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Ionization amplitudes in electron-hydrogen collisions

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Recently Zatsarinny and Bartschat [Phys. Rev. Lett. **107**, 023203 (2011)] have given an ansatz for extracting ionization amplitudes from close-coupling calculations of electron-impact ionization of atoms. They applied it with extraordinary success to a fully differential cross section of electron-helium single ionization leaving the residual ion in an $n = 2$ state. By considering electron-impact ionization of atomic hydrogen we explain the origin of the ansatz and show that it forms an effective interpolation scheme for determining the amplitudes, so long as the pseudostate energy distribution is sufficiently dense.

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I. INTRODUCTION

The last two decades have seen extraordinary progress in the field of calculating electron-impact differential ionization of atoms. Following the pioneering approach of Curran and Walters [1] the convergent close-coupling (CCC) method [2] was extended to ionization processes for hydrogen [3] and helium [4], with the goal of yielding accurate results for any total energy $E > 0$. Along the way unexpected behavior of the resulting close-coupling excitation amplitudes for positive-energy $\epsilon_n^{(N)} < E$ states was found [5]. Whenever the energy of the projectile $k_n^2/2$ was less than the energy of the target electron $E/2 < \epsilon_n^{(N)} < E$ the excitation amplitudes were shown to converge to zero with increasing N, leading to a step function [6]. This, in effect, resolved the apparent inconsistency of the close-coupling approach to ionization with the standard theory by reducing the inherent close-coupling secondary energy integration interval from $[0,E]$ to $[0,E/2]$, as would be expected for identical electrons. A detailed analysis suggested that solving the close-coupling equations is like taking a Fourier expansion of the underlying step-function complex amplitudes, with convergence to half the step height at $\epsilon_n^{(N)} = k_n^2/2 = E/2$ [7]. This explained the oscillations seen for $\epsilon_n^{(N)} < E/2$ and the stability of the results at $E/2$.

The CCC approach required interpolation of complex amplitudes available at discrete energies $\epsilon_n^{(N)}$ to yield the ionization amplitude at the measured energy of interest. This is particularly problematic using a Laguerre basis in the $E/2$ region where the energy distribution is most sparse. Attempting to avoid (at the time) impossibly large calculations, a systematic variation of the Laguerre exponential fall-off λ_l was used to ensure that $\epsilon_n^{(N)} = E/2$ for each orbital angular momentum $l \leqslant l_{\max}$. This created a systematic convergence problem [8]. However, the exterior complex scaling method [9] had no such problems and was the first computational method to show complete agreement with the measured equal energy-sharing e-H ionization differential cross sections. Soon after, when greater computational resources were available, the CCC formalism was shown to be able to do the same [10].

All of the computational methods had to deal with the vexed question of how to correctly extract the ionization amplitudes from the calculations. This topic is in itself immense. A review of the underlying formal theory has been given by Kadyrov *et al.* [11] and a connection to various computational techniques discussed by Bray *et al.* [12]. Recently Zatsarinny and Bartschat [13] have suggested a novel ansatz for the problem using the B-spline R-matrix (BSR) method with pseudostates for e-He scattering calculations with extensive comparison with experiments [14]. In particular, they yielded good agreement with the experiment of Bellm *et al.* [15,16] for e-He fully differential ionization leaving the residual ion in $n = 1$ and $n = 2$ states. Furthermore, a recent application has yielded good agreement with measurements of the e-He ionization with excitation-integrated cross sections [17].

II. THEORY

The ansatz of Zatsarinny and Bartschat [13] is as applicable to atomic hydrogen as it is to helium and appears to follow the same derivation route as for the CCC method [4,10]. Staying with the atomic hydrogen case, the total e-H Hamiltonian H is written as

$$H = K_1 + K_2 + V_1 + V_2 + V_{12}, \tag{1}$$

where the indices indicate the two electrons (1 for projectile space; 2 for target space), K is the one-electron kinetic energy operator, V is the electron-nucleus interaction, and V_{12} is the electron-electron interaction.

