Comment on "Status of the convergent close-coupling method within the framework of the rigorous Coulomb scattering theory"

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Shablov, Bilyk, and Popov [Phys. Rev. A **65**, 042719 (2002)] claimed to have analyzed the convergent close-coupling (CCC) method within the framework of the rigorous Coulomb scattering theory, but without electron exchange. They concluded that "... the amplitude obtained within the framework of this method in principle does not converge to the observable physical amplitude." We correct a misunderstanding of the origins of the CCC equations, and show that no-exchange CCC calculations exhibit no ready convergence, off or on the energy shell while those with exchange show convergence, but only on the energy shell. Since all previously published comparisons of CCC with experiment utilized on-shell amplitudes from calculations which included exchange, we question the stated conclusion.

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There appears to be a misunderstanding of the origins of the convergent close-coupling (CCC) equations. Following the original presentation of the CCC theory [2] Shablov *et al.* [1] interpreted that the CCC coupled Lippmann-Schwinger equations with pseudostates were obtained directly from those using eigenstates. This is not the case. Instead, the CCC equations may be derived using standard variational techniques resulting in stationary amplitudes. Hence, Eq. (2.4) of Ref. [1] is derived independently of Eq. (2.3), and there is no claim that for infinite N, Eq. (2.4) $\rightarrow$ Eq. (2.3). The $N\rightarrow\infty$ limiting procedure is complicated by the fact that Eq. (2.4) is solved with boundary conditions that allow only for one electron at true infinity, yet Eq. (2.3) has two such electrons. Accordingly, we suspect it is not practical to study Eq. (2.4) for finite N by reference to Eq. (2.3). Nevertheless, we welcome attempts to understand the CCC approach, particularly in the case of ionization. To facilitate this we address the issues raised by Shablov, Bilyk, and Popov [1].

The CCC ionization amplitudes were defined by Bray and Fursa [3] as

$$\langle \boldsymbol{k}_f \boldsymbol{q}_f^{(-)} | T^N | \phi_i \boldsymbol{k}_i \rangle = \langle \boldsymbol{q}_f^{(-)} | \phi_f^N \rangle \langle \boldsymbol{k}_f \phi_f^N | T^N | \phi_i \boldsymbol{k}_i \rangle, \qquad (1)$$

where we have $\epsilon_f^N = q_f^2/2$ (atomic units used throughout), and utilized the fact that $\langle \boldsymbol{q}_f^{(-)} | \phi_n^N \rangle = \delta_{fn} \langle \boldsymbol{q}_f^{(-)} | \phi_f^N \rangle$. Note that as N varies so does the energy ϵ_f^N and so some care needs to be exercised in convergence studies. From Eq. (1) Shablov, Bilyk, and Popov [1] define a half-off-shell amplitude $\langle \boldsymbol{k} \boldsymbol{q}_f^{(-)} | T^N | \phi_i^N \boldsymbol{k}_i \rangle$ and pose the question whether

$$\langle \boldsymbol{k} \boldsymbol{q}_f^{(-)} | T | \phi_i \boldsymbol{k}_i \rangle = \lim_{N\rightarrow\infty} \langle \boldsymbol{k} \boldsymbol{q}_f^{(-)} | T^N | \phi_i^N \boldsymbol{k}_i \rangle. \qquad (2)$$

This, they argue, cannot be the case because the left-hand side exists only off the energy shell, and is singular on the energy shell ($k = k_f$). We can add that the right-hand side has even the opposite on/off-shell convergence behavior. In Fig. 3 of Ref. [4] we showed that the convergence in the underlying real K-matrix elements is only on shell, and not off-shell. We shall give a similar result here, but with larger basis sizes, and also consider the effect of neglecting exchange since it is the no-exchange case that is analyzed by Shablov, Bilyk, and Popov. They state that they consider the case of

