

Convergent calculations of double ionization of helium: From $(\gamma, 2e)$ to $(e, 3e)$ processes

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The first absolute $(e, 3e)$ measurements, by Lahmam-Bennani *et al.* [Phys. Rev. A **59**, 3548 (1999)], have been recently approximately reproduced by Berakdar [Phys. Rev. Lett. **85**, 4036 (2000)] and supported by Jones and Madison [Phys. Rev. Lett. **91**, 073201 (2003)], but with widely differing conclusions. The former indirectly implied that the Born-CCC-based calculations of Kheifets *et al.* [J. Phys. B **32**, 5047 (1999)] were inaccurate due to the reliance on the first Born approximation. The latter argued that the first Born approximation was valid, but an insufficiently accurate initial state was used. We investigate these claims by performing calculations with ground states similar to those used by Jones and Madison, as well as including the second Born terms. We find the effect of the second Born terms to be negligible and that the original calculations of Kheifets *et al.* are reproduced if a ground state similar to that of Jones and Madison is used, but appropriately corrected as done by Le Sech and co-workers [J. Phys. B **23**, L739 (1990)].

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When attempting calculations of complex collision processes we have found it important to utilize a formalism where convergence of the results can be tested by substantial variation of as many of the input parameters as possible. The goal is to develop a predictive theory whose outcomes can be relied upon on scientific merit irrespective of agreement with experiment or other theory. The convergent close-coupling (CCC) method [1] was developed with this idea in mind. The total wave function is expanded utilizing a complete Laguerre basis and so greater accuracy is ensured with increasing basis size. In the Coulomb three-body problems, such as e -H scattering, once convergence is reached there is no freedom left to alter the results. Hence, when there is disagreement with experiment as discussed in Ref. [1], which may be even explained by others [2] or improved upon [3], we find that new experiments [4,5] are supportive of the original CCC results. The predictive power of the CCC approach to double photoionization (DPI or $\gamma, 2e$) was demonstrated more recently when initial disagreement with experiment [6] was resolved in favor of the CCC calculations [7].

Whereas in e -H calculations convergence considerations relate primarily to the usage of the Laguerre basis, in $(\gamma, 2e)$ calculations there is additional consideration of convergence with respect to the description of the initial state. In the more complicated Coulomb four-body problem that is electron-impact double ionization of helium $(e, 3e)$ there are further considerations of convergence with respect to the Born approximation order used to treat the case of a fast projectile. It is these issues that are of interest to us presently.

The physics of the He $(e, 3e)$ reaction in the very fast projectile mode where the incident electron has an order of magnitude or more energy than the two “slow” ejected electrons is quite similar to the case of $(\gamma, 2e)$. In both cases the initial and final atomic states are three-body problems of the He²⁺ nucleus interacting with the two slow electrons. The

application of the CCC method to $(e, 3e)$ process under these kinematical conditions is straightforward and expected to produce results as accurate as those for $(\gamma, 2e)$. However, the first Born CCC result of $(e, 3e)$ on He at 5.6 keV incident energy [8] was found significantly lower in magnitude (by factors of ~ 3 and ~ 12 for 10 and 4 eV ejected electrons, respectively) as compared with absolute measurements of Lahmam-Bennani *et al.* [9]. Such a strong disagreement could only be attributed to deviation from the first Born regime since the treatment of the initial and final states was the same in the CCC $(\gamma, 2e)$ and $(e, 3e)$ calculations. Some indications of that followed from the work of Berakdar [10] who reported good agreement with the absolute measurements [9] on the basis of a lowest-order implementation of a Faddeev-type approach. These calculations differed significantly for electron or positron impact (by about a factor of 2), thus apparently invalidating the first Born approximation.

