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# Ionization of Hydrogen Atoms by Fast Electrons

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# Ionization of hydrogen atoms by fast electrons

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We study ionization of atomic hydrogen by fast electrons using asymptotically correct two-center wave functions to describe the scattering system both initially and finally. For the final state, we employ the well-known product wave function of Redmond, which treats all three two-body Coulomb interactions exactly, albeit independently. This ''3C'' wave function is the leading term of the exact scattering wave function, regardless of how *slow* the three particles are, if any two particles have large relative *separation* [Y.E. Kim and A.L. Zubarev, Phys. Rev. A **56**, 521 (1997)]. Here we extend the analysis of Qiu *et al.* [Phys. Rev. A **57**, R1489 (1998)] to show that the 3C wave function is the leading term of the exact scattering wave function, regardless of how *close* the three particles are, if any two particles have large relative *speed*. Whereas Brauner, Briggs, and Klar [J. Phys. B **22**, 2265 (1989)], using the above wave function, demonstrated the importance of *final-state* two-center effects, we have shown that *initial-state* two-center effects must also be included to obtain accurate results at lower energies [S. Jones and D.H. Madison, Phys. Rev. Lett. **81**, 2886, (1998)]. Here we consider three different two-center approximations for the initial state, which yield nearly identical results for impact energies above 250 eV. For lower energies, the model that uses the eikonal approximation for the initial state emerges as the most accurate one, just as is observed in the case of ion impact.

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## I. INTRODUCTION

Electron-impact ionization of atoms has been a topic of considerable interest for the last three decades. Ten years ago, Brauner, Briggs, and Klar [1], using the three-body product wave function of Redmond [2,3], showed that any accurate theoretical calculation based upon first-order perturbation theory would have to include the final-state electron-electron interaction in the formation of the final-state wave function. Recently, we demonstrated that first-order perturbation theory could be extended to still lower energies by also including the initial-state electron-electron interaction in the formation of the initial-state wave function [4]. Here we study the role of initial-state correlation in more detail by comparing three different methods of including this correlation that have been proposed in the literature and by considering a wider range of energies than in our previous paper [4]. The wave functions considered for the initial state are the continuum distorted wave (CDW) approximation of Cheshire [5], the ''two-Coulomb wave'' (TCW) approximation of Dewangan [6], and the eikonal approximation of Glauber [7]. In all cases, the CDW (3C) wave function of Redmond [2,3] is used for the final state. By comparing the above results with those neglecting initial-state interactions, the effects of these interactions become clear. A further idea of the accuracy of these models is gained by comparison with nonperturbative close-coupling calculations [8,9].

We limit the scope of this study to *fast* electron-hydrogen collisions, so that a perturbative approach is appropriate. We regard a collision as fast if the projectile is faster (initially and finally) than any target electrons that participate in the collision. The 3C wave function is ideal for studying fast collisions since, as we will show, it is leading term of the exact scattering wave function in the entire coordinate space if any two particles have large relative speed.

Absolute experimental data for the triply-differential ionization cross section are available at impact energies of 54.4, 150, and 250 eV [10,11], and provide the basis for the present study. Atomic units (a.u.) are used throughout this work unless stated otherwise.

## II. THEORY

In the distorted-wave formalism, the post form of the exact transition matrix ($T$ matrix) element is given by the two-potential formula of Gell-Mann and Goldberger [12]:

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

Here $\Psi_i^+$ is the exact scattering wave function developed from the initial state satisfying exact outgoing-wave $(+)$ boundary conditions and $\chi_f^-$ is a distorted wave developed from the final state satisfying exact incoming-wave $(-)$ boundary conditions, but is otherwise arbitrary ($W_f$ is the corresponding perturbation).

In the second term of Eq. (1),

$$\beta_i=\phi_{\mathbf{k}_i}(\mathbf{r}_a)\psi_{1s}(\mathbf{r}_b) \tag{2}$$

is the unperturbed initial state, where $\psi_{1s}$ is the wave function for the hydrogen atom, $\mathbf{k}_i$ is the wave vector for the incident electron, and

$$\phi_{\mathbf{k}}(\mathbf{r})=(2\pi)^{-3/2}\exp(i\mathbf{k}\cdot\mathbf{r}). \tag{3}$$

 

The vectors $\mathbf{r}_a$ and $\mathbf{r}_b$ are the coordinates of the two electrons relative to the nucleus, which we take to be infinitely massive. The initial-state channel interaction $V_i$ in Eq. (1) is given by

$$V_i = -\frac{1}{r_a} + \frac{1}{r_{ab}}. \tag{4}$$

Here $r_{ab} = |\mathbf{r}_{ab}|$, where $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$.

For the final state, we use the CDW wave function (in electron-atom literature, this is usually called the 3C wave function) [1–3,13,14]:

$$\chi_f^- = \psi_{\mathbf{k}_a}^-(\mathbf{r}_a)\psi_{\mathbf{k}_b}^-(\mathbf{r}_b)C^-(1/k_{ab}, \mu\mathbf{k}_{ab}, \mathbf{r}_{ab}). \tag{5}$$

Here $\mathbf{k}_a$ and $\mathbf{k}_b$ are the wave vectors for the two final-state electrons and $\mathbf{k}_{ab} = \mathbf{k}_a - \mathbf{k}_b$. The reduced mass of two electrons is denoted by $\mu = 1/2$. The wave functions

$$\psi_{\mathbf{k}}^{\pm}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r})C^{\pm}(-1/k, \mathbf{k}, \mathbf{r}) \tag{6}$$

are continuum states of the hydrogen atom. They satisfy

$$\left(-\frac{1}{2}\nabla^2 - \frac{1}{r}\right)\psi_{\mathbf{k}}^{\pm}(\mathbf{r}) = \frac{1}{2}k^2\psi_{\mathbf{k}}^{\pm}(\mathbf{r}). \tag{7}$$

Distortion effects of the Coulomb potential are contained in the function

$$C^{\pm}(\alpha, \mathbf{k}, \mathbf{r}) = N^{\pm}(\alpha)\,{}_1F_1(\mp i\alpha, 1; \pm ikr - i\mathbf{k}\cdot\mathbf{r}). \tag{8}$$

Here ${}_1F_1$ is the confluent hypergeometric function and $N^{\pm}(\alpha) = \Gamma(1 \pm i\alpha)\exp(-\pi\alpha/2)$, where $\Gamma$ is the gamma function.

