Comment on "Dirac *R*-matrix method for the calculation of x-ray line polarization"

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In a recent article by Chen *et al.* [Phys. Rev. A **79**, 062715 (2009)], reference is made to magnetic sublevel collision strengths in an earlier relativistic distorted-wave (RDW) article by Zhang *et al.* [Phys. Rev. A **41**, 198 (1990)]. In the former reference, Chen *et al.* carried out Dirac *R*-matrix calculations that suggest the polarization of the $3C$ and $3D$ lines of Fe XVII, which can be computed from the magnetic sublevel collision strengths, differ from RDW results by as much as 20%. We have recently carried out a variety of RDW and Dirac *R*-matrix calculations of the $3C$ and $3D$ polarizations that demonstrate this quantity to be relatively insensitive to the size and details of the atomic model. Moreover, the polarizations obtained from these recent RDW and Dirac *R*-matrix calculations agree well, and they also agree well with the polarizations that can be obtained from the fundamental collision data published by Zhang *et al.* This good agreement between RDW and Dirac *R*-matrix polarizations contradicts the behavior reported by Chen *et al.*

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Chen *et al.* have raised the question of whether perturbative, relativistic distorted-wave (RDW) theory is sufficiently accurate to calculate the polarization associated with the $3C$ and $3D$ transitions in Fe XVII, in light of results from a recently implemented Dirac *R*-matrix (DRM) magnetic sublevel code [1]. In this Comment, we consider this central issue and also address further concerns, such as the manner in which the earlier work of Zhang *et al.* [2] was represented in Ref. [1] and the apparent lack of direct verification of the magnetic sublevel method that was implemented in Ref. [1], before outlining our approach to resolving this issue.

As described by Chen *et al.* [1], calculations of the polarization associated with the $3C$ and $3D$ transitions of Fe XVII are necessary in interpreting electron-beam ion trap (EBIT) measurements. Theoretical predictions of the degree of linear polarization (measured at an angle of 90° with respect to the beam direction) for these transitions can be obtained from the fundamental cross sections for electron-impact excitation (EIE) between magnetic sublevels (MS) according to Eq. (2.2) of Ref. [1]. We reproduce this expression for convenience:

$$P(E) = [\sigma_0(E) - \sigma_1(E)]/[\sigma_0(E) + \sigma_1(E)]\,, \qquad (1)$$

where E represents the energy of the impact electrons and σ_{M_f} represents the cross section associated with collisional excitation from the ground state to a particular excited magnetic sublevel associated with the final level of the $3C$ or $3D$ fine-structure transitions. This excited sublevel is denoted by the magnetic quantum number $M_f = 0$ or 1.

According to Chen *et al.* [1], they carried out DRM calculations of σ_0 and σ_1 for both the $3C$ and $3D$ transitions. Relatively large discrepancies were reported between the background values of the DRM results (collision strengths, rather than cross sections, were actually compared) and the earlier RDW results of Zhang *et al.* [2] "as much as 40% for $3C$ and up to 30% for $3D$." However, these DRM versus RDW comparisons were not performed in a self-consistent manner, the details of which will be discussed below. For the moment, we note that in Ref. [1] it was stated that the discrepancies with the earlier RDW collision strengths resulted in a difference that was generally "20% larger" when polarization comparisons were made. To be completely accurate, it should be noted that there were *no* polarization data actually presented in Ref. [2], but we assume that the authors employed the formula given by Eq. (1) in order to obtain those results. In fact, the purpose of Ref. [2] was to present the theory and computational approach for computing fully relativistic distorted-wave (RDW) MS collision strengths. Zhang *et al.* clearly stated their belief that "no other fully relativistic program [was] available with which we could compare results for this type of cross section." Therefore, the data published in Ref. [2] represent model calculations that were provided only to compare with the best, then-available, semirelativistic calculations [3,4] in order to verify that the RDW approach had been implemented correctly. For practical applications, such as the polarization results currently under consideration, more elaborate calculations are needed to ensure convergence and consistency in computed results with respect to increased atomic-model size.