This conclusion, however, was challenged by the recent work of Jones and Madison [11] who managed to get good agreement, both in shape and magnitude, with the experiment of Lahmam-Bennani *et al.* [9], and the calculations of Berakdar [10], while staying entirely within the first Born formalism. As in the first Born calculations presented by Lahmam-Bennani *et al.* [9], Jones and Madison [11] used a well-known three Coulomb wave (3C) final state, but with a different helium ground state. They argued that Hylleraas-based ground states, as employed earlier [8,9], fail to satisfy the Kato cusp conditions [12] and are inaccurate when the two electrons are close together. In support of their argument, Jones and Madison [11] employed the Pluvillage ground state [13] which treated the interelectron interaction to all orders of perturbation theory and satisfied Kato’s cusp conditions exactly. This combination of the 3C final state and the Pluvillage ground state restored agreement with experiment of Lahmam-Bennani *et al.* [9] within the first Born model.

Here we review our earlier ($e, 3e$) calculations [8] in the light of these new theoretical findings [10,11]. Following the implementation of the second Born term [14] we are able to test the contribution of this term for the kinematics considered here. We have also implemented the Pluvillage ground state and its improved version as prescribed by Le Sech and co-workers [15,16], who argued that the former lacked the screening of two-particle interactions by the third particle. Finally, we used a much bigger CCC expansion, than that used previously [8], in describing the final state. The new initial and final states are first applied to helium DPI to check the gauge dependence as a function of energy. Subsequently, we consider the corresponding ($\gamma, 2e$) and ($e, 3e$) cases with two 10 eV outgoing electrons. Given the relatively low momentum transfer in the ($e, 3e$) experiment, we expect it to be close to the optical limit.

The probability of the ($e, 3e$) reaction is given by the fully differential cross section (FDCS),

$$\frac{d\sigma}{d\Omega' d\Omega_1 d\Omega_2 dE_2} = (2\pi)^4 \frac{k' k_1 k_2}{k_0} |T_{fi}|^2, \quad (1)$$

where indices 0, 1, and 2 are assigned to the incident and two ejected electrons, respectively. We treat the projectile as a plane wave and write the double ionization amplitude

$$T_{fi} = \frac{4\pi}{q^2} \frac{1}{(2\pi)^3} \langle \Psi_{k_1 k_2} | e^{iq \cdot r_1} + e^{iq \cdot r_2} - Z | \Psi_0 \rangle \quad (2)$$

as the Fourier transform of the Coulomb interaction $V = |\mathbf{r}_0 - \mathbf{r}_1|^{-1} + |\mathbf{r}_0 - \mathbf{r}_2|^{-1} - Z/r_0$ between the projectile and the target. Here $Z=2$ is the nuclear charge and $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}'$ is the momentum transfer. By setting $\mathbf{q} \rightarrow 0$ we reach the optical limit. In this limit angular correlations of the two ejected electrons are the same in ($e, 3e$) and ($\gamma, 2e$) reactions if we align the vector \mathbf{q} with the polarization axis of light. The magnitudes of the corresponding cross sections differ by a simple kinematic factor.

Following the successful application of the CCC formalism to ($e, 2e$) equal energy-sharing cross sections [17] we take Laguerre basis exponential fall-off parameters to be the same for all $l \leq 4$ and basis sizes $N_l = 60 - l$. All open plus lowest three closed states were included in the calculations. Previously [8], with smaller computational resources, we were restricted to $N_l = 17 - l$ and had to vary the exponential fall-off parameters for each $l \leq 4$ to avoid inaccuracy associated with interpolation of the complex amplitudes. Some minor variation of the present results from those published previously is due to the very different choices of the Laguerre bases used here.

In our earlier paper [8] we calculated only the first Born amplitude (2) using two accurate ground-state wave functions: a 15-term multiconfiguration Hartree-Fock and a 20-term Hylleraas. These two wave functions produced nearly identical results in the two gauges of the Born operator—length and velocity. In the present investigation we begin with the Pluvillage ground state,

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2) = 8\pi^{-1} e^{-Z(r_1+r_2)} N(k) \Phi_0(\eta, k r_{12}), \quad (3)$$

where

$$\Phi_0(\eta, k r_{12}) = e_1^{-ikr_{12}} F_1(1 - i\eta, 2, 2ikr_{12}).$$

The noncorrelated part of the ground state (3) is the product of the two hydrogenic orbitals in the field $Z=2$. The correlation factor $\Phi_0(\eta, k r_{12})$ with $\eta = (2k)^{-1}$ describes the center-of-mass motion of the electron pair unimpeded by the nucleus.