The perturbation $W_f$ in Eq. (1) is determined from the Schrödinger equation

$$(H - E)\chi_f^- = W_f\chi_f^-, \tag{9}$$

where

$$H = -\frac{1}{2}\nabla_{\mathbf{r}_a}^2 - \frac{1}{2}\nabla_{\mathbf{r}_b}^2 - \frac{1}{r_a} - \frac{1}{r_b} + \frac{1}{r_{ab}} \tag{10}$$

is the full Hamiltonian and

$$E = \frac{1}{2}k_a^2 + \frac{1}{2}k_b^2 \tag{11}$$

is the total energy. Substituting $\chi_f^-$ [the CDW (3C) wave function of Eq. (5)] into the Schrödinger equation (9), we obtain (previously obtained by Klar [15,16]) [17]

$$W_f = \mathbf{K}_{ab}\cdot\mu(\mathbf{K}_a - \mathbf{K}_b), \tag{12}$$

where

$$\mathbf{K}_a \equiv \mathbf{K}(-1/k_a, \mathbf{k}_a, \mathbf{r}_a), \tag{13}$$

$$\mathbf{K}_b \equiv \mathbf{K}(-1/k_b, \mathbf{k}_b, \mathbf{r}_b), \tag{14}$$

$$\mathbf{K}_{ab} \equiv \mathbf{K}(1/k_{ab}, \mu\mathbf{k}_{ab}, \mathbf{r}_{ab}), \tag{15}$$

and where

$$\mathbf{K}(\alpha, \mathbf{k}, \mathbf{r}) \equiv \frac{{}_1F_1(1 + i\alpha, 2; -ikr - i\mathbf{k}\cdot\mathbf{r})}{{}_1F_1(i\alpha, 1; -ikr - i\mathbf{k}\cdot\mathbf{r})}(\hat{\mathbf{k}} + \hat{\mathbf{r}}), \tag{16}$$

where $\hat{\mathbf{k}}$ and $\hat{\mathbf{r}}$ are unit vectors in the directions of $\mathbf{k}$ and $\mathbf{r}$, respectively.

The perturbation (12), a complex scaler, is a six-dimensional three-body interaction of shorter range than the Coulomb interaction. It represents interactions *between* two-body subsystems since the distortion effects of each two-body Coulomb potential have been treated exactly, but independently, in $\chi_f^-$.

Kim and Zubarev [18], building on work by Alt and Mukhamedzhanov [19] and Mukhamedzhanov and Lieber [20], showed that the CDW (3C) wave function (5) is asymptotically correct in *all* asymptotic domains of coordinate space. This means that the above wave function is the leading term of the exact scattering wave function if any two particles are far apart.

Qiu *et al.* [21], on the other hand, studied the behavior of the 3C wave function in the *entire* coordinate space. They wrote the following high-energy ansatz for the exact scattering wave function developed from the final state:

$$\Psi_f^- = \psi_{\mathbf{k}_a}^-(\mathbf{r}_a)\psi_{\mathbf{k}_b}^-(\mathbf{r}_b)\mathcal{C}(\mathbf{r}_{ab}), \tag{17}$$

where the $\psi_{\mathbf{k}}(\mathbf{r})$ are given by Eq. (6) and $\mathcal{C}(\mathbf{r}_{ab})$ is a function to be determined. Substituting $\Psi_f^-$ (17) into Schrödinger's equation, $(H - E)\Psi_f^- = 0$, one obtains the following equation for $\mathcal{C}(\mathbf{r}_{ab})$:

$$\left[\nabla_{\mathbf{r}_{ab}}^2 + (i\mathbf{k}_{ab} + \mathbf{K}_b - \mathbf{K}_a)\cdot\boldsymbol{\nabla}_{\mathbf{r}_{ab}} - \frac{1}{r_{ab}}\right]\mathcal{C}(\mathbf{r}_{ab}) = 0, \tag{18}$$

where $\mathbf{K}_a$ and $\mathbf{K}_b$ are given by Eqs. (13) and (14), above. Qiu *et al.* [21] considered the case where $k_{ab} \gg 1$ and $k_a \gg k_b$. For large $k_{ab}$, Eq. (18) reduces, to leading order in $1/k_{ab}$, to

$$\left[\nabla_{\mathbf{r}_{ab}}^2 + i\mathbf{k}_{ab}\cdot\boldsymbol{\nabla}_{\mathbf{r}_{ab}} - \frac{1}{r_{ab}}\right]\mathcal{C}(\mathbf{r}_{ab}) = 0, \tag{19}$$

since the functions $\mathbf{K}_a$ and $\mathbf{K}_b$ are bounded in the entire coordinate space [21]. Equation (19) is just the usual equation for the confluent hypergeometric function; thus

$$\mathcal{C}(\mathbf{r}_{ab}) = C^-(1/k_{ab}, \mu\mathbf{k}_{ab}, \mathbf{r}_{ab}), \tag{20}$$

where $C^-(\alpha, \mathbf{k}, \mathbf{r})$ is given by Eq. (8). As a result, $\Psi_f^-$ reduces to the 3C wave function (5) for $k_a \to \infty$ and finite $k_b$. Obviously, the same result is also obtained if $k_{ab} \gg 1$ and $k_b \gg k_a$, or if all three momenta are large. This leaves only the case where $k_a \gg k_{ab}$ and $k_b \gg k_{ab}$ (not considered by Qiu *et al.* [21]). In this limit, $\mathbf{K}_a$ (13) vanishes as $1/k_a$ and $\mathbf{K}_b$ (14) vanishes as $1/k_b$, so we still obtain the 3C wave function. This follows from the asymptotic form of $\mathbf{K}(\alpha, \mathbf{k}, \mathbf{r})$ [22]:

$$\mathbf{K}(\alpha,\mathbf{k},\mathbf{r}) \underset{k\to\infty}{\sim} \frac{\hat{\mathbf{k}}+\hat{\mathbf{r}}}{ikr(1+\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})}. \tag{21}$$

Equation (21) is, of course, not valid in the singular direction $\hat{\mathbf{k}}=-\hat{\mathbf{r}}$. In this case, we have to consider the full $\mathbf{K}(\alpha,\mathbf{k},\mathbf{r})$ given by Eq. (16), which is identically zero for $\hat{\mathbf{k}}=-\hat{\mathbf{r}}$. Thus the exact scattering wave function developed from the final state reduces to the CDW (3C) wave function (5) in the full coordinate space for high energies $E$, no matter how this energy is shared between the two final-state electrons.

