Evidence of Initial-State Two-Center Effects for $(e, 2e)$ Reactions

S. Jones* and D. H. Madison
Physics Department, University of Missouri-Rolla, Rolla, Missouri 65401
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Coincidence, or $(e, 2e)$, measurements of electron-impact ionization of atoms have established that the largest values of triply differential cross sections are obtained in collisions involving small momentum transfer to the target. Absolute measurements for these reactions are now available for hydrogen at 54.4-eV impact energy, and relative data have recently been reported at 27.2 eV. Previous theoretical works have concentrated on employing asymptotically correct two-center wave functions for the final state, leaving the initial state described by the Born approximation. Here we report results for which asymptotically correct two-center wave functions are used for *both* the initial and final states of the scattering system. Comparison of these results with experiment reveals that two-center effects (projectile-target correlations) are also important in the initial state. [S0031-9007(98)07114-2]

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In 1966, Dodd and Greider [1] wrote the following: "The problem of obtaining a convergent solution for three-body scattering processes has been investigated extensively by Faddeev, Lovelace, Weinberg, Rosenberg, and Amado [2–6]. The conclusions reached by these authors are essentially the same: in order to obtain a nondivergent solution for the three-body amplitude, it is necessary to replace the Lippmann-Schwinger equation by a set of coupled integral equations. The kernel in the coupled equations is a 3×3 matrix which, when squared, contains no dangerous diagrams. These equations, originally proposed by Faddeev, were the first that gave a mathematically sound formulation of the three-body scattering problem."

Dodd and Greider [1] then showed that a simplification of the Faddeev equations is obtained when the mass of one particle is either much larger or much smaller than the other two. When this mass restriction applies, the scattering amplitude is determined by a *single* integral equation that can be cast as a perturbation series. Gayet [7] showed that an existing perturbation series, the continuum distorted-wave (CDW) series, could be derived from Dodd and Greider's three-body scattering theory. Thus, the CDW series offers a convergent approach for solving three-body scattering problems.

The CDW approximation was originally proposed in 1964 by Cheshire [8] for ion-atom charge exchange. In 1978, Belkić [9], starting from Dodd and Greider's distorted-wave formalism [1], extended the method to ion-atom ionization. Unfortunately, as shown by Crothers [10], the initial-state wave function in the CDW approximation is not properly normalized. Consequently, the now firmly established CDW-EIS (CDW final state, eikonal initial state) approximation for ion-atom ionization was proposed by Crothers and McCann [11] in 1983.

The above ideas grasped a foothold in electron-atom literature in 1989, when Brauner, Briggs, and Klar [12] reported $(e, 2e)$ calculations for electron-hydrogen ionization where the final-state wave function satisfied the exact asymptotic boundary conditions. This correlated "3C" wave function has received much attention and is identical (mass and charge enter as parameters) to the final-state wave function in the CDW [9] and CDW-EIS [11] approximations. To our knowledge, it first appeared in a 1973 paper by Rosenberg [13] (quoting an unpublished work of Redmond).

Since 1989, there have been numerous attempts to improve the 3C wave function for $(e, 2e)$ reactions. In each of these papers, however, the uncorrelated, single-center Born approximation was still made for the initial state. One would expect that the convergence properties of perturbation series should be improved by also including correlation in the initial state (CDW-EIS approximation). That this is indeed the case is demonstrated here for the first time for the $(e, 2e)$ process.

In the distorted-wave formalism, the exact transition amplitude is given in post interaction form by [14,15]

$$T_{fi} = \langle \chi_f^- | W_f^\dagger | \Psi_i^+ \rangle + \langle \chi_f^- | V_i - W_f^\dagger | \beta_i \rangle . \quad (1)$$

Here Ψ_i^+ is the exact scattering wave function developed from the initial state satisfying exact outgoing-wave boundary conditions and χ_f^- is a distorted wave developed from the final state satisfying exact incoming-wave boundary conditions, but is otherwise arbitrary. The perturbation W_f is the difference between the exact final-state interaction between all three particles and the approximate scattering potential used to calculate χ_f. In the second term of Eq. (1),

$$\beta_i = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_a)\psi_{1s}(\mathbf{r}_b)$$

is the unperturbed initial state, where ψ_{1s} is the wave function for the hydrogen atom and $\mathbf{k}_i$ is the wave vector for the incident electron. The corresponding channel interaction is $V_i = 1/r_{ab} - 1/r_a$. The vectors $\mathbf{r}_a$ and $\mathbf{r}_b$ are the coordinates of the two electrons relative to the nucleus and $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$ is their relative coordinate. We use atomic units (a.u.), except where noted otherwise, and take the mass of the nucleus to be infinite.