As stated above, the claims of 30–40% discrepancies in the DRM versus RDW MS collision strengths presented in Ref. [1] were made within an *inconsistent* framework. More specifically, the two calculations employed different lists of atomic configurations in determining the atomic structure of the target ion and the subsequent matrix elements required to compute the collision strengths. Chen *et al.* claim to have used "target states up to $n = 5$" in their atomic structure calculations, while Zhang *et al.* used configurations up to only $n = 3$. This type of incongruity between two structure calculations that differ by an order of magnitude in scale can compromise comparisons of the resulting MS collision strengths. In fact, in earlier work [5], Chen himself emphasized

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and demonstrated the importance of consistency in attempting to provide verification of his DRM and RDW calculations when calculating fine-structure collision strengths for *the very same system* of Fe XVII currently under consideration. He stated, "This agreement is an indication for the mutual validation of both the present RDW calculation and my previous DRM work." He then concluded with, "Our RDW procedures are therefore adequate to be used for the calculation of $3C$ and $3D$ direct or background collision strengths in EIE of Fe XVII".

Therefore, it remains unclear why the choice was made in Ref. [1] to compare a large-scale DRM MS calculation with a modest 20-year-old RDW calculation, when there existed a clear inconsistency in the list of configurations employed in the two models. A comparison involving a consistent set of configurations would have provided a more direct verification for those calculations in Ref. [1], but, instead, only "indirect proof" was provided to support the verification of those DRM MS calculations. For example, it was mentioned that the results obtained from the summing of those MS cross sections in Ref. [1] were compared with the fine-structure results previously calculated by Chen [5,6]. However, good agreement for this type of summation comparison is a necessary, but not a sufficient, condition to ensure that a magnetic sublevel algorithm has been implemented correctly. It is well known (see, for example, the discussions in Refs. [2,7]) that *an arbitrary choice* for the Coulomb phase shifts σ_{l_i} appearing in Eq. (3.7) of Ref. [1] would still allow this condition to be true. This outcome will always occur for Eq. (3.7) because the angular coefficients in that expression will automatically remove any dependence on the Coulomb phase shifts after the appropriate sums have been performed [see Eqs. (14)–(16) of Ref. [2] for details]. A more stringent, direct verification could have been accomplished by Chen *et al.* if they had compared with other MS calculations that had been carried out in a consistent manner, similar to the comparisons in Ref. [2].

A final, perplexing statement from Ref. [1] that we would like to address is the assertion, "It is known, however, that the RDW method has difficulty treating channel coupling effects and the interacting Rydberg resonances when compared with the ... DRM method." This statement is unwarranted for the strong transitions and the highly charged species under consideration here. The RDW approach typically exhibits the above inadequacies for neutral or near-neutral species. It is well known from fundamental theoretical considerations that the DW and RDW approaches are quite suitable for obtaining accurate results for highly charged systems, for which the weak-coupling approximation is valid. In an earlier paper [5], involving one of the authors of Ref. [1], strong arguments for the validity of the RDW method, as applied to electron-impact excitation of Fe XVII, were provided. This validity was independently confirmed for that same system by the earlier configuration-average DW calculations of Pindzola *et al.* [8]. It is, again, unclear what new information has been presented in the intervening period to undermine this position. As far as resonance contributions are concerned, once again, it is well known that the DW and RDW approaches can adequately incorporate resonance behavior for highly charged systems via the independent-process, isolated-resonance (IPIR) method (e.g. [9]). Comparisons that display favorable agreement between various DW and R-matrix results with resonances can be found, for example, in Refs. [7,9] and the references therein. Also, a specific capability to include resonances in RDW EIE calculations was presented in Ref. [10]. For the purposes of the present work, we will focus on only the direct contribution of the RDW collision strengths and how they compare with the background contribution of the corresponding DRM results.

In view of the above considerations, we expect that RDW and DRM results should compare favorably in the present context of magnetic sublevel transitions for Fe XVII, provided that a *consistent* comparison is performed. Therefore, we have embarked on our our own study to determine what, if any, discrepancies might exist between results computed with the two methods. Detailed results of this study will be provided in a forthcoming article. In the present work, we simply provide a small, but relevant, sample of these results in order to highlight some key features. We focus here on the $3C$ transition, which displayed broader variations between RDW and DRM results in Ref. [1] than were observed for the $3D$ results. In general, our RDW and DRM results agree better for the $3D$ transition than for the $3C$ transition, so focusing on the latter transition provides an upper bound on the discrepancies that are observed between the two types of calculations.