It is instructive to rewrite the exact $T$-matrix element (1) in an alternative form:

$$T_{fi}=\langle\chi_f^-|V_i|\beta_i\rangle+\langle\chi_f^-|W_f^\dagger|(\Psi_i^+-\beta_i)\rangle. \tag{22}$$

The first amplitude in Eq. (22) is the 3C approximation of Brauner, Briggs, and Klar [1] and the second term contains all higher-order corrections to this approximation since the sum of the two terms is exact. The 3C approximation is obtained from the exact $T$-matrix element (22) by approximating the exact scattering wave function $\Psi_i^+$ by the unperturbed state $\beta_i$ (the Born approximation). In the present approach, $\Psi_i^+$ is approximated by a two-center wave function containing electron-electron correlation. From Eq. (22), we see that this correlation introduces physical effects contained in higher-order terms of a 3C perturbation series. In the following, we discuss in detail three different methods proposed in the literature for including this correlation.

### A. CDW approximation

The CDW approximation was introduced by Cheshire [5] for ion-atom charge exchange and extended to ion-atom ionization by Belkić [13]. In the CDW approximation, the CDW (3C) wave function (5) describes the final state, while the exact scattering wave function in Eq. (1) is approximated by the initial-state CDW wave function [the analog of the 3C wave function (5)]:

$$\Psi_i^+\approx\psi_{\mathbf{k}_i}^+(\mathbf{r}_a)\psi_{1s}(\mathbf{r}_b)C^+(1/k_i,\mu\mathbf{k}_i,\mathbf{r}_{ab})\mu^{-i/k_i}. \tag{23}$$

The factor $\mu^{-i/k_i}$ is needed here so that the wave function (23) asymptotically goes over to the unperturbed initial state (2).

The primary flaw of the CDW initial-state wave function (23) is that it ignores the binding energy of the atomic electron [23] (by treating it as a continuum electron with zero energy when calculating the electron-electron Coulombic-distortion factor). For sufficiently high impact energies, the binding energy can be ignored. For lower energies we found that neglecting binding causes the cross sections corresponding to binary collisions to be grossly overestimated, as one might expect. A possible remedy is to ''bind'' the atomic electron to the nucleus by adding the nuclear mass to the atomic-electron mass when calculating the initial-state Coulombic-distortion factor for the electron-electron interaction. If we do this, we obtain Dewangan's ''two Coulomb waves'' (TCW) wave function [6].

### B. CDW-TCW approximation

Dewangan and Bransden [24], studying proton-hydrogen excitation, showed that the use of the CDW wave function for the initial state almost, but not quite, yields a fully closed second-Born term when the scattering amplitude is evaluated using the Born approximation for the final state. Accordingly, Dewangan [6] proposed a ''two Coulomb waves'' (TCW) approximation for the initial state that does lead to a fully closed second-Born term. For the case of electrons colliding with hydrogen atoms it is given by

$$\Psi_i^+\approx\psi_{\mathbf{k}_i}^+(\mathbf{r}_a)\psi_{1s}(\mathbf{r}_b)C^+(1/k_i,\mathbf{k}_i,\mathbf{r}_{ab}). \tag{24}$$

We label the choice (5), together with the approximation (24), the CDW-TCW approximation (CDW final state, TCW initial state).

We note that the difference between the CDW wave function (23) and Dewangan's wave function (24), is that the latter effectively replaces the two-electron reduced mass $\mu=1/2$ with unity in the electron-electron correlation function of Eq. (23). This is equivalent to adding the nuclear mass to the atomic-electron mass, as discussed above. Thus, in Dewangan's wave function, the relative wave vector between projectile and *atom* determines the extent of electron-electron Coulomb distortion, whereas in the CDW wave function (23) of Cheshire [5], it is the relative wave vector between *two free electrons* that determines this distortion.

### C. CDW-EIS approximation

Crothers [25], using the time-dependent theory, has shown that the CDW initial-state wave function is not properly normalized. (We believe this normalization problem stems from the neglect of atomic binding energy.) To overcome this problem, Crothers and McCann [26] employed the eikonal approximation [7] for the initial state. For electrons colliding with H($1s$), the eikonal approximation to the exact scattering wave function $\Psi_i^+$ is given by

$$\Psi_i^+\approx\tilde{\psi}_{\mathbf{k}_i}^+(\mathbf{r}_a)\psi_{1s}(\mathbf{r}_b)\tilde{C}^+(1/k_i,\mu\mathbf{k}_i,\mathbf{r}_{ab})\mu^{-i/k_i}. \tag{25}$$

Here

$$\tilde{\psi}_{\mathbf{k}}^\pm(\mathbf{r})=\phi_{\mathbf{k}}(\mathbf{r})\tilde{C}^\pm(-1/k,\mathbf{k},\mathbf{r}) \tag{26}$$

is the asymptotic form of a Coulomb wave [Eq. (6)] and

$$\tilde{C}^\pm(\alpha,\mathbf{k},\mathbf{r})=\exp[\mp i\alpha\ln(kr\pm\mathbf{k}\cdot\mathbf{r})] \tag{27}$$

is the asymptotic form of a Coulombic-distortion factor [Eq. (8)]. Since the eikonal approximation affects only the *phase* of the unperturbed wave function (2), there can be no normalization problems. The choice (5), together with the approximation (25), is called the CDW-EIS approximation (CDW final state, eikonal initial state). It has been hugely successful in the case of *ion*-impact ionization of atoms [26–28]. Recently we showed that this approximation leads to considerable improvement over the 3C approximation of Brauner, Briggs, and Klar [1] in the case of *electron*-impact ionization of hydrogen at intermediate energies [4].