The Schrödinger equation $(H - E)|\Psi_{Si}^{(+)}\rangle = 0$, where S is the total spin and i is the initial state, is solved by firstly obtaining the N target (pseudo)states via

$$\langle \phi_m^{(N)} | K_2 + V_2 | \phi_n^{(N)} \rangle = \epsilon_n \delta_{mn}, \tag{2}$$

in a Laguerre basis in the case of the CCC method [2]. Box-basis states [18], which are similar in their energy distribution to those in the BSR method, may also be used. The completeness of the states ensures that for

$$I_2^{(N)} = \sum_{n=1}^{N} |\phi_n^{(N)}\rangle\langle\phi_n^{(N)}| \tag{3}$$

we have

$$\lim_{N\to\infty} I_2^{(N)} = I_2, \tag{4}$$

the true identity operator in target space.

The close-coupling expansion may be written as

$$\begin{aligned} 0 &= (H - E)|\Psi_{Si}^{(+)}\rangle \\ &\approx (H - E)(1 + (-1)^S P_r) I_2^{(N)} |\psi_{Si}^{(+)}\rangle, \end{aligned} \tag{5}$$

where the space exchange operator P_r ensures the required symmetry for the total (spin-dependent) wave function $\Psi_{Si}^{(+)}$, irrespective of the symmetry of the numerically obtained $\psi_{Si}^{(+)}$.

In the CCC method [2] the resulting close-coupling equations are solved directly for the transition amplitudes $\langle \boldsymbol{k}_f \phi_f^{(N)} | V_S I_2^{(N)} | \psi_{Si}^{(+)} \rangle \equiv \langle \boldsymbol{k}_f \phi_f^{(N)} | T_S | \phi_i^{(N)} \boldsymbol{k}_i \rangle$ via

$$\begin{aligned} \big\langle \boldsymbol{k}_f \phi_f^{(N)} \big| T_S \big| \phi_i^{(N)} \boldsymbol{k}_i \big\rangle &= \big\langle \boldsymbol{k}_f \phi_f^{(N)} \big| V_S \big| \phi_i^{(N)} \boldsymbol{k}_i \big\rangle \\ &\quad + \sum_{n=1}^{N} \int d^3k \frac{\big\langle \boldsymbol{k}_f \phi_f^{(N)} \big| V_S \big| \phi_n^{(N)} \boldsymbol{k} \big\rangle \big\langle \boldsymbol{k} \phi_n^{(N)} \big| T_S \big| \phi_i^{(N)} \boldsymbol{k}_i \big\rangle}{E^{(+)} - \epsilon_n^{(N)} - k^2/2}, \end{aligned} \tag{6}$$

where $V_S = V_1 + V_{12} + (-1)^S (H - E) P_r$.

For discrete excitation ($\epsilon_f^{(N)} = \epsilon_f < 0$) the T_{fi} amplitudes are used to calculate the physically observable processes. For ionization amplitudes $F_{Si}(\boldsymbol{k}_f, \boldsymbol{q}_f)$, with outgoing electron energies satisfying $q_f^2/2 + k_f^2/2 = E$, we begin with [4,10,11]

$$\begin{aligned} F_{Si}(\boldsymbol{k}_f, \boldsymbol{q}_f) &\equiv \langle \Phi_f^{(-)} | \overleftarrow{H} - E | \Psi_{Si}^{(+)} \rangle \\ &\approx \langle \Phi_f^{(-)} | I_2^{(N)} (H - E) [1 + (-1)^S P_r] I_2^{(N)} | \psi_{Si}^{(+)} \rangle \\ &= \langle \boldsymbol{k}_f \boldsymbol{q}_f^{(-)} | I_2^{(N)} [H - E + (-1)^S (H - E) P_r] I_2^{(N)} | \psi_{Si}^{(+)} \rangle \\ &= \langle \boldsymbol{k}_f \boldsymbol{q}_f^{(-)} | I_2^{(N)} [V_1 + V_{12} + (-1)^S (H - E) P_r] I_2^{(N)} | \psi_{Si}^{(+)} \rangle \\ &= \sum_{n=1}^{N} \big\langle \boldsymbol{q}_f^{(-)} \big| \phi_n^{(N)} \big\rangle \big\langle \boldsymbol{k}_f \phi_n^{(N)} \big| T_S \big| \phi_i^{(N)} \boldsymbol{k}_i \big\rangle. \end{aligned} \tag{7}$$

The main assumption is that the close-coupling expansion ensures that the total wave function has the projectile-space electron always shielded by the target-space one due to the utilization of $I_2^{(N)}$. In other words, the asymptotic Hamiltonian is simply $K_1 + H_2$, and so the asymptotic state is a product of a plane wave $\boldsymbol{k}_f$ and a pure Coulomb wave $\boldsymbol{q}_f$.

