Scaling behavior of the fully differential cross section for ionization of hydrogen atoms by the impact of fast elementary charged particles

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Ionization of hydrogen atoms by the impact of fast charged particles can be accurately treated theoretically using simple two-center wave functions to describe the scattering system both initially and finally. For the final state, we use a continuum distorted wave (CDW) that contains the product of three Coulombic distortion factors (one for each two-body interaction), hence it is called the 3C wave function. This CDW (3C) wave function is ideal for studying fast collisions since it is asymptotically correct in all asymptotic domains of momentum space for all configurations of the three particles in coordinate space [S. Jones and D. H. Madison, Phys. Rev. A **62**, 42 701 (2000)]. Coulomb distortion in the entrance channel is provided by an eikonal initial state (EIS), and this CDW-EIS approximation, introduced by Crothers and McCann [J. Phys. B **16**, 3229 (1983)], has proven to be the most accurate perturbative method ever devised within a two-state approximation. The first fully differential cross sections for ion-atom ionization in the CDW-EIS approximation are presented. In addition, by considering projectiles of different mass and charge, it will be shown that although the charge of the projectile is important, the mass of the projectile plays virtually no role in the vast majority of fast ionizing collisions.

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I. INTRODUCTION

In previous works [1,2], we studied ionization of atomic hydrogen by electron impact using asymptotically correct two-center wave functions to describe the scattering system both initially and finally. Here we use the same theoretical model to study ionization of H(1*s*) by the impact of elementary particles of different mass and charge. In the entrance channel, the Coulomb distortion is provided by an eikonal initial state (EIS) [3–5]. For the final state, we use a continuum distorted wave (CDW) that contains the product of three Coulombic distortion factors [6], hence it is called the 3C wave function. For the case of electrons of impact speed v_i ionizing hydrogen atoms, it has been shown [2] that the Schrödinger equation reduces, to leading order in $1/v_i$ in the full coordinate space, to the eigenequation for the 3C wave function (here, and throughout this work, atomic units are used except where stated otherwise). The above result is also obtained for other projectiles of charge $Z_P = \pm 1$. The case of multiply charged ions as projectiles ($Z_P > 1$) demands special care. We will show below that if the multiply charged ion is fast relative to both the residual target ion and the ionized electron (the dominant mode of ionization at intermediate and higher energies), then the Schrödinger equation reduces, to leading order in $1/v_i$, to the 3C eigenequation. If the initially fast projectile becomes slow relative to either the residual ion or the ionized electron, the Schrödinger equation still reduces to the 3C eigenequation, but to leading order in Z_P/v_i. Thus the 3C wave function is asymptotically correct in all asymptotic domains of *momentum space* for all configurations of the three particles in coordinate space. This result complements that of an earlier work [7], which showed that the 3C wave function is asymptotically correct in all asymptotic domains of *coordinate space* for all configurations of the three particles in momentum space.

Absolute measurements for the fully differential cross section (FDCS) for electron-impact ionization of atomic hydrogen are available at impact energies of 54.4, 150, and 250 eV [8,9], and the collision geometries from these experiments are used for reference in the present study of projectiles of different mass and charge. Although there exists as yet no FDCS measurements for other projectiles in the case of atomic hydrogen as target, recent advances in experimental techniques have rendered such measurements feasible. Indeed, FDCS measurements for ion-impact ionization of helium [10] and positron-impact ionization of molecular hydrogen [11] have been recently reported in the literature.

Here we report fully differential CDW-EIS cross sections for ionization of H(1*s*) by the impact of elementary charged particles. The FDCS provides the most stringent test of theoretical models since the momentum of the projectile, the ionized electron, and the residual target ion is fully determined. Comparison of FDCS for ionization of hydrogen by the impact of electrons and antiprotons, as well as positrons and protons, reveals that the mass of the projectile is not important in fast ionizing collisions (with final projectile speeds greater than 2–3 a.u.) for the dominant case of small momentum transfer to the target. This result extends groundbreaking work by Berakdar, Briggs, and Klar [12], who proposed a scaling law for the FDCS where different projectiles have the same *final* speed. They considered a reference-electron-impact energy of 250 eV and exposed a limitation of their scaling law in that projectile mass effects cannot always be scaled out if the momentum transfer is large, even for very fast projectiles. The 3C approximation [13,14] employed by Berakdar, Briggs, and Klar [12], which uses the CDW (3C) wave function for the final state but neglects distortion of the initial state, is believed to be reasonably accurate for impact energies above about 100 eV for electron or positron impact [14] (200 keV/amu for singly charged ion impact). Here we test the scaling law of Berakdar, Briggs, and Klar [12] against the CDW-EIS approximation, which allows us to consider lower impact energies with confidence, e.g., a reference-electron-impact energy of 54.4 eV, where the validity of CDW-EIS has recently been established [1,2].

