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

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(Received 12 July 2010; published 22 September 2010)

In response to the Comment written by Zhang *et al.* [Phys. Rev. A **82**, 036701 (2010)] we show that the main ideas and results (about the physics and method) reported in our paper [Phys. Rev. A **79**, 062715 (2009)] still appear to be correct. Although none of the conjectures given in the Comment about the potential problems in our code are correct, there was a small error in our code, so the part of our paper with numerical data, presented to support our method, appears to be incorrect. The wealth of resonance features in the x-ray line $3D$ demonstrated in our paper still appears to be real and is reconfirmed by a revised calculation with the error fixed.

DOI: 10.1103/PhysRevA.82.036702 PACS number(s): 34.80.Dp, 32.30.Rj, 34.80.Nz

We have found a small error or "bug" in the subroutine used to calculate the Coulomb phase shift. The consequence of this bug in our code MSJJ is that the part of our paper [1] with numerical data, presented to support our method, appears to be incorrect.

On the other hand, the main ideas and results (about the physics and method) reported in our paper still appear to be correct.

(1) For applications to the Fe XVII x-ray spectrum measured on an EBIT (electron-beam ion trap) [2], we point out and demonstrate that x-ray line polarization is a function of *both* the electron energy *and* the electron-beam width [as per Eqs. (2.2) and (2.5) given in our paper [1]]. Our paper works out the physics and shows that proper treatment of polarization is necessary for EBIT spectral analysis [2] and for further astrophysics applications [3].

(2) To address the problem we defined in point (1), we have developed a method within the framework of Dirac *R*-matrix theory to calculate x-ray line polarization. This method appears to be correct (regardless of the mistake in our code). There are, however, two typographical errors: the factor $\frac{k_j}{2k_i}$ should be replaced by $\frac{k_f}{2k_i}$ in Eq. (3.6); and $\sigma_{l'_f}$ should be replaced by σ_{l_f} in Eq. (3.7). (This second error is also pointed out in the Comment by Zhang *et al.* [4].) These two errors did not enter into our code MSJJ [see point (4) below].

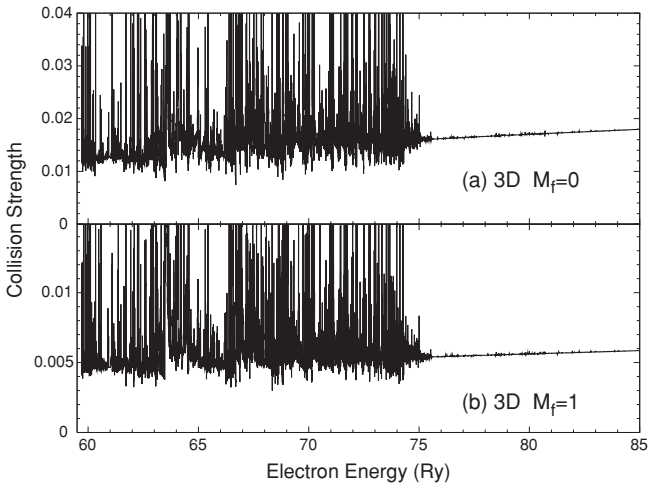

FIG. 1. Collision strength Ω (black) calculated without the bug fixed in our code for electron impact excitation (EIE) to $3D$ magnetic sublevels of Fe XVII: (a) $M_f = 0$, (b) $M_f = 1$. M_f is the magnetic quantum number of the upper level of $3D$.