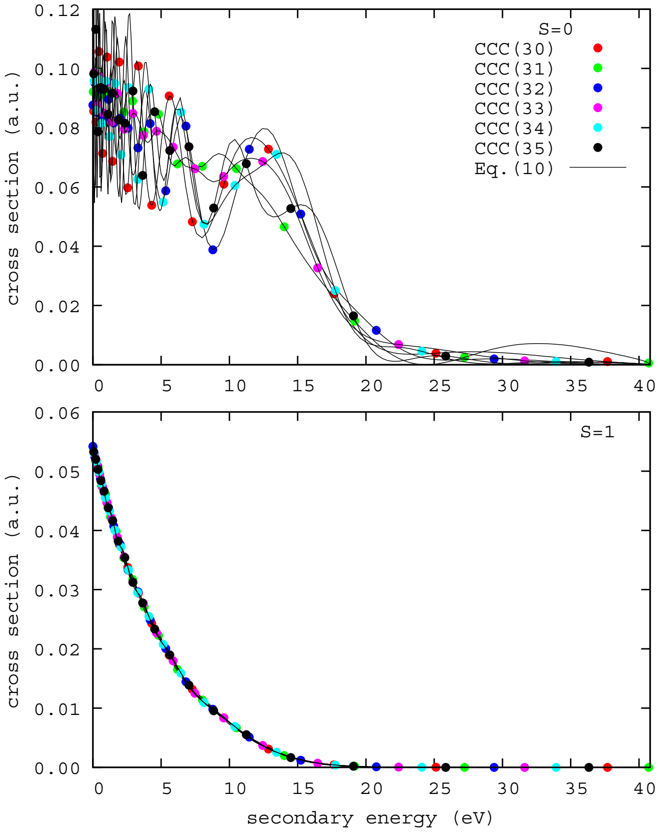

FIG. 1. (Color online) Singly differential cross sections for 54.4 eV electron-impact ionization of atomic hydrogen in the S-wave model. The results are presented for six separate CCC(N) calculations with $N = 30, \ldots, 35$. The solid points arise from using Eq. (9), and the corresponding lines are obtained via the usage of Eq. (10).

As Eq. (7) stands it cannot be used because $\langle \boldsymbol{k}_f \phi_n^{(N)} |$ is not on the energy shell. In the CCC method we take advantage of the fact (see the Appendix of Abdurakhmanov *et al.* [19]) that