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For the final state, we make the CDW (3C) choice:

$$\chi_f^- = (2\pi)^{-3}\exp(i\mathbf{k}_a\cdot\mathbf{r}_a + i\mathbf{k}_b\cdot\mathbf{r}_b)C(\alpha_b,\mathbf{k}_b,\mathbf{r}_b) \times C(\alpha_a,\mathbf{k}_a,\mathbf{r}_a)C(\alpha_{ab},\mathbf{k}_{ab},\mathbf{r}_{ab})\,. \quad (2)$$

Here $\mathbf{k}_a$ and $\mathbf{k}_b$ are the wave vectors for the two final-state electrons and $\mathbf{k}_{ab} = \mu(\mathbf{k}_a - \mathbf{k}_b)$ is their relative wave vector, where $\mu = 1/2$ is their reduced mass. The Sommerfeld parameters are given by $\alpha_a = -1/k_a$, $\alpha_b = -1/k_b$, and $\alpha_{ab} = \mu/k_{ab}$. Distortion effects of the Coulomb potential are contained in the function

$$C(\alpha,\mathbf{k},\mathbf{r}) \equiv \Gamma(1 - i\alpha)\exp(-\pi\alpha/2) \times {}_1F_1(i\alpha,1;-ikr - i\mathbf{k}\cdot\mathbf{r})\,,$$

where ${}_1F_1$ is the confluent hypergeometric function and Γ is the gamma function. It is well known that the wave function (2) is asymptotically correct for large separations between all three particles. It has recently been shown [16] that this wave function also remains valid if only two interparticle separations are large. Thus, the wave function (2) is asymptotically correct in *all* asymptotic domains.

The perturbation W_f in Eq. (1) is determined from the Schrödinger equation: $(H - E)\chi_f^- = W_f\chi_f^-$, where H is the Hamiltonian and E is the energy. Substituting χ_f^- into the Schrödinger equation, we obtain

$$W_f = \mathbf{K}(\alpha_{ab},\mathbf{k}_{ab},\mathbf{r}_{ab}) \cdot \mu[\mathbf{K}(\alpha_a,\mathbf{k}_a,\mathbf{r}_a) - \mathbf{K}(\alpha_b,\mathbf{k}_b,\mathbf{r}_b)]\,,$$

where

$$\mathbf{K}(\alpha,\mathbf{k},\mathbf{r}) \equiv \frac{{}_1F_1(1 + i\alpha,2;-ikr - i\mathbf{k}\cdot\mathbf{r})}{{}_1F_1(i\alpha,1;-ikr - i\mathbf{k}\cdot\mathbf{r})}\left(\frac{\mathbf{k}}{k} + \frac{\mathbf{r}}{r}\right).$$

For the exact scattering wave function Ψ_i^+, we make the eikonal approximation [17] (z axis along $\mathbf{k}_i$):

$$\Psi_i^+ \approx \beta_i \exp\left[-\frac{i}{k_i}\ln\left(\frac{r_a - z_a}{r_{ab} - z_{ab}}\right)\right]. \quad (3)$$

The eikonal phase factor, like the product of the last two Coulombic-distortion factors in Eq. (2), introduces projectile-target correlations (two-center effects). The choice (2) together with the approximation (3) is the CDW-EIS approximation. The 3C approximation of Brauner, Briggs, and Klar [12] is obtained by omitting the eikonal phase factor in Eq. (3). For sufficiently high energies, the eikonal approximation is valid for small momentum transfer to the target (small scattering angles of the projectile) [15,17]. As a result, we consider only momentum transfer less than one (a.u.) and ignore electron

