being considered in Ref. [3], so we do not know the basis for Roberts and Ginges referring to it as the HF value from Ref. [3]. Nonetheless, it is possible to find a one to one correspondence between the RPA terms and certain terms of the many-body perturbation theory (MBPT) as have been shown in Refs. [14,15]. Since RCC theory is an all-order perturbation theory, it contains all the RPA contributions and also takes into account the interplay between the RPA and the non-RPA effects. The RPA, however, misses out many contributions that appear in the RCC theory. In Fig. 1, we show a few selected lowest-order non-RPA correlation effects from the second-order MBPT method using the Goldstone diagram representation that are present to all-orders in the determination of Core contributions to $E1_{\rm PV}$ using the RCC theory. We find huge cancellations among the contributions from the non-RPA and the RPA correlation effects. The final small Core contribution to $E1_{\rm PV}$ in Cs is the result of these strong cancellations. A perusal of the final result for $E1_{\rm PV}$, listed in Table I, from Refs. [1,4] suggests that it uses the scaled wave functions from the combined BO + RPA methods to obtain the Core contribution, whereas the Main result is taken from the RCC calculations of Ref. [3]. A large difference can also be noticed between the Main contribution from the RCC theory with the combined BO + RPA calculations. However, only a small difference between the *ab initio* results for the Core contributions from RPA and the combined BO + RPA methods is noticed. It suggests that perhaps the strong cancellation seen for the Core

TABLE I. Comparison of contributions from the "Core" and "Virtual" orbitals to the $E1_{\mathrm{PV}}$ amplitude [in $-i(Q_W/N)ea_0 \times 10^{-11}$] of the $6s^2S_{1/2} - 7s^2S_{1/2}$ transition in ^{133}Cs using the Dirac-Coulomb Hamiltonian from various works. We have also mentioned the many-body methods and approaches employed in determination of these contributions. The signs of the Core orbital contributions from Refs. [1,4], marked in bold fonts, differ from the other works.

Method	Approach	Core	Virtual	Reference
HF	*ab initio*	−0.00174		[1]
RPA	*ab initio*	**0.00170**		[1]
RPA	Scaled	**0.00259**		[1]
BO + RPA	*ab initio*	**0.00181**		[1]
BO + RPA	Scaled	**0.00181**		[1]
HF	*ab initio*	−0.0017	0.7401	[2]
RCCSD	*ab initio*	−0.0019	0.9006	[2]
RCCSDT	*ab initio*	−0.0018	0.9011	[2]
Lower order		−0.0020		[3]
RCCSDT	*sum-over*		0.9073	[3]
RCCSDT	*sum-over + scaled*		0.9018	[3]
HF	*ab initio*	−0.00174		[4]
RPA	Scaled	**0.00259**		[4]
BO + RPA	*ab initio*	**0.00170**	0.8949	[4]
BO + RPA	Scaled	**0.00182**	0.8920	[4]
	Earlier reported Core contributions			
RCCSD	*ab initio*	−0.002		[8]
RCCSD	*ab initio*	−0.002		[9]
RCCSD	*ab initio*	−0.0019		[10]
Lower order		−0.002(2)		[13]

contribution from the RPA and non-RPA effects in the RCC theory is not happening through the scaled BO + RPA approaches. Also, we find that the scaling of contributions from the Virtuals, which also contains both RPA and non-RPA contributions and are the dominant ones, change by about 0.3% while the scaled RPA contributions to the Core contributions are almost 34%. So we have doubts over the efficacy of these scaling approaches, which are meant to capture the missing physical effects in the determination of wave functions using the BO + RPA methods. In fact, another follow-up work by Roberts *et al.* [16] mentions that they had missed out double-core polarization effects in Ref. [4], which appear naturally in the RCC theory. In addition, we find that there is about 1% difference in the Virtual contributions between Refs. [3,4]. This corroborates the point we had made above that the RPA and non-RPA contributions using the hybrid BO + RPA methods are inadequate.