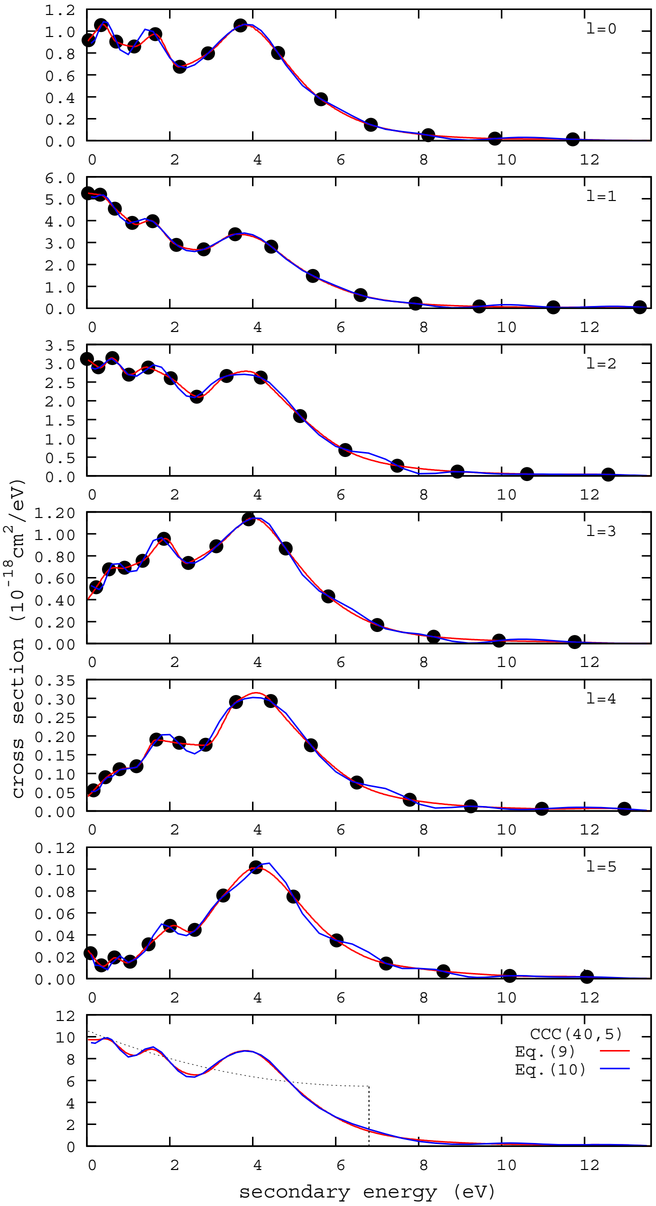

FIG. 2. (Color online) Singly differential cross sections for 27.2 eV electron-impact ionization of atomic hydrogen, calculated with the $N_0 = 40$ and $l_{\max} = 5$ CCC calculation of Bray [21]. Individual $l \leqslant 5$ components are given together with the sum (bottom panel). The cubic spline interpolations over the presented solid points arising from Eq. (9) are compared with those obtained via the usage of Eq. (10). The step function estimate (as $N_0 \to \infty$) [21] is also given in the bottom panel.

if $q_f^2/2 = \epsilon_m^{(N)}$ for some m, then

$$\langle \boldsymbol{q}_f^{(-)}|\phi_n^{(N)}\rangle = \delta_{mn}\langle \boldsymbol{q}_f^{(-)}|\phi_n^{(N)}\rangle, \tag{8}$$

in which case

$$F_{Si}(\boldsymbol{k}_f,\boldsymbol{q}_f) \approx \langle \boldsymbol{q}_f^{(-)}|\phi_f^{(N)}\rangle\langle \boldsymbol{k}_f\phi_f^{(N)}|T_S|\phi_i^{(N)}\boldsymbol{k}_i\rangle, \tag{9}$$

where it is implicit that $q_f^2/2 = \epsilon_f^{(N)}$, and so the ionization amplitudes are available only at the energies of the pseudostates in the CCC calculations. To obtain amplitudes at any other energies, interpolation over the available complex amplitudes is required.

The ansatz suggested by Zatsarinny and Bartschat [13] avoids any interpolation by simply replacing $\langle \boldsymbol{k}_f\phi_n^{(N)}|$ with $\langle \boldsymbol{k}_n\phi_n^{(N)}|$ in Eq. (7) and performing the full sum

$$F_{Si}(\boldsymbol{k}_f,\boldsymbol{q}_f) \approx \sum_{n=1}^{N}\langle \boldsymbol{q}_f^{(-)}|\phi_n^{(N)}\rangle\langle \boldsymbol{k}_n\phi_n^{(N)}|T_S|\phi_i^{(N)}\boldsymbol{k}_i\rangle. \tag{10}$$

While we are unable to derive Eq. (10) from first principles, it is much more convenient to use since no interpolation is required to obtain an ionization amplitude at any secondary energy $q_f^2/2$. Furthermore, it still yields Eq. (9) whenever $q_f^2/2 = \epsilon_n^{(N)}$.