To remain consistent with our previous papers on electron impact [1,2], we neglect the mass of an electron relative to the mass of a proton. In this case, the electron-proton reduced mass is unity, the reduced mass μ of the colliding partners (projectile and target *atom*) is identical to the reduced mass of projectile and target *ion*, and the center of mass of the target *atom* coincides with the center of mass of the target *ion*; thus the Jacobi coordinates $(\mathbf{r}_a, \mathbf{r}_b)$, where $\mathbf{r}_a$ $(\mathbf{r}_b)$ refers the projectile (atomic electron) to the target ion, are appropriate to describe the collision process.

II. THEORY

In the distorted-wave formalism, the post form of the exact transition matrix (T matrix) element is given by [15]

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

Here Ψ_i^+ is the exact scattering wave function developed from the initial asymptotic state satisfying exact outgoing-wave $(+)$ boundary conditions, χ_f^- is a distorted wave developed from the final asymptotic state satisfying exact incoming-wave $(-)$ boundary conditions, but is otherwise arbitrary (W_f is the corresponding perturbation), and β_i is the initial asymptotic state (V_i is the corresponding channel interaction).

We now consider the ionization of atomic hydrogen by the impact of a projectile P of mass M_P and charge Z_P. In the center-of-mass (c.m.) system, the initial asymptotic state is given by

$$\beta_i = (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_a) \psi_i(\mathbf{r}_b), \tag{2}$$

and the corresponding channel interaction is

$$V_i = Z_P / r_a - Z_P / r_{ab}, \tag{3}$$

where $\mathbf{k}_i$ is the relative momentum of the incident projectile with respect to the target atom (assumed initially at rest), ψ_i is the wave function for the target atom, and $r_{ab} = |\mathbf{r}_{ab}|$, where $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$.

A. CDW-EIS approximation

For the final state, we use the CDW (3C) wave function [6]

$$\chi_f^- = (2\pi)^{-3} \exp(i\mathbf{k}_a \cdot \mathbf{r}_a + i\mathbf{k}_b \cdot \mathbf{r}_b) C^-(-1/v_b, \mathbf{k}_b, \mathbf{r}_b) \times C^-(Z_P/v_a, \mathbf{k}_a, \mathbf{r}_a) C^-(-Z_P/v_{ab}, \mathbf{k}_{ab}, \mathbf{r}_{ab}). \tag{4}$$

Here $\mathbf{k}_a(\mathbf{k}_b)$ is the final relative momentum of the projectile (ionized electron) with respect to the target ion, $\mathbf{k}_{ab}$ is the final relative momentum of the projectile with respect to the ionized electron, and v_a, v_b, and v_{ab} are the final relative speeds within the projectile–target-ion, electron–target-ion, and projectile-electron subsystems, respectively. Distortion effects of the Coulomb potential are contained in the function

$$C^-(\eta, \mathbf{k}, \mathbf{r}) = N(\eta)\, {}_1F_1(i\eta, 1; -ikr - i\mathbf{k} \cdot \mathbf{r}). \tag{5}$$

Here $\mathbf{r}$ $(\mathbf{k})$ is the relative coordinate (momentum) and η is the Sommerfeld parameter for the two-body subsystem under consideration, ${}_1F_1$ is the confluent hypergeometric function, and $N(\eta) = \Gamma(1 - i\eta)\exp(-\pi\eta/2)$, where Γ is the gamma function.

The perturbation W_f in Eq. (1) is defined by the relation

$$(H - E)\chi_f^- = W_f \chi_f^-, \tag{6}$$

where

$$H = -\frac{1}{2\mu}\nabla^2_{\mathbf{r}_a} - \frac{1}{2}\nabla^2_{\mathbf{r}_b} + \frac{Z_P}{r_a} - \frac{1}{r_b} - \frac{Z_P}{r_{ab}} \tag{7}$$

is the full Hamiltonian (neglecting the total c.m. motion) and

$$E = k_i^2/(2\mu) + \epsilon_i = k_a^2/(2\mu) + k_b^2/2 \tag{8}$$

is the total energy in the c.m. frame, where ϵ_i is the binding energy of the target atom. Substituting χ_f^- (4) into Eq. (6), we obtain