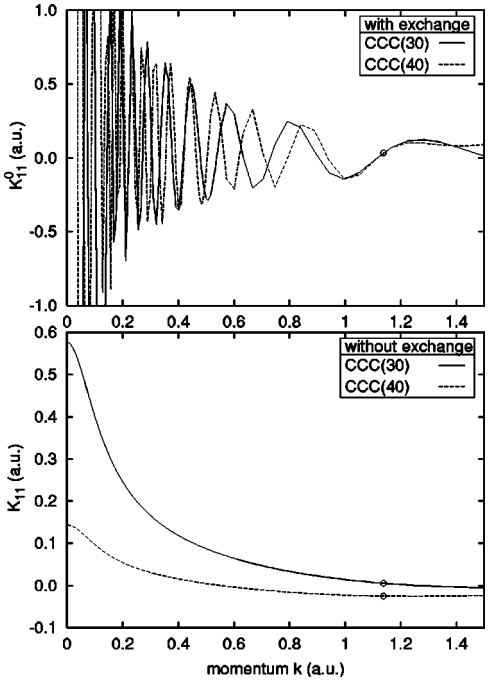

FIG. 1. 17.6 eV e-H elastic K-matrix element (singlet when with exchange) calculated with and without exchange using the specified CCC(N) calculations in the S-wave model. The on-shell point from both calculations is plotted with the open circle, and is indistinguishable for the with-exchange calculation.

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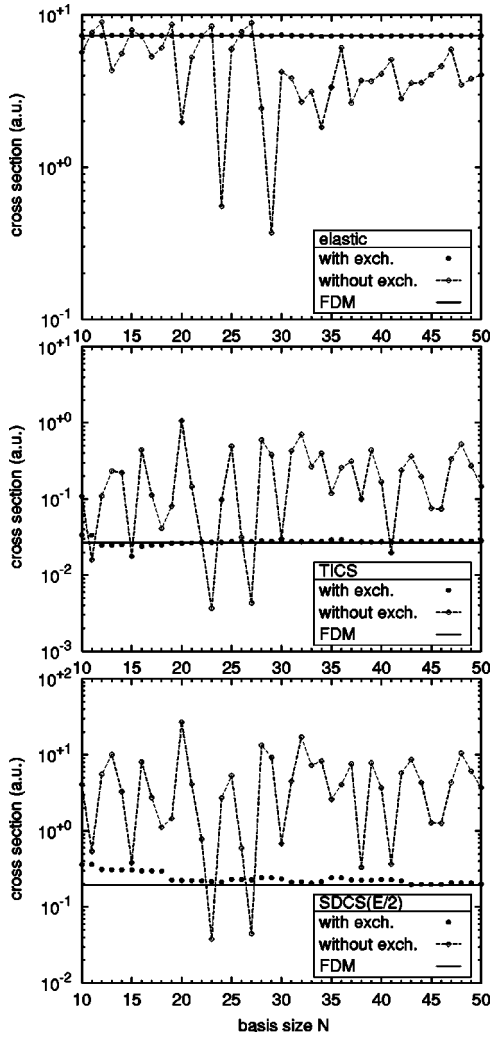

FIG. 2. 17.6 eV *e*-H elastic, total ionization (TICS), and equal-energy singly differential [SDCS($E/2$)] spin-averaged cross sections in the *S*-wave model with and without electron exchange. The dots are the results of CCC(N) calculations, where N is the size of the Laguerre basis. In the case of the no-exchange calculations the open dots have been connected by straight lines to help guide the eye. The finite-difference method (FDM) of Jones and Stelbovics [6] gives near exact solutions.

distinguishable electrons with no rearrangement. In the CCC formalism this amounts to dropping electron exchange.

We see in Fig. 1 that in the with-exchange calculations there is no convergence away from the on-shell point. Oscillations increase with N, as was shown earlier [4], and are due to the energy-dependent exchange potentials necessary to ensure uniqueness of the close-coupling expansion [2]. In contrast, the no-exchange calculations yield very smooth behavior with k, but show no convergence with N, on or off the energy shell. Consequently the question of convergence with N in the CCC method critically depends on whether exchange is or is not included.

To show this in more detail, in Fig. 2 we give an on-shell convergence study, with and without exchange. We see that even the elastic scattering cross section shows no convergence if exchange is neglected. However, once exchange is included convergence is evident, and most importantly, to the independently evaluated accurate results [5,6], including the ionization case where the two outgoing electrons have the same energy.

We suggest that the present examples indicate the importance of including exchange when attempting to study the CCC theory. The fact that CCC amplitudes show no convergence off the energy shell has been previously stated [4]. However, in the CCC method a lack of convergence, off the energy shell is of no consequence since stable on-shell K-matrix elements are obtained. The on-shell real symmetric K matrix is in turn used to define the unitary on-shell T matrix. Understanding of the convergence with N in the CCC method must incorporate exchange and use the same limiting procedures [7]. This was not done by Shablov, Bilyk, and Popov [1]. Consequently, we suspect that they have not identified any formal problems with the CCC approach to excitation or ionization.

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