In this study, we have paid specific attention to comparing RDW and DRM calculations that were computed from the same, consistent list of atomic configurations in order to make meaningful comparisons. Our method for computing RDW MS collision strengths has been published previously [2], and a new capability to compute DRM MS collision strengths has been developed by one of us (C.P.B.) specifically for this study. The DRM structure calculations were performed with the Dirac-Fock atomic structure program GRASP [11,12] and the corresponding scattering calculations were performed with the Dirac atomic R-matrix codes (DARC) [13,14]. Comparing results from two independently developed computational schemes reduces the chances of systematic error and provides an excellent method for direct verification of the numerical implementations when choosing an appropriate test case.

As an initial, proof-of-principle calculation, we present in Fig. 1 a comparison of MS collision strengths, associated with the $3C$ transition, that were computed from the nominal target configuration list originally implemented by Zhang *et al.* [2]. This list includes the following configurations: $1s^22s^22p^6$, $1s^22s^22p^53l$, and $1s^22s^12p^63l$ (with $l = s,p,d$), which results in 37 fine-structure levels, including all excited levels resulting from a single promotion of an electron in the $n = 2$ shell to the $n = 3$ shell. We shall refer to these calculations as the $n = 3$ model. The RDW results computed from this model in Fig. 1 are essentially a reproduction of the RDW results from Zhang *et al.* [2], while the DARC results are new. The expected agreement between the RDW values and the background of the DARC results provides some verification that these two independent approaches have been implemented correctly. The x- and y-axis bounds for this figure, and all others in this work, were chosen to coincide with those of Ref. [1] in order to facilitate comparisons with the figures in that work. We note that the DARC collision strengths presented in this figure were calculated with a relatively coarse energy mesh, so much of the detailed resonance structure is not captured. This choice

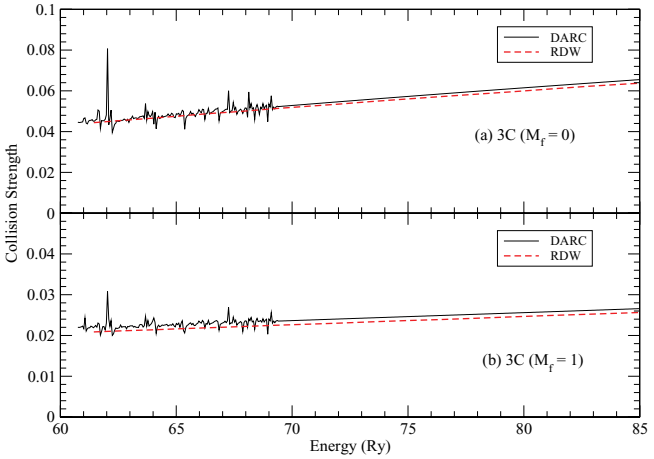

FIG. 1. (Color online) Collision strengths, computed with the $n = 3$ model, vs electron impact energy for magnetic sublevel transitions associated with the $3C$ transition of Fe XVII: (a) $M_f = 0$ and (b) $M_f = 1$. The solid line represents DARC results and the dashed line represents RDW results.

was made in order to reduce the required computing time and does not detract from the verification procedure in any way.

In Fig. 2, we again present magnetic sublevel collision strengths associated with the $3C$ transition, but this time the results were obtained from a more extensive list of configurations than was used for the $n = 3$ model. In this case, additional excited configurations of the form $1s^2 2s^2 2p^5 4l$ and $1s^2 2s^1 2p^6 4l$ (with $l = s,p,d,f$) were obtained from the promotion of a single electron in the $n = 2$ shell to the $n = 4$ shell. Two extra, double-promotion configurations of the form $1s^2 2s^2 2p^4 4s^2$ and $1s^2 2s^2 2p^4 4p^2$ were also included in order to ensure convergence in the GRASP atomic structure calculations. For consistency, these latter two configurations were also included in the Dirac-Fock-Slater atomic structure calculations that were employed in the generation of the RDW collision strengths. We shall refer to these calculations as the