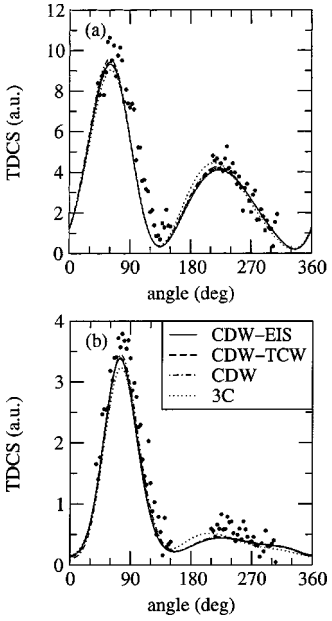


FIG. 1. Scattering-plane triply differential cross section (TDCS) for an impact energy of 250 eV vs the angle (clockwise from forward direction) of the slower (5 eV) electron. Circles are absolute experimental data of Ehrhardt *et al.* [10]. The fixed observation angle (counterclockwise) for the faster electron is (a) 3° or (b) 8°.

## III. RESULTS AND DISCUSSION

We evaluate the scattering amplitude (1) by direct six-dimensional numerical (Gauss-Legendre) quadrature [22]. Spherical coordinates are used for $\mathbf{r}_b$ and cylindrical coordinates are used for $\mathbf{r}_a$, with the $z$ axis taken along the direction of the momentum transfer $\mathbf{q}=\mathbf{k}_i-\mathbf{k}_a$. We estimate that our numerical uncertainty is less than 2% at the peak values.

For the kinematics considered here, the effects of electron exchange are small and are neglected. Therefore we refer to the faster final-state electron as the scattered electron and to the slower final-state electron as the ejected electron. The triply differential cross section (TDCS) measurements [10,11] fix the energy and angle of the scattered electron, thus fixing the energy of the ejected electron which is observed over the full range of experimentally accessible angles in the scattering plane. In the angular distribution of the ejected electrons, two peaks are found: a binary peak centered near the direction of the momentum transfer $\mathbf{q}$ and a recoil peak approximately in the opposite direction.

In order to make a meaningful comparison with the absolute experimental data, it is necessary to understand that there are two independent sources of experimental error—error for the internormalization of data points (for the shape of the angular distribution) and error for the overall normalization of the data points (for putting the relative data on an absolute scale). Experimental TDCS for different angles of the outgoing electrons are internormalized to $\pm 10\%$. TDCS for different energies of the outgoing electrons are *not* internormalized and therefore must be put on an absolute scale independently. For impact energies of 150 and 250 eV, Ehrhardt *et al.* [10] put their relative TDCS on an absolute scale ($\pm 15\%$) by extrapolating the corresponding generalized oscillator strengths to zero momentum transfer and comparing with known photoionization results. The relative TDCS for 54.4-eV impact energy [29], on the other hand, was brought on absolute scale ($\pm 35\%$) directly by measurement [11]. In the first part of this section we study the role of initial-state correlation and in the second part we compare with close-coupling calculations and make a detailed comparison between theory and experiment.

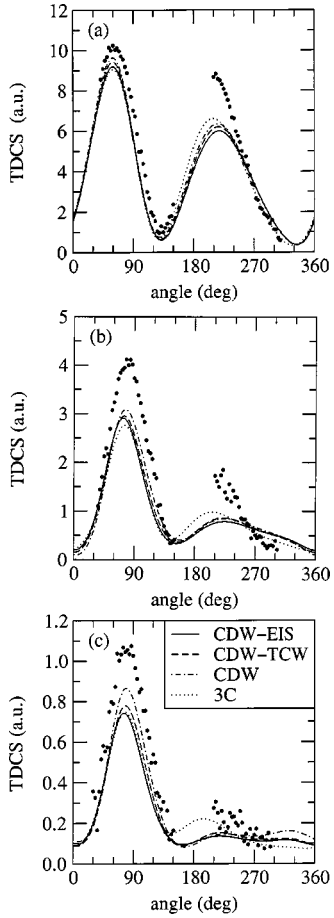


FIG. 2. Scattering-plane triply differential cross section (TDCS) for an impact energy of 150 eV vs the angle (clockwise from forward direction) of the slower (3 eV) electron. The solid circles are absolute experimental data of Ehrhardt *et al.* [10]. The fixed observation angle (counterclockwise) for the faster electron is (a) 4°, (b) 10°, or (c) 16°.

### A. Role of initial-state correlation

The 3C, CDW, CDW-TCW, and CDW-EIS results are compared with the absolute experimental measurements [10] for an impact energy of 250 eV in Fig. 1. The first thing to note from Fig. 1 is that the CDW, CDW-TCW, and CDW-EIS results are nearly identical. All of these calculations have 3C as the first term and involve different approximations for the higher-order terms of a 3C perturbation series. If we assume that these higher-order terms have been *accurately* approximated, then the small differences between these results and the 3C results means that the higher-order terms of a 3C perturbation series are small at 250 eV. Nevertheless, it

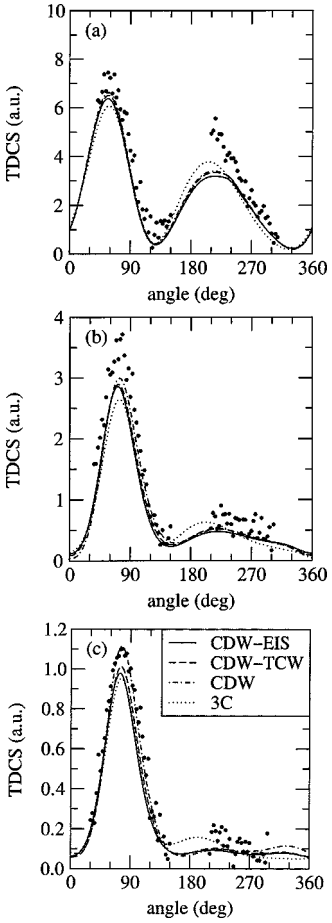


FIG. 3. Same as Fig. 2 for a slow-electron energy of 5 eV.