In Table II, we present Breit contributions to electron affinities (EAs) of the low-lying states of Cs from the previous works including from our RCCSDT method. In Ref. [3], these contributions were borrowed from Ref. [17] that had employed the third-order relativistic many-body perturbation theory [RMBPT(3)]. As can be seen from this

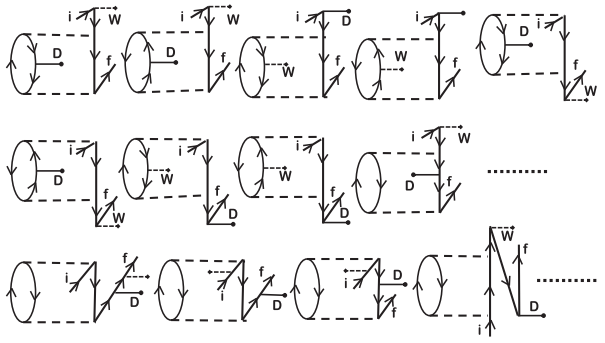

FIG. 1. A few examples of Goldstone diagrams representing non-RPA effects to the Core contributions in the determination of $E1_{\mathrm{PV}}$ amplitude in the one-valence atomic systems. Contributions from such diagrams to $E1_{\mathrm{PV}}$ of the $6s^2S_{1/2} - 7s^2S_{1/2}$ transition in ^{133}Cs cancel out strongly with that arise due to RPA. Here lines with upward arrows denote virtuals, lines with downward arrows denote occupied orbitals, i and f are the initial and final valence orbitals respectively, lines with D represent the E1 operator, lines with W correspond to the H_{weak} operator and the dashed lines stand for H_{em} operator.

table, there are substantial differences among these results and they are mainly due to the electron correlation effects. Similarly, we also give the Breit contributions to the magnetic dipole hyperfine structure constants (A_{hfs}) in Table III from different works and observe striking differences in the results. From Ref. [7], one can observe how the Breit contributions to EAs and A_{hf} vary from lower- to higher-order methods and these variations are different for both properties. This clearly indicates that the same scaling of wave functions may not give the correct results for properties described by operators with different ranks and radial behavior (see also Ref. [18]).

TABLE II. The estimated contributions from the Breit interaction to the EAs (in cm^{-1}) in Cs reported in various works.

Method	$6S$	$6P_{1/2}$	$7S$	$7P_{1/2}$	$8P_{1/2}$
RMBPT(3) [17]	2.6	−7.1	0.26	−2.5	
RMBPT [19]	4.39	−8.78	0.0	−2.19	
SD [20]	1.1	−6.9	−0.72	−2.6	
RCCSD [21]	1.0	−7.0	0.0	−3.0	
RCCSDT [2]	−0.60	−7.81	−0.65	−2.61	−1.21

TABLE III. The reported Breit interaction contributions to the A_{hyf} values (in MHz) in ^{133}Cs from different methods.

Method	$6S$	$6P_{1/2}$	$7S$	$7P_{1/2}$	$8P_{1/2}$
RMBPT(3) [6]	4.87	−0.52	1.15	−0.15	
RMBPT [19]	5.0	−0.2	0.8	0.0	
SD [20]	−4.64	−0.87	−0.83	−0.29	
Analytic [22]	4.6		1.09		
RPA [23]	0.0	−1.25	−0.05	−0.39	
RCCSDT [2]	4.65	−0.18	0.83	−0.04	−0.02

It is desirable to have an exact expression to account for the QED effects for the determination of the atomic wave functions. However, there is no well-defined approach for incorporating the QED interactions to high precision in many-electron systems and they are mostly accounted for using model potentials. To the best of our knowledge, the QED model potential defined in Refs. [24,25], which include contributions from the local and nonlocal potentials to represent the self-energy (SE) interactions, are fairly reliable for estimating SE effects. In Ref. [2], we had used the expression for the SE interaction model potential defined in Refs. [26,27] and the vacuum polarization effects were included in a manner similar to that used in Refs. [25,26]. As provided by Ref. [24], the expression for estimating the SE contributions to the A_{hf} constants can be divided into "irreducible" and "reducible" parts. The reducible part, which contains ultraviolet divergences, has two terms. Each of the terms of the reducible part may contribute significantly in the property evaluation, but the two contributions strongly cancel each other (e.g., see Ref. [24]) resulting in the largest contribution arises mainly from the irreducible part. The contribution of the QED model potential included in H_{em} comes mainly from this irreducible part.