Le Sech and co-workers [15,16] suggested that the original Pluvillage ground state [13] could be improved by introducing the screening of the interelectron interaction by the nucleus. This can be implemented by changing the effective strength of the Coulomb interaction to $\eta = q(2k)^{-1}$ where $q < 1$. In addition, the screening of the electron-nucleus interaction by another electron can be accommodated by introducing the shielding factor $\cosh(\lambda r_1) + \cosh(\lambda r_2)$ in the noncorrelated part of the ground state with $\lambda < 1$.

In Fig. 1 we show the double-to-single photoionization cross-section ratio for He from threshold to intermediate energies where it is highly sensitive to electron correlation in the ground state. We performed calculations with three different ground-state wave functions: Pluvillage, Le Sech, and Hylleraas. Should the ground and final states be exact, the calculations in the three gauges of the electromagnetic operator—the length r , velocity $\partial/\partial r$, and acceleration Z/r^2 —would be identical. Numerical difference between the three gauges is an indicator of the lack of accuracy in the wave functions. As the final state is identical in all three calculations, variation in the results is due to the choice of the ground-state description. The gauge convergence is worst for the Pluvillage ground state. Only the acceleration gauge, which takes most of its strength at small distances near the nucleus, gives good results. The two other gauges, the length and velocity, which are saturated at large and intermediate distances, respectively, are in strong disagreement with each other and the experiment [18]. The Le Sech ground state brings significant reduction in the gauge variation, particularly at the energy of interest to us here of 20 eV above threshold. The Hylleraas ground state yields excellent agreement between the three gauges and the experiment.

To investigate the ground-state effects further, we calculate the angular distribution of the two equal-energy photoelectrons $E_1 = E_2 = 10$ eV in the form of the triply differential cross section (TDCS) which is obtained from FDCS (1) in the optical limit $q \rightarrow 0$. This TDCS is the counterpart of the FDCS reported in the experiments of Lahmam-Bennani *et al.* [9]. In Fig. 2 we show the TDCS for a fixed angle of one of the photoelectrons whereas the second electron is detected on the full angular range. We choose $\theta_1 = 60^\circ$ where the TDCS is largest in magnitude. As in the case of the total DPI cross section, the Pluvillage ground state gives the worst results, especially in the length form. Gauge invariance and agreement with experiment is much better with the Le Sech and Hylleraas ground states.

Complete failure of the length gauge with the Pluvillage ground state in DPI has severe implications for ($e, 3e$) calculations which are also performed in the length gauge of the