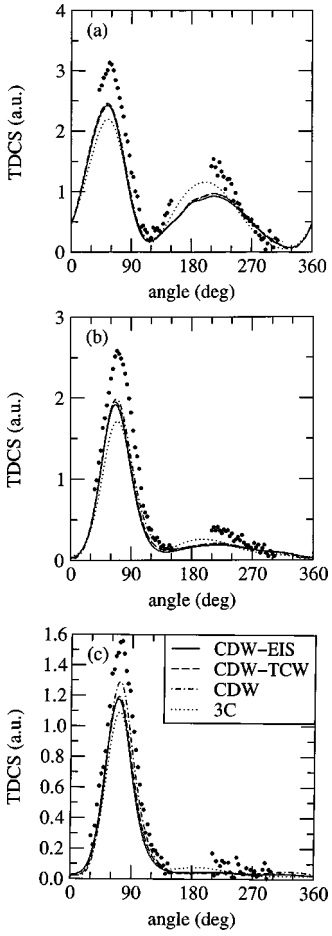


FIG. 4. Same as Fig. 2 for a slow-electron energy of 10 eV.

is seen that the higher order terms increase the magnitude of the binary peak, decrease the magnitude of the recoil peak and shift the recoil peak to a smaller angle between the two outgoing electrons. As we will see, these same effects simply become more pronounced for lower energies.

Figures 2–4 contain the same comparison for 150-eV incident electrons and ejected-electron energies of 3, 5, and 10 eV. At 150-eV impact energy, the CDW-EIS and CDW-TCW results remain very similar but are now more noticeably different from the 3C results, which neglect initial-state correlation. Although the larger binary peak predicted by CDW is in better agreement with the experiment at 150 eV, the following comparison at 54.4 eV strongly suggests that this agreement is fortuitous.

For 54.4-eV incident electrons, similar results are shown in Fig. 5. As the incident energy is lowered, more noticeable differences between the theories become evident. Nevertheless, the general trend of the 3C being smaller for the binary peak, and larger and shifted to larger angles between the electrons for the recoil peak remains. At this energy, it is clearly seen that the position of the recoil peak as predicted using the higher-order terms of a 3C perturbation series is in better accord with experiment than that predicted by the first term. When the higher-order calculations are compared, it is seen that the magnitude of the binary peak predicted by the CDW calculation is much too large as compared to experiment [11], particularly for larger momentum transfer. This is because the CDW approximation, as discussed in the previous section, neglects the binding energy of the atomic electron. Overall, CDW-EIS is in best accord with the absolute experimental data [11] at 54.4 eV. Therefore we use CDW-EIS in the following detailed comparison with close-coupling calculations and experiment.

### B. Comparison with close-coupling results

The CDW-EIS results are compared with a very recent convergent close-coupling (CCC) calculation [9], labeled CCC99, for 250-eV incident electrons in Fig. 6. It is seen that the two very different approaches yield almost identical results and that where experiment [10] and theory differ, the two theories are in better agreement with each other than with experiment. The CCC results should be accurate if a sufficient number of terms are included in the expansion of the wave function and the CDW-EIS results should be accurate if the important physical effects are included to all contributing orders of perturbation theory. As described in the theory section, the CDW-EIS calculation contains contributions from all orders of a perturbation series that has the 3C approximation as the first term. When a close-coupling calculation and a perturbation series calculation yield the same results, this suggests that the close-coupling calculation has included a sufficient number of terms in the expansion of the

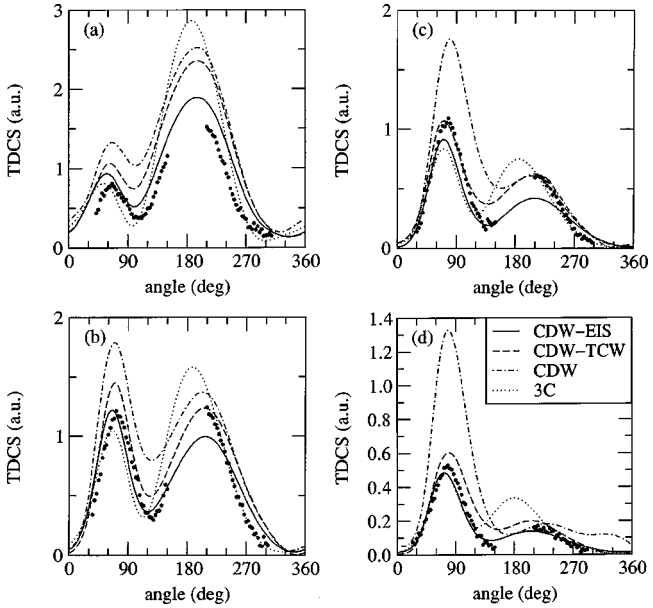


FIG. 5. Scattering-plane triply differential cross section (TDCS) for an impact energy of 54.4 eV vs the angle (clockwise from forward direction) of the slower (5 eV) electron. Circles are absolute experimental data of Ehrhardt and Röder [11]. The fixed observation angle (counterclockwise) for the faster electron is (a) 4°, (b) 10°, (c) 16°, or (d) 23°.

wave function and the perturbation series has the important physical effects contained to all contributing orders. The closeness of the present CDW-EIS and CCC calculations thus strongly suggests that theory has converged and both

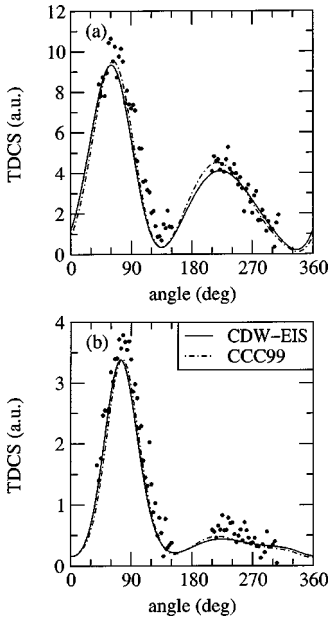


FIG. 6. Scattering-plane triply differential cross section (TDCS) for an impact energy of 250 eV vs the angle (clockwise from forward direction) of the slower (5 eV) electron. The solid circles are absolute experimental data of Ehrhardt *et al.* [10]. The calculations labeled CCC99 are from Bray [9]. The fixed observation angle (counterclockwise) for the faster electron is (a) 3° or (b) 8°.