In Tables IV and V, we present our estimated QED contributions to EA and A_{hf} values, respectively, of the important low-lying states. Here, we have neglected the reducible contribution of the SE interaction to A_{hf}. As can be seen, there are large differences in the estimated QED contributions to EAs from the previously reported calculations. Thus, the electron correlation effects also change the magnitudes of the QED contributions. Therefore, it was imperative to give the estimated QED contribution from our RCC theory only rather than borrowing from another work in order to assess the quality of the calculated wave functions more reliably. This is why we had included the model QED potential through H_{em} for the determination of atomic wave functions and the spectroscopic properties were evaluated using these wave functions. It was found that the estimated QED contribution to the ground state A_{hf} value from this approach is −7.28 MHz, which is comparable to the more accurate calculations −9.7 MHz [28,29] and −8.8(1.5) MHz [30]. It can also be seen from Table VI that our estimated QED contribution to $E1_{\mathrm{PV}}$ is −0.0028(3), which is comparable to −0.0024(3) used in Ref. [3] from Ref. [31] and −0.0029(3) used in Ref. [4] from Ref. [26]. Here, we have quoted uncertainty only from the electron correlation effects by taking the difference in the results from the RCCSD and RCCSDT methods. Since our estimated QED contributions match reasonably well with the previous estimations using other methods and they were treated in a consistent manner along with the DC and Breit interactions in Ref. [2], we did not focus on the missing small QED contributions to different properties. Since uncertainties for the many-body calculations cannot be estimated reliably, their accuracies are analyzed by comparing the final calculated results with their experimental values. These comparisons are further used to estimate the uncertainty of $E1_{\mathrm{PV}}$, which accounts for all possible missing physical effects including the higher level excitations and neglected QED effects. This is exactly what has been done in Ref. [2] and is along the same lines as Ref. [3]. If Roberts and Ginges feel that this is an issue then the accuracy of our calculated QED contribution to $E1_{\mathrm{PV}}$ amplitude can be determined by taking the QED correction either from Ref. [31] or Ref. [26] as was done in Refs. [3,4]. In such a scenario, the final conclusion of our study would still remain the same.

TABLE IV. The estimated QED interaction contributions to the EAs (in cm^{-1}) in the previous works.

Reference	$6S$	$6P_{1/2}$	$7S$	$7P_{1/2}$	$8P_{1/2}$
[26]	−17.6	0.4	−4.1	0.1	0.05
[32]	−0.069%	0.006%	−0.040%	0.004%	0.003%
[27]	−25.28	1.18			
[2]	−20.53	1.31	−5.09	0.57	0.71

TABLE V. The reported QED interaction contributions to the A_{hyf} values (in MHz) from the earlier calculations.

Reference	$6S$	$6P_{1/2}$	$7S$	$7P_{1/2}$	$8P_{1/2}$
[28,29]	−9.7	−0.05	−2.30	−0.02	
[30]	−8.8(1.5)				
[2]	−7.28	0.05	−1.51	0.01	∼0.0

TABLE VI. Comparison of contributions from the Breit and QED interactions to the $E1_{\mathrm{PV}}$ amplitude [in $-i(Q_W/N)ea_0\times 10^{-11}$]) of the $6s^2S_{1/2}-7s^2S_{1/2}$ transition in ^{133}Cs from various methods employed in different works.

Breit	QED	Method	Reference
−0.0055(5)	−0.0028(3)	RCCSDT	[2]
	−0.0029(3)	Correlation potential	[26]
−0.0054		RMP(3)	[17]
−0.0045	−0.27(3)%	Local DHF potential	[31]
−0.004		Optimal energy	[19]
	−0.33(4)%	Radiative potential	[33]
−0.0055		Correlation potential	[34]

IV. SUMMARY

We have given possible reasons for the large differences between the core contributions to the parity violating electric dipole transition amplitude in Cs between Refs. [2,3] and [1,4]. This was the *prime motive* of carrying out our calculation of $E1_{\mathrm{PV}}$ in Ref. [2]. We have also explained why we have added both the Breit and QED

interactions to the DC Hamiltonian in our calculations rather than borrowing them from previous works. Since they are included in our calculations in a consistent manner, *albeit* the QED part being approximate, it would not be accurate to say that the uncertainty due to the QED effects in our result is larger than that in Ref. [4]. In fact, it is straightforward to use our results from the DC Hamiltonian and combine with the earlier estimated Breit and QED contributions to determine the uncertainty in the parity violating electric dipole transition amplitude of the Cs atom as has been done in Refs. [3,4]. In our view, that would not be appropriate owing to the fact that the many-body methods and basis functions used in those calculations would not be consistent. Even in such a case, our final result will not change significantly. However, it would be more important at this stage to include the neglected contributions from the Dirac-Coulomb Hamiltonian rigorously through the triple and quadruple excitations in the RCC theory in order to probe new physics beyond the Standard Model. Therefore, the concerns expressed by Roberts and Ginges in their Comment are misplaced.

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