III. RESULTS

Here we wish to investigate why the formulation in Eq. (10) has worked so well [13,17], and if there are any limitations to its application. We begin by considering the S-wave model for e-H ionization, where the singly differential cross section (SDCS) has all of the (nonphase) ionization information. The CCC-calculated SDCS is expected to converge to a step function with increasing Laguerre basis size N, for both singlet ($S = 0$) and triplet ($S = 1$) scattering [6]. In the latter case owing to the Pauli exclusion principle the height of the step is zero, and so no oscillations are expected in the SDCS for $\epsilon_n^{(N)} \leqslant E/2$. In the singlet case the height of the step at $\epsilon_n^{(N)} = E/2$ should be $1/4$ the true result, even in not fully convergent calculations, with extensive oscillations for $\epsilon_n^{(N)} < E/2$ [7].

In Fig. 1 we present the SDCS arising from 54.4 eV e-H CCC(N) calculations for the S-wave model with $N = 30,\ldots,35$. Exact results for this case have been given by Bartlett *et al.* [20]. The dots are the raw data points, from all six CCC(N) calculations, arising via Eq. (9), and the corresponding lines are from Eq. (10) calculated on a dense energy mesh. In the singlet case we see consistency of the raw CCC results in the vicinity of $E/2$. However, those obtained via Eq. (10) show substantial variation in this energy region. This is rather problematic given that the exact result at $E/2$