$$W_f = \mathbf{K}_{ab} \cdot (\mathbf{V}_b - \mathbf{V}_a), \tag{9}$$

where

$$\mathbf{V}_a \equiv \mathbf{K}(Z_P/v_a, \mathbf{k}_a, \mathbf{r}_a)/\mu, \tag{10}$$

$$\mathbf{V}_b \equiv \mathbf{K}(-1/v_b, \mathbf{k}_b, \mathbf{r}_b), \tag{11}$$

$$\mathbf{K}_{ab} \equiv \mathbf{K}(-Z_P/v_{ab}, \mathbf{k}_{ab}, \mathbf{r}_{ab}), \tag{12}$$

and where

$$\mathbf{K}(\eta, \mathbf{k}, \mathbf{r}) \equiv \frac{\nabla_{\mathbf{r}} C^-(\eta, \mathbf{k}, \mathbf{r})}{C^-(\eta, \mathbf{k}, \mathbf{r})}. \tag{13}$$

The complex vector function $\mathbf{K}(\eta, \mathbf{k}, \mathbf{r})$ is given explicitly by

$$\mathbf{K}(\eta, \mathbf{k}, \mathbf{r}) = \eta k \left[\frac{{}_1F_1(1 + i\eta, 2; -ikr - i\mathbf{k} \cdot \mathbf{r})}{{}_1F_1(i\eta, 1; -ikr - i\mathbf{k} \cdot \mathbf{r})} \right] (\hat{\mathbf{k}} + \hat{\mathbf{r}}), \tag{14}$$

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

For the exact scattering wave function Ψ_i^+ in Eq. (1) we make the eikonal approximation [3],

$$\Psi_i^+ \approx (2\pi)^{-3/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_a) \psi_i(\mathbf{r}_b) \times \exp\left[i\frac{Z_P}{v_i} \ln\left(\frac{v_i r_a - \mathbf{v}_i \cdot \mathbf{r}_a}{v_i r_{ab} - \mathbf{v}_i \cdot \mathbf{r}_{ab}} \right) \right]. \tag{15}$$

Here $\mathbf{v}_i = \mathbf{k}_i / \mu$ is the velocity of the incident particle with respect to the target. The choice (4), together with the approximation (15), is the CDW-EIS [CDW (3C) final state and eikonal initial state] approximation [5,1]. The 3C approximation [13,14], which neglects projectile-target interactions in the initial state, may be obtained from the CDW-EIS approximation by replacing Z_P with zero in Eq. (15). If we further neglect projectile-target interactions in the final state by replacing Z_P with zero in χ_f^- (4), we obtain the first Born approximation (FBA).

B. Fully differential cross section and scaling law

The FDCS for the process

$$P+\mathrm{H}(1s)\rightarrow P+\mathrm{H}^+ + \mathrm{e}^- \tag{16}$$

is given in the c.m. frame by [16]

$$\frac{d^5\sigma}{d\Omega_a d\Omega_b dE_b}=(2\pi)^4\mu^2\frac{v_a v_b}{v_i}|T_{fi}|^2. \tag{17}$$

Here $E_b=k_b^2/2$ is the energy of the ionized electron and Ω_b (Ω_a) is the solid angle for the ionized electron (projectile). In this work, we calculate the FDCS in the scattering plane as a function of the angle between $\mathbf{k}_b$ and $\mathbf{q}$ for fixed $\mathbf{q}$ and $|\mathbf{k}_b|$, where $\mathbf{q}=\mathbf{k}_i-\mathbf{k}_a$ is the momentum transferred from the projectile to the target atom and $\hat{\mathbf{q}}=\mathbf{q}/|\mathbf{q}|$ is our quantization axis.

From the analytic properties of the FDCS in the FBA, it can be seen that both $\mathbf{q}$ and $\mathbf{k}_b$ should be the same when comparing the impact of different projectiles. In addition, we scale the FDCS for the projectile P to that of some reference projectile P' (reduced mass μ', charge $Z_{P'}$) such that, in the FBA, the scaled FDCS for the projectile P is the same as the FDCS for the reference projectile P':

$$\frac{d^5\sigma_{\mathrm{scaled}}}{d\Omega_a d\Omega_b dE_b}=\frac{v_i v_{a'}}{v_{i'} v_a}\left(\frac{\mu' Z_{P'}}{\mu Z_P}\right)^2\frac{d^5\sigma}{d\Omega_a d\Omega_b dE_b}. \tag{18}$$