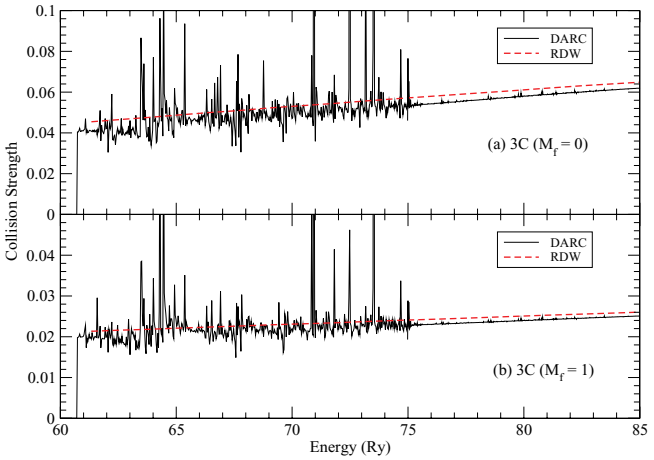

FIG. 2. (Color online) Collision strengths, computed with the $n = 4$ model, vs electron impact energy for magnetic sublevel transitions associated with the $3C$ transition of Fe XVII: (a) $M_f = 0$ and (b) $M_f = 1$. The solid line represents DARC results and the dashed line represents RDW results.

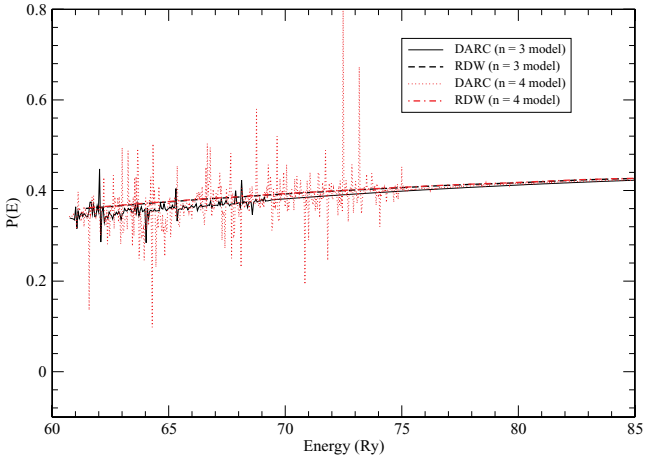

FIG. 3. (Color online) Polarization vs electron impact energy for the $3C$ transition of Fe XVII. Results: solid black curve, $n = 3$ DARC results; dashed black curve, $n = 3$ RDW results; dotted red curve, $n = 4$ DARC results; dot-dashed curve, $n = 4$ RDW results.

$n = 4$ model, which contains 256 fine-structure levels. We note that the RDW curves in the $n = 4$ model are now higher than the background of the corresponding DARC curves in Fig. 2, while the situation was reversed in the $n = 3$ model results of Fig. 1. While there is a slightly broader separation between the RDW curves and the background of the DARC curves in Fig. 2 as compared to Fig. 1, the overall agreement between the two results is excellent and remains within a few percent over the entire range.

Next, we present in Fig. 3 the polarization, computed from Eq. (1), of the $3C$ transition, which results from the excitation cross sections of the $n = 3$ and $n = 4$ models described above. Overall, the two RDW curves agree very well with the background of the two DARC curves, particularly at the higher energies. Furthermore, as will be shown in more detail in a forthcoming article, this good agreement between polarizations calculated with the RDW and DARC codes persists for more complicated target descriptions that include excited configurations containing occupied shells beyond $n = 4$, such as $n = 6$ type models similar to those considered previously by Chen [5] in studying the convergence of fine-structure collision strengths for Fe XVII. Not only does a particular list of configurations result in RDW and DARC polarizations that agree well with each other, but these polarizations agree well *across all of the models* that we have investigated, including the $n = 6$ model mentioned above. Stated plainly, while the fundamental MS cross sections, or collision strengths, undergo changes as the target description is expanded in order to obtain converged results, the cross sections associated with the $M_f = 0$ and $M_f = 1$ magnetic sublevel transitions that arise from a particular fine-structure transition move in tandem. If one MS cross section increases or decreases due to a change in the atomic model, the other cross section changes in a similar manner. Thus, we have observed that the polarization, which is calculated from a *ratio* of sums and differences of MS cross sections, is relatively *insensitive* to the size of the atomic model. Moreover, as illustrated in Fig. 3, the RDW and background DARC polarizations for the $3C$ and $3D$ lines obtained from all of the models that we have