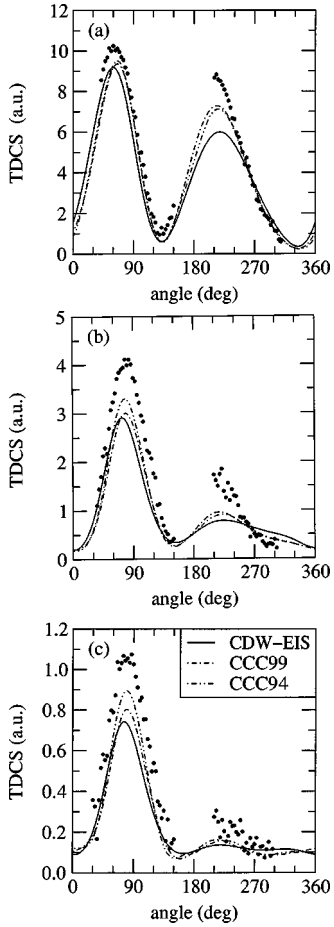


FIG. 7. Scattering-plane triply differential cross section (TDCS) for an impact energy of 150 eV vs the angle (clockwise from forward direction) of the slower (3 eV) electron. The solid circles are absolute experimental data of Ehrhardt *et al.* [10]. The calculations labeled CCC99 are from Bray [9] and those labeled CCC94 are from Bray *et al.* [8]. The fixed observation angle (counterclockwise) for the faster electron is (a) 4°, (b) 10°, or (c) 16°.

results are accurate. Following this logic, one would conclude that theory is probably more accurate than the experiment at this energy.

For 150-eV incident electrons (Figs. 7–9), the present CDW-EIS results are compared with two different CCC calculations. The older results, labeled CCC94 [8], incorporated higher target orbital angular momentum than that used within the close-coupling equations. The newer CCC99 calculations [9], which are believed to be more accurate, are based only on the target angular momentum actually retained in these equations. From Figs. 7–9, it is seen that the CCC99 calculations are in significantly better agreement with the CDW-EIS results than the CCC94 calculations, which are as much as 23% larger than CCC99 for the binary peak.

Although the agreement between CDW-EIS and CCC99 is excellent at 150 eV, the agreement between theory and experiment does not appear so good, and a more careful analysis is needed. In Tables I–III, we have listed the heights of the experimental [10] and theoretical (CDW-EIS and CCC99) binary peaks at 150 eV as well as the ratio of each theory to experiment at these peaks. This ratio is just the

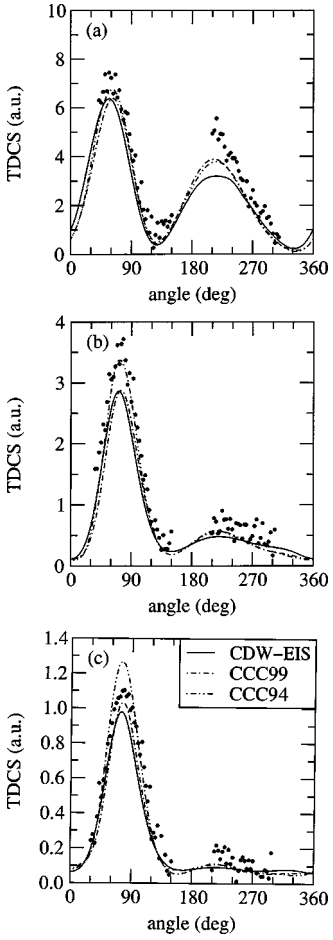


FIG. 8. Same as Fig. 7 for a slow-electron energy of 5 eV.

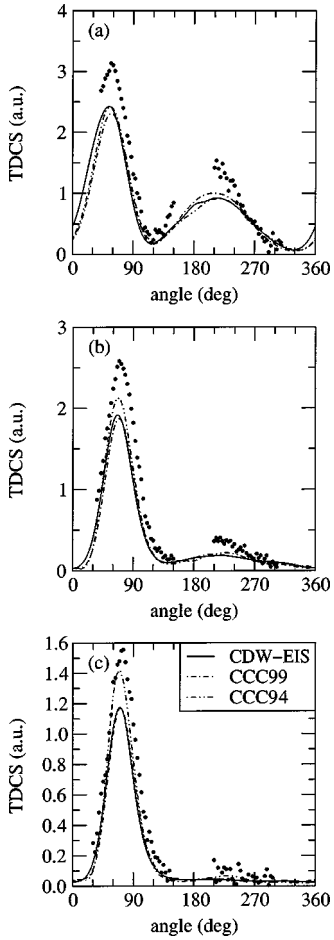


FIG. 9. Same as Fig. 7 for a slow-electron energy of 10 eV.

scaling factor that experiment would need to be multiplied by to agree with the theory for the height of the binary peak. From Table I (ejected electrons with an energy of 3 eV), the scaling factors for CCC99 are 0.91, 0.73, and 0.75 for scattering angles of 4°, 10°, and 16°, respectively. The median of these three scaling factors is 0.82 (18% less than unity) and the range of deviation about this median value is $\pm 0.09$, which is $\pm 11\%$ of the median value. Thus, as far as CCC99 is concerned, the overall normalization of experiment is 18% too large and the internormalization error is 11%. These errors are just slightly outside the experimental limits of 15 and 10 %, respectively and therefore we would argue that CCC99 is in quantitative agreement with the experimental binary peak for an impact energy of 150 eV and an ejected-electron energy of 3 eV. Making the same analysis for CDW-EIS, we get scaling factors of $0.80 \pm 0.10$ ($\pm 12\%$); that is, a 20% overall error and a 12% relative error, which is very similar to what CCC99 predicts.

