

### Comment on “Theoretical Confirmation of the Low Experimental $3C/3D$ $f$ -Value Ratio in Fe xvii”

Recently, Mendoza and Bautista (MB) published configuration interaction calculations of the debated  $2p^6 1S_0 - 2p^5 3d^3 D_1^o$  ( $3D$ ) and  $2p^6 1S_0 - 2p^5 3d^1 P_1^o$  ( $3C$ ) transitions in Fe xvii [1]. Taking fine-tuning and  $2p$ -orbital relaxation into account, MB obtained the ratio  $f(3C)/f(3D) = 2.82$ , in good agreement with the measured ratio  $2.61 \pm 0.23$  [2] and concluded that there is no need to consider nonlinear dynamical modeling [3,4] or nonequilibrium plasma effects [5,6] when interpreting experiments. We argue that the inaccurate energy structure in Ref. [1] is due to a limited and unbalanced treatment of correlation, and the methods used to correct for this leads to unreliable results for the  $f(3C)/f(3D)$  ratio. These corrections consist of (i) the use of a fine-tuning procedure that is questionable when applied to limited expansions, and (ii) the use of nonorthogonal orbitals to represent unphysical  $2p$ -orbital relaxation effects. Thus, the conclusion that the measured ratio is correct, with no need to include nonlinear effects in the interpretation, cannot be drawn.

Several large-scale calculations have been performed for Fe xvii [4,7–10] all in remarkable agreement, giving  $f(3C)/f(3D) = 3.55$ . These calculations are accurate as judged by (i) agreements with observed energy separations—to within 0.05% for transition energies and 0.2% for the important  $2p^5 3d^1 P_1^o - ^3 D_1^o$  term splitting (implying that there is no need for the two corrections used in Ref. [1]), (ii) completeness of the basis expansions and convergence of computed properties with respect to increasing orbital sets ( $n \leq 10$  rendering well-converged results with expansions reaching  $10^6$  configuration state functions for the odd parity  $J = 1$  states [9]), (iii) stability with respect to QED and higher-order corrections (correlation in the  $1s^2$  core and inclusion of triple and quadruple excitations [4,7–9]), and (iv) agreement between transition rates in length and velocity form to within 1% for a whole range of transitions [7–9].

The calculations in Ref. [1] are limited and unbalanced since the excited state expansions lack the  $2s^2 2p^3 3snln'l'$  and  $2s^2 2p^3 3dnln'l'$  configurations obtained by double excitations, which are needed to balance the included  $2s^2 2p^4 nln'l'$  double excitations from the ground state. This unbalance, as well as the arguably even more important  $n \leq 3$  orbital set limitation, yields poor energy separations ([1], Table II). Two procedures, fine-tuning and nonorthogonal orbitals ( $2p$  relaxation), are introduced in Ref. [1] by which the originally inaccurate wave functions are changed to reproduce experimental energies. Fine-tuning, or term energy correction (TEC), is a way to compensate for the fact that a calculation has failed to accurately predict energy separations by omitting

important contributions to the wave functions. In contrast to this, TEC corrections for the large-scale calculations (e.g., Ref. [7]) give negligible changes to transition rates and thereby their ratios.

The main explanation for the low  $f(3C)/f(3D)$  ratio obtained in Ref. [1] is the use of different  $2p$  orbitals in the  $2p^6$ ,  $2p^5 3s$ , and  $2p^5 3d$  configurations. The orbitals are computed using the AUTOSTRUCTURE code [11] with a model potential, where scaling parameters are obtained by minimizing the difference between computed and observed term energies, a process referred to as  $2p$ -orbital relaxation. In the large-scale calculations, which reproduce the experimental energy structure accurately, any physical relaxation will be included through a large number of  $np$  orbitals (up to  $n = 10$  in Ref. [7]), together with independently optimized odd and even states. In atomic calculations, accurate transition energies and rates are obtained by properly accounting for static and dynamic electron correlation. Dynamic electron correlation corrects for the cusps in the wave functions as  $r_{ij} \rightarrow 0$ . It is a local effect that can only be described by large basis expansions based on extended orbital sets [12]. In the calculations by MB, the lack of dynamic electron correlation, as reflected in the poor energy separations, is compensated for by changing the model potential governing the shape of the  $2p$  orbitals. Thus, the local effect of correcting the wave function for the cusp behavior is traded for a modification of the  $2p$  orbital, which is a global rearrangement of the wave function. The effect of such a procedure on the  $f(3C)/f(3D)$  is huge, but the procedure itself is neither physically nor mathematically justified. Independent calculations for this highly ionized ion show that the  $2p$  orbital is weakly configuration and term dependent, further emphasizing that the  $2p$  relaxation is questionable.

To conclude, we argue that the method proposed in Ref. [1] does not explain the difference between large-scale, converged calculations and experiments for the  $f(3C)/f(3D)$  ratio.

The authors would like to acknowledge discussions with Dr. Yuri Ralchenko. K. W. is grateful for initial discussions with Dr. Zhanbin Chen. T. B., J. E. and P. J. acknowledge support from the Swedish Research Council under contract No. 2015-04842.

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Received 11 July 2017; published 30 October 2017  
DOI: [10.1103/PhysRevLett.119.189301](https://doi.org/10.1103/PhysRevLett.119.189301)

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