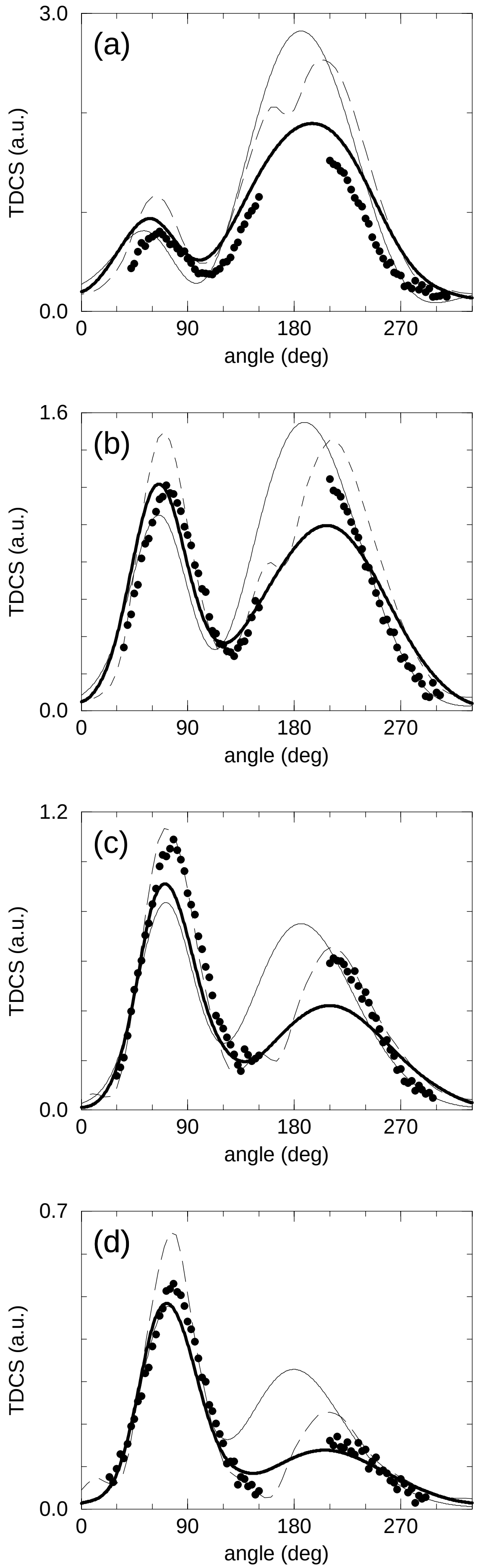

FIG. 1. Scattering-plane TDCS at 54.4 eV vs the angle (clockwise from forward direction) of the slower (5 eV) electron. The angle (counterclockwise) of the faster electron is (a) 4°, (b) 10°, (c) 16°, or (d) 23°. Thick line: CDW-EIS. Thin line: 3C. Broken line: CCC [19]. Circles: experiment [20].

exchange, which involves large momentum transfer. For the kinematics considered here, the cross section is primarily determined by small momentum-transfer collisions and therefore exchange is relatively unimportant.

We use six-dimensional numerical quadrature [18] to evaluate the scattering amplitude. In Fig. 1, the present triply differential cross section (TDCS) results both with initial-state correlation (CDW-EIS) and without initial-state correlation (3C) are compared with the absolute ($\pm 40\%$) measurements [20] at 54.4 eV as well as the convergent close-coupling (CCC) results of Bray *et al.* [19]. The TDCS experimental data characteristically has two maxima with the one at smaller angles being referred to as the binary peak since it is near the angle that an atomic electron would emerge after a single collision with the projectile. The second peak is called the recoil peak since it results from the atomic electron further colliding with the recoiling ion. Comparing the CDW-EIS and 3C results, it is seen that initial-state correlation is important; particularly for the recoil peak where it significantly