Now we should also include the recoil peak in the above analysis; however, in Fig. 7(b), the experimental recoil peak is about a factor of 2 larger than theory, which is clearly well outside acceptable limits. Nevertheless, in this case there is very good agreement between CDW-EIS and CCC99 and therefore we believe theory is more accurate than experiment. Furthermore, at 150 eV, the recoil data is rather noisy for the larger scattering angles and therefore would require smoothing to sensibly determine the necessary scaling factors.

The largest difference between CCC99 and CDW-EIS for 150-eV impact energy lies in the recoil peak for an ejected-electron energy of 3 eV and a scattering angle of 4° [Fig. 7(a)], where the CCC results are larger and closer to the experimental data. It is odd that the two theories should disagree for this particular case since an eikonal approximation would be expected to be most accurate for small scattering angles. Nevertheless, CDW-EIS is smaller relative to experi-

TABLE I. Comparison of the present CDW-EIS results, the CCC99 results [9], and experiment (expt.) [10] for an impact energy of 150 eV and an ejected-electron energy of 3 eV for scattering angles of 4°, 10°, and 16°. The data are experimental and theoretical values for the height of the binary peak in atomic units and the ratio of theory to experiment at this peak.

| | 4° | 10° | 16° |
|---|---|---|---|
| CDW-EIS | 9.18 | 2.91 | 0.74 |
| CCC99 | 9.36 | 3.01 | 0.80 |
| Expt. | 10.24 | 4.12 | 1.07 |
| (CDW-EIS)/(expt.) | 0.90 | 0.71 | 0.69 |
| (CCC99)/(expt.) | 0.91 | 0.73 | 0.75 |

TABLE II. Same as Table I for an ejected-electron energy of 5 eV.

| | 4° | 10° | 16° |
|---|---|---|---|
| CDW-EIS | 6.37 | 2.86 | 0.98 |
| CCC99 | 6.39 | 2.87 | 1.03 |
| Expt. | 7.45 | 3.72 | 1.10 |
| (CDW-EIS)/(expt.) | 0.86 | 0.77 | 0.89 |
| (CCC99)/(expt.) | 0.86 | 0.77 | 0.94 |

ment by about the same amount here as it is for the binary peak of Fig. 7(c). This means that the preceding error analysis, which only included binary peaks, would be unaffected if the recoil peak of Fig. 7(a) were also included in the analysis.

For 5-eV ejection energy (Fig. 8 and Table II) we obtain scaling factors of $0.86\pm0.08$ ($\pm7\%$) for CCC99 and $0.83\pm0.06$ ($\pm7\%$) for CDW-EIS. At this point we should mention that it is not strictly necessary to take the median scaling factor as the overall scaling factor that determines the difference between theory and experiment for the overall normalization. One can take the largest or smallest scaling factor, or anything inbetween. For example, in the above case of CDW-EIS, the scaling factors may be written as $0.86\pm0.09$ ($\pm10\%$) rather than $0.83\pm0.06$ ($\pm7\%$). As a result, both CCC99 and CDW-EIS are within the stated experimental uncertainties for ejected electrons with an energy of 5 eV. Unless stated otherwise, however, the median scaling factor, which minimizes the internormalization error, will be used.

For 10-eV ejected electrons (Fig. 9 and Table III), we obtain scaling factors of $0.74\pm0.01$ ($\pm1\%$) for CCC99 and $0.76\pm0.01$ ($\pm1\%$) for CDW-EIS. Thus, CCC99 and CDW-EIS predict that the experimental data is 26% and 24% too large, respectively, which is now fairly large compared to the stated experimental uncertainty of 15%. The closeness of the two theories suggests, however, that theory is more accurate than the experiment and therefore we believe that the overall experimental normalization is about 25% too large for 10-eV ejected electrons.

Figure 10 compares the present CDW-EIS results with the two CCC calculations and the absolute experimental data [11] for 54.4-eV incident electrons. The newer CCC99 results do not exhibit the double recoil peak structure that was present in CCC94. The binary peaks exhibit the same behavior for 54.4 eV as was seen for the higher energies, with CCC94 larger than CCC99 (as much as 29%) and with

TABLE III. Same as Table I for an ejected-electron energy of 10 eV.

| | 4° | 10° | 16° |
|---|---|---|---|
| CDW-EIS | 2.42 | 1.91 | 1.17 |
| CCC99 | 2.31 | 1.87 | 1.17 |
| Expt. | 3.13 | 2.58 | 1.56 |
| (CDW-EIS)/(expt.) | 0.77 | 0.74 | 0.75 |
| (CCC99)/(expt.) | 0.74 | 0.72 | 0.75 |