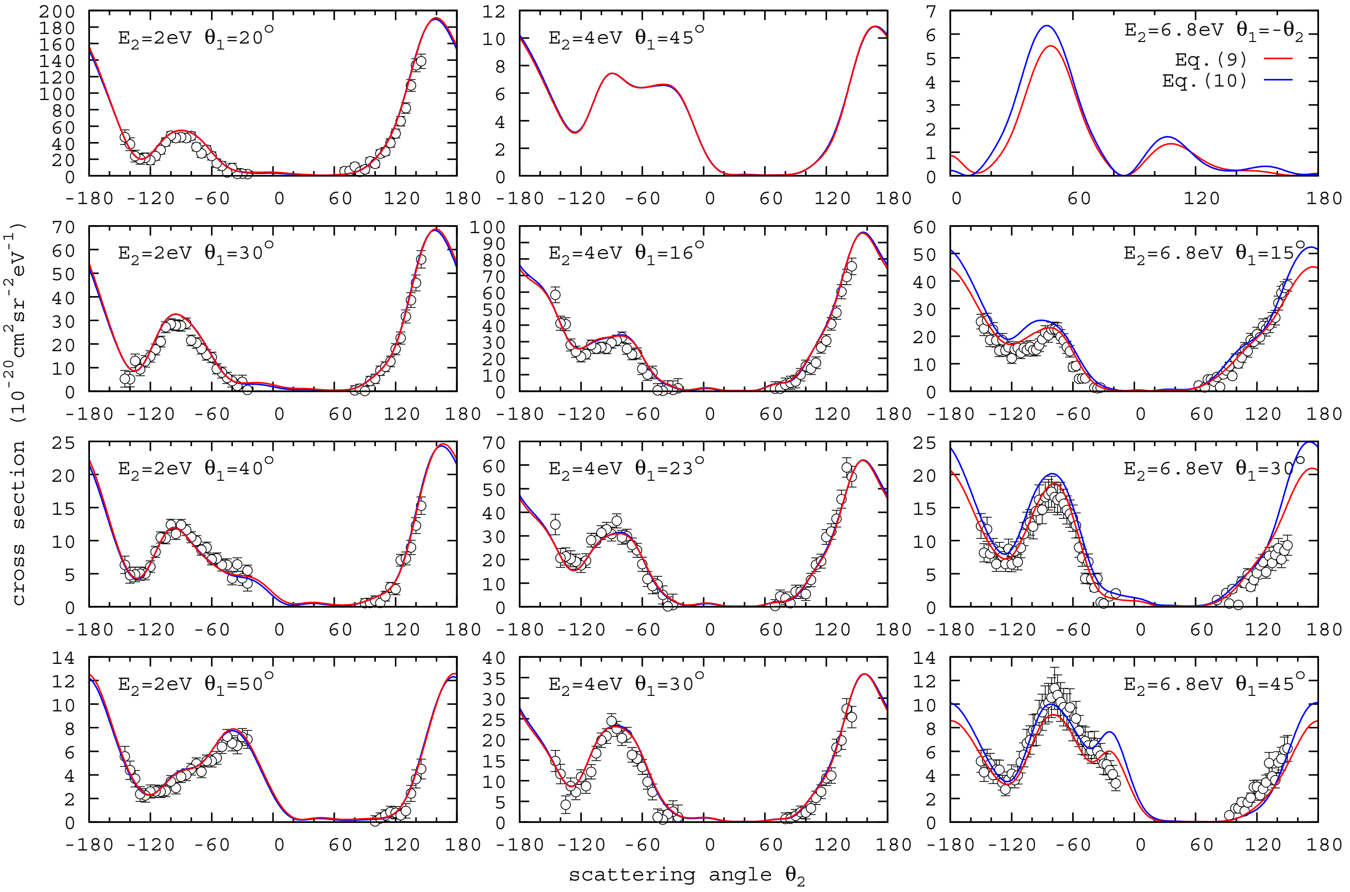

FIG. 3. (Color online) Fully differential cross sections for 27.2 eV electron-impact ionization of atomic hydrogen. The CCC calculations are the $N_0 = 40$ and $l_{\max} = 5$ ones from Bray [21]. The original results utilizing Eq. (9) are compared with those obtained via the usage of Eq. (10). Experimental data are as presented by Berakdar *et al.* [22].

is four times the raw result. In other words, the procedure given by Eq. (10) is not guaranteed to go through the correct result at $q_f^2/2 = E/2$. This suggests that this equation may not have any fundamental origin, but in effect is yet another interpolation scheme whose application requires some care. Furthermore, the oscillations in the asymmetric energy sharing case will require a rescaling procedure as for the CCC method [21] to yield the correct smooth results of Bartlett *et al.* [20]. No problems are seen in the S-wave model triplet case.

Having considered application of Eq. (10) to the S-wave model we now consider the full problem for the case of 27.2 eV electron-impact ionization fully differential cross sections. This is a particularly convenient case due to measurements existing for three separate energy sharing cases of $E_B = 2$, 4, and 6.8 eV ($E_A = 13.6 - E_B$), and the convergence study of the CCC method has already been considered in some detail [21].

We begin by first considering the SDCS, which now comprises several $l \leqslant l_{\max}$ components obtained from the integrated cross sections for positive-energy pseudostates $\phi_n^{(N)}$ with $l \leqslant l_{\max}$. As an example we take the CCC calculations with $N_0 = 40$, and $l_{\max} = 5$ [21]. In Fig. 2 the solid dots are the results obtained directly from Eq. (9) and connected using cubic splines. Also given are the results using Eq. (10), performed on a fine energy mesh. We see very good agreement between the two approaches, though a little variation can occasionally be seen (e.g., around 7 eV for $l = 2$, and around 6 eV for $l = 5$). Note that Eq. (8) (when partial-wave expanded) ensures that the SDCS obtained via Eq. (10) has to pass through the solid dots. At other energies Eq. (8) is approximately satisfied with the $\langle \boldsymbol{q}_f^{(-)}|\phi_n^{(N)}\rangle$ peaking for $\epsilon_n^{(N)}$ closest to $q_f^2/2$. We believe this is the reason why Eq. (10) works so well.

Having found good agreement for the SDCS it is not surprising that a similarly good agreement is found for the fully differential cross sections presented in Fig. 3. Any variation for the asymmetric energy-sharing case is barely visible. For the equal energy-sharing case there is some minor variation, perhaps due to the minor variation visible in the individual SDCS components. Note that to get accurate absolute cross sections the same rescaling technique, to the step function of Fig. 2, has been applied to the usage of Eq. (10) as for the CCC method [21].

IV. CONCLUSIONS

To summarize, we believe the ansatz presented by Zatsarinny and Bartschat [13] is in effect a useful interpolation procedure for generating ionization amplitudes at any secondary energy, but it has no formal origin and still requires a rescaling procedure as for the CCC method to yield accurate absolute cross sections. So long as the pseudostate energy mesh is sufficiently dense it will yield accurate answers due to the approximate satisfaction of Eq. (8), which improves with increasing energy density. Its advantage is that it requires no interpolation over the underlying complex amplitudes and may be readily applied to multichannel final states, which occur in e-He ionization with excitation problems. This will be the next area of our focus.

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