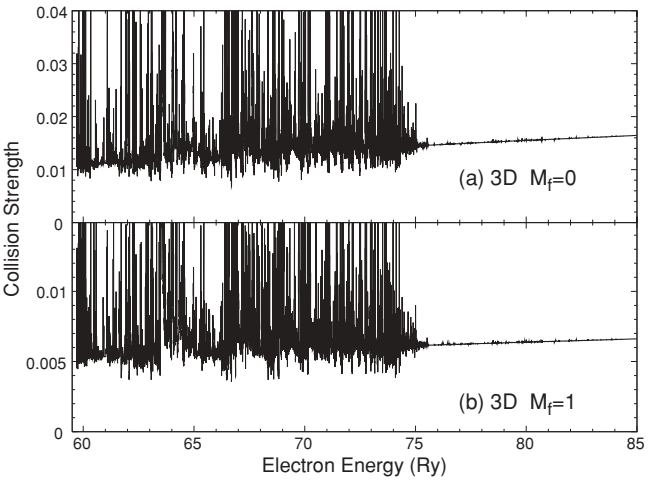

FIG. 2. Collision strength Ω (black) calculated with the bug fixed in our code for EIE to $3D$ magnetic sublevels of Fe XVII: (a) $M_f = 0$, (b) $M_f = 1$.

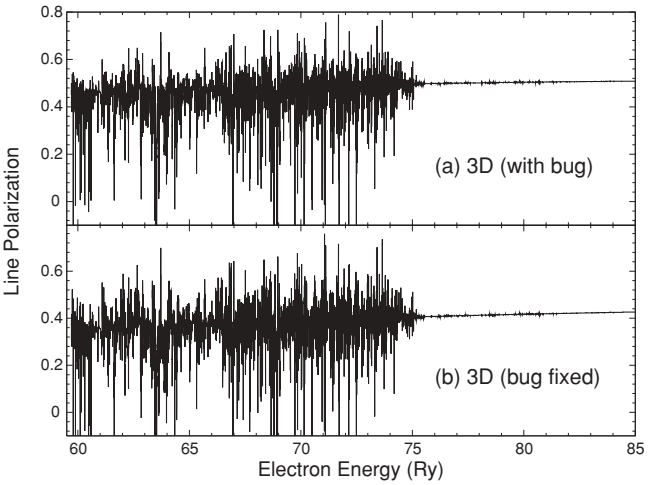

FIG. 3. Polarization $P(E)$ (black) defined in [1] for $3D$ of Fe XVII: (a) with the bug in our code and (b) with the bug fixed in our code.

(3) We have written a new code MSJJ to implement our method, along the lines delineated in points (1) and (2) above and in more detail in our paper [1], to calculate the x-ray line polarization in Fe XVII. In fact, our code is more general than for the case treated in our paper. Our code can be used for general calculations of x-ray polarization within the framework of Dirac *R*-matrix theory, with the *T* matrix or *K* matrix provided from Dirac *R*-matrix theory.

(4) Finally, for Fe XVII, the resonance features in magnetic sublevel cross sections and oscillation features in polarization are pointed out, reported, and demonstrated. The effect of resonance features for the $3D$ x-ray line appears to be real and is found to be more pronounced than for the $3C$ line.

Although *none* of the conjectures given in the Comment [4] about the potential problems in our code MSJJ are correct, the value of this Comment is that it points out *independently* (from us!) that there might be a bug in our code MSJJ. In particular, the implication of this Comment is that there might be a bug in the Coulomb phase-shift subroutine in our MSJJ code. Another contribution of this Comment is that Zhang *et al.* also find one of the two typographical errors, i.e., the error that appears in Eq. (3.7), as already stated above.

Figures 1–3 show a smaller calculation than was used in our paper (with principal quantum number n up to 4 given in [5]) to demonstrate and reconfirm here the wealth of resonance features in $3D$. Once the more complete and larger calculations using our code with the bug fixed are finished, we will further report more numerical results to support our method.

[1] G. X. Chen, K. Kirby, N. S. Brickhouse, T. Lin, and E. Silver, Phys. Rev. A **79**, 062715 (2009).
[2] J. N. Tan, E. Silver, J. Pomeroy, J. M. Laming, and J. Gillaspy, Phys. Scr. T **119**, 30 (2005).
[3] R. K. Smith, N. S. Brickhouse, D. A. Liedahl, and J. C. Raymond, Astrophys. J. **556**, L91 (2001).
[4] H. L. Zhang, C. J. Fontes, and C. P. Ballance, Phys. Rev. A **82**, 036701 (2010).
[5] G. X. Chen, A. K. Pradhan, and W. Eissner, J. Phys. B **36**, 453 (2003).