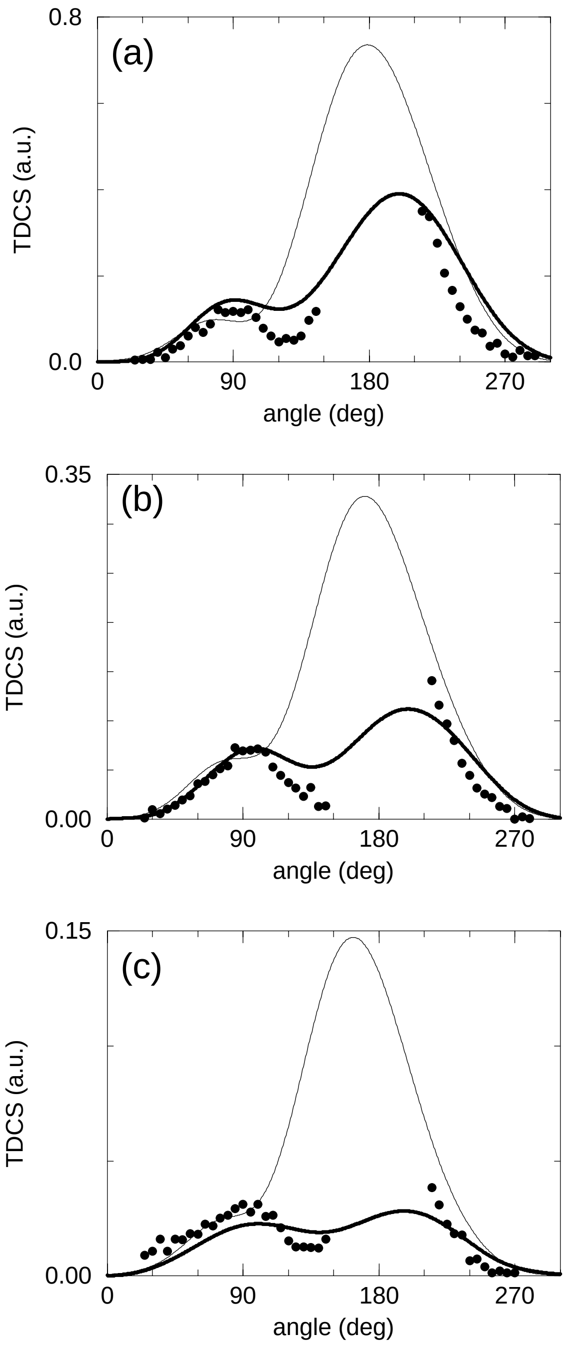

FIG. 2. Same as Fig. 1 for an impact energy of 27.2 eV and a slower-electron energy of 2 eV. The fixed observation angle for the faster electron is (a) 20°, (b) 30°, or (c) 40°.