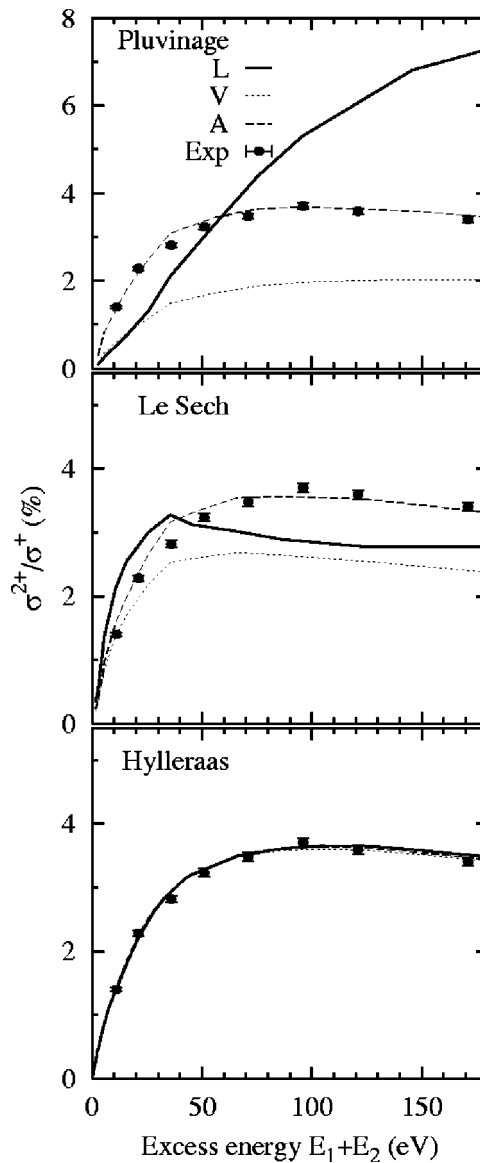


FIG. 1. Double-to-single photoionization cross-section ratio σ^{2+}/σ^+ as a function of the electron pair energy $E_1 + E_2$. The CCC calculations with different ground states (top, Pluvinage; middle, Le Sech; bottom, Hylleraas) are shown in the length, velocity, and acceleration (L , solid line; V , dotted line; and A , dashed line) gauges. The experimental data are from Dörner *et al.* [18].

Born operator (2). Results of the CCC calculations of the $(e, 3e)$ FDCS are shown on the top row of panels in Fig. 3. As in Figs. 1 and 2, we show calculations with three ground-state wave functions: Pluvinage, Le Sech, and Hylleraas. In addition, the calculations were performed utilizing the first and second Born approximations [14] and found to be different by less than 10% (although not quantified, a similar conclusion was reached in Ref. [20]). We choose the fixed ejected electron angles at the values where the four-body Green's function calculations of [10] are available. Results of this calculation along with the 3C-Pluvinage calculation of Jones and Madison [11] are shown on the bottom panels.

In the top panel, scaling factors of 2.2 and 1.8 have to be applied to the CCC calculations with the Hylleraas and Le

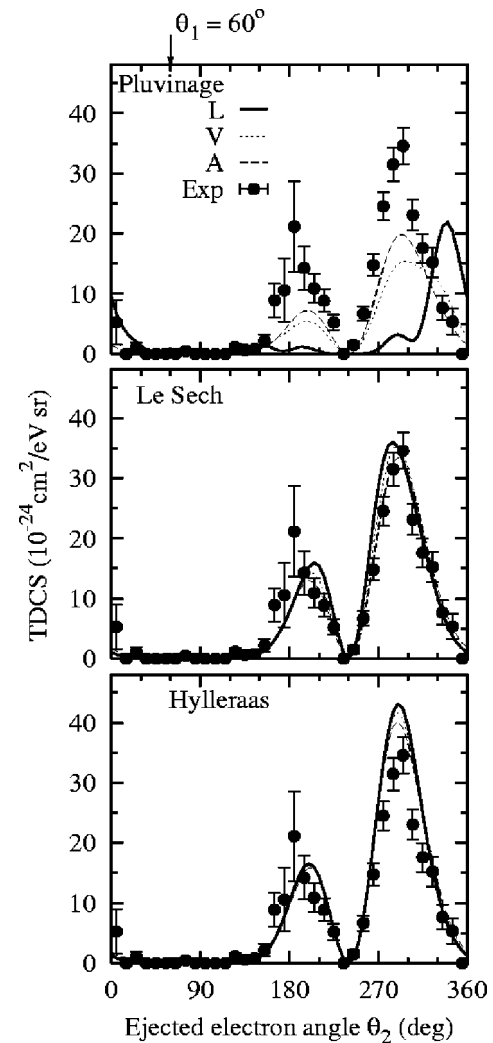


FIG. 2. Triply differential cross section (TDCS) in the polarization plane of light for $(\gamma, 2e)$ on He at $E_1 = E_2 = 10$ eV and the Stokes parameter $S_1 = 0.98$. As in Fig. 1, the CCC calculations with different ground states (top, Pluvinage; middle, Le Sech; bottom, Hylleraas) are shown in the length, velocity, and acceleration (L , V , and A) gauges. The line styles are as in Fig. 1. The experimental data are from Bräuning *et al.* [19].

Sech ground states, respectively, to match the experiment. The shape of the FDCS calculated with the Pluvinage ground state is very different from the experiment and the other two calculations. A scaling factor of six was applied to this calculation to put it approximately on the same scale as the experiment. On the other hand, in the bottom panel, the two 3C-based calculations of Berakdar [10] and Jones and Madison [11] agree between themselves and with the absolute measurements of Lahmam-Bennani *et al.* [9] without any additional scaling. However, we must recall that simply changing the charge of the projectile will destroy the good agreement between the two 3C-based calculations.