considered in this study are confined to a relatively narrow band that is centered about a value 0.4, which is consistent with the value that has been used in the interpretation of earlier EBIT experiments [15,16].

This clustering of the polarization about a value of 0.4 contradicts the recently published results in Fig. 3 of Chen *et al.* [1]. For example, in that figure, a difference of ~20% is displayed at an impact energy of approximately 75 Ry between their 3*C* DRM polarization and the corresponding RDW result, which they apparently derived from the collision strengths of Zhang *et al.* [2]. We have observed no such discrepancies in our studies, even for more detailed models that include occupied orbitals up to $n = 6$. Instead, the agreement between our RDW and background DARC polarizations is consistently very good over the entire range of energies for all of the atomic models that we have considered.

While it is difficult to discern why there are differences between the results from the present study and those of Ref. [1], we offer the following four considerations in hopes of resolving this issue:

(1) There is an error in the expression for the MS cross section in Eq. (3.7) of Ref. [1]. The Coulomb phase shift represented as $\sigma_{l'_f}$ should really be $\sigma_{l'_i}$. We do not know if this incorrect expression was implemented in their MSJJ program, but the MS cross section can be very sensitive to the phase shifts that are employed in the summation.

(2) As stated above, Ref. [1] claimed to have used a "target states up to $n = 5$" type of model in their DRM calculations and referred to earlier papers by Chen [5,6] for details. However, there is an inconsistency in the description of the "mode $n = 5$" models in those two references. Reference [5] lists the $2s^1 2p^6 4l$ configurations as being included in the $n = 5$ model, while Ref. [6] does not. It is unclear which of these "$n = 5$" models was used in the MS calculations of Ref. [1].

(3) The situation is further complicated by the "mode $n = 5+$" model described in Refs. [5,6]. This model additionally includes the $2s^2 2p^4 3d^2$ configuration and also pseudostates. Since there is no explicit mention of pseudostates in Ref. [1], one would assume that the mode "$n = 5+$" model was not used in that work. If that is the case, then, according to our present study, one would expect the polarizations in Ref. [1] to agree well with the results presented in this comment, and yet, significant differences are observed. If, on the other hand, pseudostates were employed and they contributed in a significant manner to the differences in RDW and DRM polarizations that were reported in Ref. [1], then that issue is an important point that was not stated or verified in that work. Furthermore, if pseudostates were employed in Ref. [1], it does not appear that any detailed description of the method for incorporating these states in the structure calculations has been provided in Refs. [5,6], which makes independent verification of the MS DRM results rather difficult. All that is mentioned in this regard is that "pseudo-orbitals with the relativistic quantum number $|\underline{\kappa}| = 1$–3" were included [5]. That statement provides a description of the angular characteristics of the pseudo-orbitals that were employed, but there is no mention of the specific form of the radial functions that were used. Nor is there any indication of how many different sets of radial functions were employed, which is sometimes denoted by an "apparent" principal quantum number or the symbol $\overline{n}$. These details are typically provided when describing the use and implementation of pseudostates within an *R*-matrix context (see, for example, Refs. [17,18]).

(4) As stated previously, we did not observe much sensitivity of the 3*C* and 3*D* polarizations as the complexity of the atomic model was increased. This observation makes it difficult to understand how the polarizations in Ref. [1], *regardless of what atomic model was used*, could differ by 20% from the RDW and DRM results calculated in the present work.

Based on the above considerations, the results of Chen *et al.* [1] deserve further scrutiny. A direct verification of their MS approach, via comparisons such as those described in the present work, would help to understand their reported discrepancies. However, in order to perform such a verification, a clear description of their atomic model, as well as their method of implementation for pseudostates (assuming they were used), would have to be provided.

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