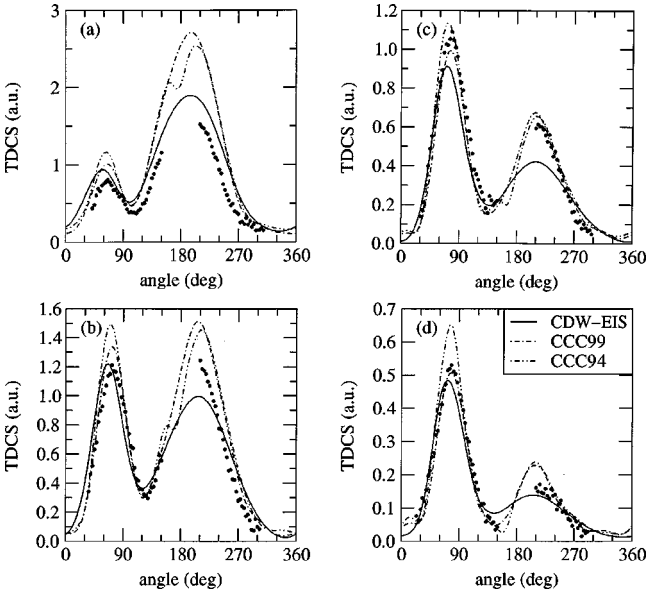


FIG. 10. Scattering-plane triply differential cross section (TDCS) for an impact energy of 54.4 eV vs the angle (clockwise from forward direction) of the slower (5 eV) electron. The solid circles are absolute experimental data of Ehrhardt and Röder [11]. The calculations labeled CCC99 are from Bray [9] and those labeled CCC94 are from Bray *et al.* [8]. The fixed observation angle (counterclockwise) for the faster electron is (a) 4°, (b) 10°, (c) 16°, or (d) 23°.

CCC99 much closer to CDW-EIS. The difference between CCC99 and CDW-EIS at the binary peak is less than 10% in all cases. The recoil peak is a bit of a mixed bag. CDW-EIS is consistently smaller (about 35%) than CCC99 and in half the cases, CDW-EIS is in better agreement with experiment and in the other half CCC99 is in better agreement. These results are summarized in Table IV. Using the binary data *only* gives scaling factors of $1.00\pm0.16$ ($\pm16\%$) for CDW-EIS and $1.08\pm0.17$ ($\pm16\%$) for CCC99. Clearly, both theories are well within the overall normalization uncertainty of 35%. Both theories, however, predict that the internormalization error is 16%, rather than 10%. If we include the recoil data as well, we get scaling factors of $0.95\pm0.25$ ($\pm26\%$) for CDW-EIS and $1.30\pm0.39$ ($\pm30\%$) for CCC99. Note that for scattering angles of 4° and 10°, the center of the recoil peak was not accessible in the experiment and therefore we compare theory and experiment at the angle (210° in both cases) where the experimental recoil data is the largest. Now both theories predict that the internormalization error is considerably larger than the experimental estimate of 10%. Furthermore, agreement between the two theories is poor for the height of the recoil peak. For these reasons, we believe it is more reasonable to assume that the experiment is more accurate than either theory for the relative size of the peaks (height of the recoil peak relative to the height of the binary peak). If this is indeed the case, then CDW-EIS is underestimating the recoil peak relative to the binary peak by about 20% for scattering angles of 10° and 16°, while CCC99 is overestimating the same by about 36% for 4°, 20% for 16°, and 47% for 23°.

TABLE IV. Comparison of the present CDW-EIS results, the CCC99 results [9], and experiment (expt.) [11] for an impact energy of 54.4 eV and an ejected-electron energy of 5 eV for scattering angles of 4°, 10°, 16°, and 23°. The data are the experimental and theoretical values for the height of the binary (bin) and recoil (rec) peaks in atomic units and the ratio of theory to experiment at these peaks.

| | 4° | | 10° | | 16° | | 23° | |
|---|---|---|---|---|---|---|---|---|
| | bin | rec | bin | rec | bin | rec | bin | rec |
| CDW-EIS | 0.94 | 1.83 | 1.22 | 0.99 | 0.91 | 0.42 | 0.48 | 0.14 |
| CCC99 | 1.01 | 2.58 | 1.34 | 1.51 | 0.99 | 0.67 | 0.51 | 0.24 |
| Expt. | 0.81 | 1.52 | 1.21 | 1.24 | 1.09 | 0.61 | 0.53 | 0.17 |
| (CDW-EIS)/(expt.) | 1.16 | 1.20 | 1.01 | 0.80 | 0.84 | 0.69 | 0.91 | 0.82 |
| (CCC99)/(expt.) | 1.25 | 1.70 | 1.11 | 1.22 | 0.91 | 1.10 | 0.96 | 1.41 |

## IV. SUMMARY AND CONCLUSION

In studies of electron-atom ionization, much of the theoretical effort has naturally focused on the use of asymptotically correct two-center wave functions for the final state, since the simple Born approximation for the initial state already satisfies the asymptotic boundary conditions exactly. On the other hand, the important contributions to the $T$ matrix come from intermediate and close range where electron-electron interactions are significant. From this point of view, one may question the neglect of correlation in the initial channel.

We have examined three different methods of including electron-electron correlation in the initial state. Although all three two-center wave functions are valid high-energy approximations, we found that the use of the eikonal approximation yields the best agreement with experiment for lower energies, just as is observed in the case of ion impact [26]. In our opinion, the CDW-EIS approximation is the most accurate first-order perturbative approach currently available for fast collisions between charged particles and atoms.

The role of initial-state correlation was clearly evident in this work. Including initial-state correlation introduces physical effects contained in higher-order terms of a 3C perturbation series. These higher-order terms increase the magnitude of the binary peak, decrease the magnitude of the recoil peak, and shift the recoil peak to a smaller angle between the two final-state electrons. These effects increase in size with decreasing impact energy and are especially important for impact energies below 100 eV. We note that the above effects of initial-state correlation are opposite those of final-state correlation.

When the CDW-EIS results are compared with the recent CCC99 calculations, it is found that the two theories predict almost identical binary peaks for impact energies of 54.4 eV and higher. At 150 and 250 eV, the recoil peaks are also almost the same except for small ejection energies and small scattering angles for the projectile, where they differ by up to 18%. For an impact energy of 54.4 eV, there is a relatively large difference between the two theories in the recoil peak region and neither theory is in quantitative agreement with the experiment for all scattering angles.

It would be hard to find two theoretical approaches as different as CDW-EIS and CCC. Whereas CDW-EIS is a first-order perturbative approach, CCC is a nonperturbative method and whereas CDW-EIS uses a final-state wave function that satisfies correct asymptotic boundary conditions, the CCC formalism precludes this. For these reasons, we regard the level of agreement between the two theories as encouraging for both theories.

## ACKNOWLEDGMENTS

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