Thus, we encounter the extraordinary situation where we have confidence in our results even though they disagree with experiment and two other theories, all of which agree with each other. We do not agree with the implicit conclusion of [10] that the first Born approximation is insufficient for

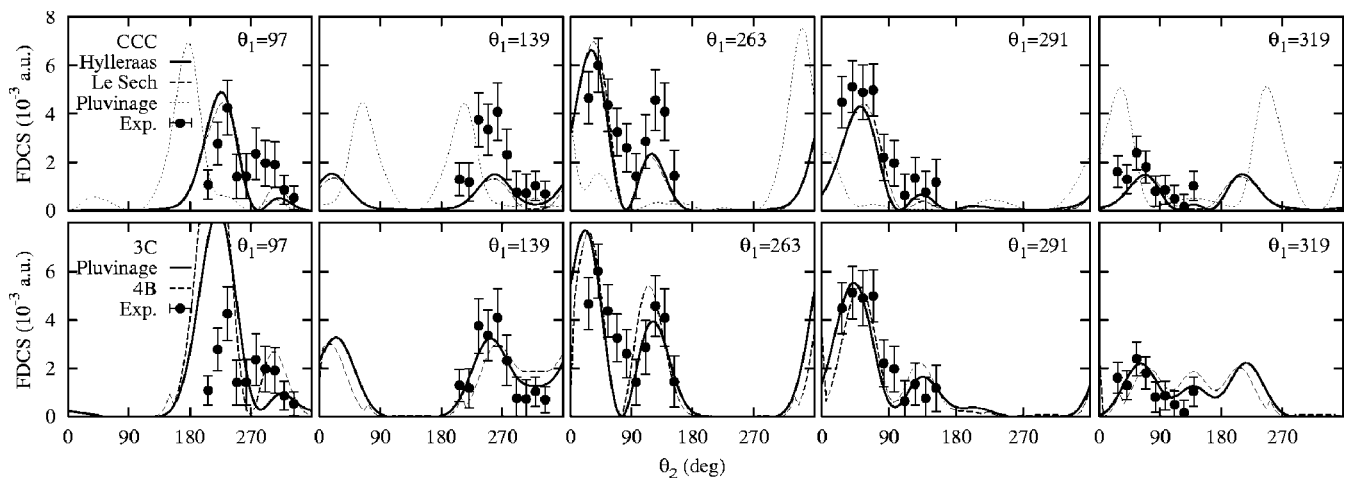


FIG. 3. Fully differential cross section (FDACS) in the scattering plane for $(e,3e)$ on He at $E_0=5.6$ keV, $E_1=E_2=10$ eV, and $q=0.24$ a.u. for selected fixed ejected electron angles θ_1 . The CCC calculations with different ground-state wave functions are shown on the top row of panels. The Pluvintage, Le Sech, and Hylleraas ground-state results are shown by the dotted, dashed, and solid lines and multiplied by factors of 6, 1.8, and 2.2, respectively, to match the experiment of Lahmam-Bennani *et al.* [9]. On the bottom row of panels we show the Pluvintage-3C calculation of Jones and Madison [11] and the four-body (4B) Green's function calculation of Berakdar [10].

the problem at hand. While Jones and Madison [11] also argue this, they use the Pluvintage ground state which we have shown here not to work for DPI or $(e,3e)$ when combined with the CCC final state. However, when this ground state was improved to yield the Le Sech state, which still satisfies the Kato's cusp conditions, the results yielded good agreement with the originally used Hylleraas ground state. We do not accept that the 3C final state can work better than the CCC final state for the kinematics considered irrespective of the initial state. Finally, we have checked the absolute relations between the $(\gamma,2e)$ and $(e,3e)$ calculations and find them consistent. Consequently, we stand by the original ap-

proach to the problem [8]. Fundamentally, we argue that the physics of the $(e,3e)$ process of the type considered here is closely related to the corresponding $(\gamma,2e)$ process. We are hopeful that this work will stimulate further experimental and theoretical study of the subject.

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