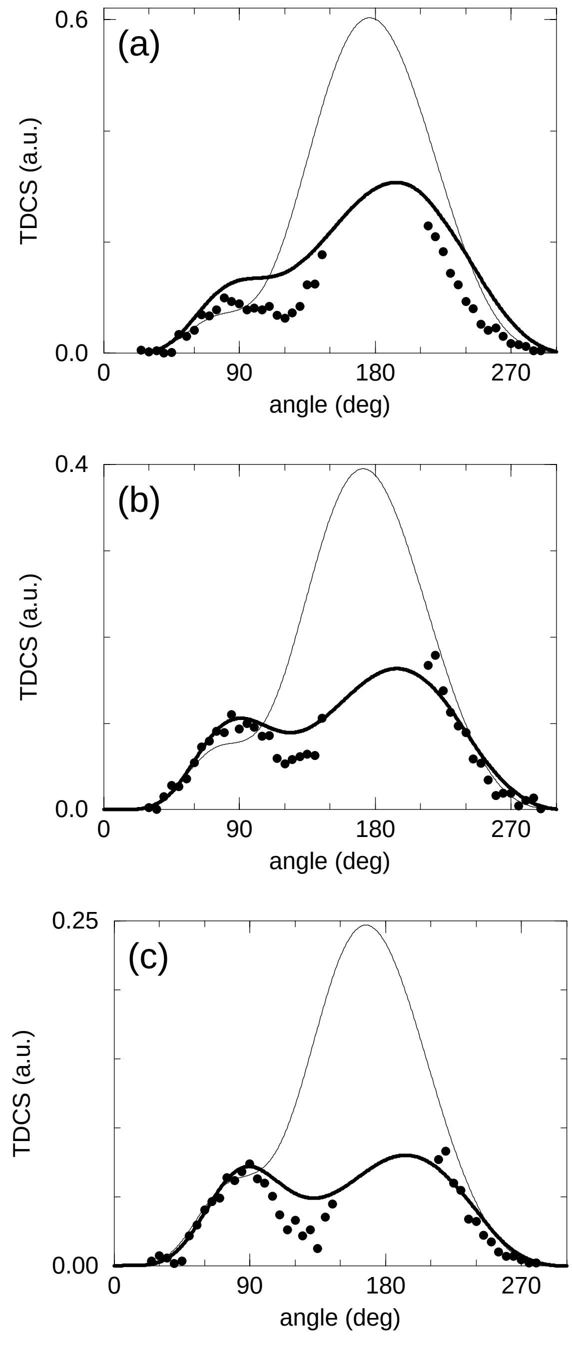

FIG. 3. Same as Fig. 2 for a slower-electron energy of 4 eV. The fixed observation angle for the faster electron is (a) 16°, (b) 23°, or (c) 30°.

decreases the magnitude of the TDCS and shifts the peak position to larger scattering angles, leading to much better agreement with the shape of the data. CCC results are also in excellent agreement with the shape of the data, but are about $1/3$ larger than CDW-EIS predictions.

In Figs. 2–4, we present our results for an impact energy of 27.2 eV (CCC results are not available). The relative experimental data [20] are normalized to our CDW-EIS results by multiplying by the same factor for each scattering angle of the faster electron for a fixed slower-electron energy, since these data are on the same scale. It is seen that initial-state correlation is even more important for the lower-energy incident electrons. Whereas the experimental data still exhibit the characteristic double-peak structure, the binary peak is either missing or only a small shoulder in the 3C results. Initial-state correlation, on the other hand, brings back the double-peak structure.

In conclusion, we have evaluated the first term of the CDW-EIS perturbation series for electron-hydrogen ionization. Our results show that two-center effects in $(e, 2e)$ reactions are important *before* the atomic electron is ejected into the continuum. Including initial-state correlation significantly improved agreement with experiment particularly for the lower impact energy. Since the measurements at 27.2 eV are not absolute, absolute measurements are necessary to determine the validity of these predictions since the magnitude of the cross section can be extremely sensitive to the theoretical model. Nevertheless, we are encouraged by the fact that the CDW-EIS binary- to recoil-peak ratios are in reasonable agreement with experiment. Finally, we note that this work is based upon satisfying both initial-state and final-state asymptotic boundary conditions whereas the CCC method is not. Absolute measurements and CCC calculations for 27.2 eV would provide additional insight into the importance of satisfying boundary conditions.

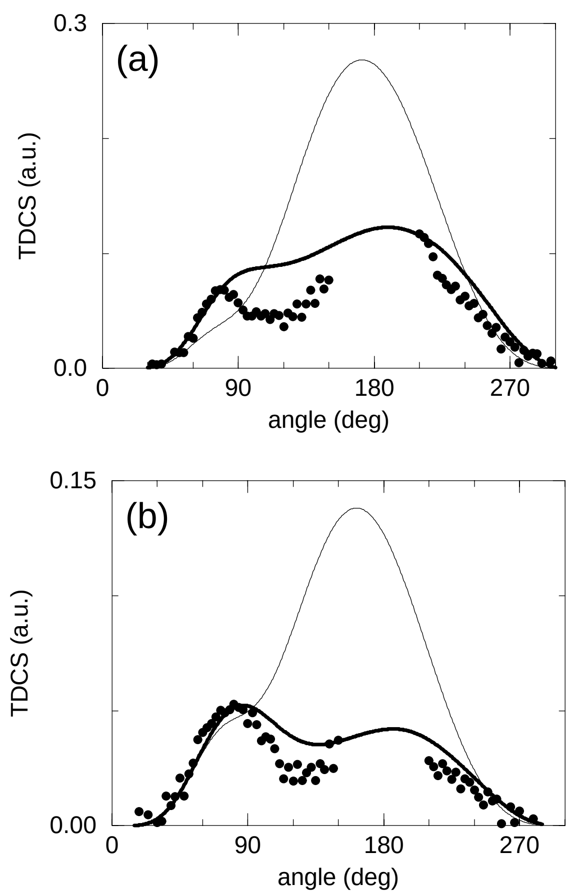

FIG. 4. Same as Fig. 2 except that here each final-state electron has an energy of 6.8 eV. The fixed observation angle is (a) 15°, or (b) 30°.

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*Present address: Centre for Atomic, Molecular and Surface Physics, Murdoch University, Perth 6150, Australia.

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