Furthermore, following Berakdar, Briggs, and Klar [12], we take both projectiles to have the same final speed; thus $v_a = v_{a'}$. Then, assuming the collision geometry for the reference projectile P' is known, the (c.m.) collision energy $E_i = k_i^2/(2\mu)$ for the projectile P is given by energy conservation,

$$E_i=(\mu/\mu')E_{i'}-(\mu/\mu'-1)(E_b-\epsilon_i), \tag{19}$$

where $E_{i'}=k_{i'}^2/(2\mu')$ is the collision energy for the reference projectile P'. The c.m. scattering angle for the projectile P, $\theta_a=\cos^{-1}(\hat{\mathbf{k}}_a\cdot\hat{\mathbf{k}}_i)$, can be found from the law of cosines,

$$q^2=k_i^2+k_a^2-2k_ik_a\cos\theta_a. \tag{20}$$

Then the momentum transfer direction $\theta_q=\cos^{-1}(\hat{\mathbf{q}}\cdot\hat{\mathbf{k}}_i)$ is determined from the law of sines, $q\sin\theta_q=k_a\sin\theta_a$. In the following, we take the reference projectile P' to be an electron. In this case, $\mu'=1$ and Eq. (19) reduces to the corresponding equation in Berakdar, Briggs, and Klar [12]. Finally, we note that it is not always possible to make both $\mathbf{q}$ and $\mathbf{k}_b$ the same for projectiles differing in mass since the range of allowed values of q is mass dependent. For the electron-impact collision geometries considered by Ehrhardt and co-workers [8,9] at impact energies of 54.4, 150, and 250 eV, there is one case (impact energy 54.4 eV, ejected-electron energy of 5 eV, and scattering angle of 4°) where the momentum transfer for electron impact is smaller than the minimum momentum transfer in the case of ion impact. Thus, no comparison is made for this case, which is not so important since, as we will see, mass effects can no longer be scaled out for this low value of impact energy.

C. Asymptotic domains of momentum space

We now investigate the validity of the CDW (3C) final-state wave function in different asymptotic domains of momentum space. Before the various possibilities are considered, we first obtain some necessary limiting values.

The maximum magnitude of the function $\mathbf{K}(\eta,\mathbf{k},\mathbf{r})$, given by Eq. (14), is of the order of $|\eta k|$, i.e., $O(|\eta k|)$, since the ratio of confluent hypergeometric functions (the square-bracketed term) in Eq. (14) is of order unity for small values of $kr+\mathbf{k}\cdot\mathbf{r}$, where the magnitude of $\mathbf{K}(\eta,\mathbf{k},\mathbf{r})$ is maximum. Thus

$$|\mathbf{K}(\eta,\mathbf{k},\mathbf{r})|_{\max}=O(|\eta k|). \tag{21}$$

We note that ηk is finite even if k is infinite. We also need to know the asymptotic behavior of $\mathbf{K}(\eta,\mathbf{k},\mathbf{r})$ for $k\rightarrow\infty$ at any fixed value of $r\neq 0$. Using

$$C^-(\eta,\mathbf{k},\mathbf{r})\underset{kr+\mathbf{k}\cdot\mathbf{r}\rightarrow\infty}{\widetilde{\quad}}(kr+\mathbf{k}\cdot\mathbf{r})^{-i\eta} \tag{22}$$

and Eq. (13), it is easily shown that

$$\mathbf{K}(\eta,\mathbf{k},\mathbf{r})\underset{kr+\mathbf{k}\cdot\mathbf{r}\rightarrow\infty}{\widetilde{\quad}}-\frac{i\eta}{r}\left[\frac{\hat{\mathbf{k}}+\hat{\mathbf{r}}}{1+\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}}\right]. \tag{23}$$

Now if $k\rightarrow\infty$, then $kr+\mathbf{k}\cdot\mathbf{r}\rightarrow\infty$, unless $\hat{\mathbf{k}}=-\hat{\mathbf{r}}$. In this case, Eq. (23) is not valid and Eq. (14) has to be used instead, giving $\mathbf{K}(\eta,\mathbf{k},\mathbf{r})\equiv 0$ for $\hat{\mathbf{k}}=-\hat{\mathbf{r}}$. Thus

$$|\mathbf{K}(\eta,\mathbf{k},\mathbf{r})|=O(|\eta|)\quad\text{for}\quad k\rightarrow\infty\quad\text{at fixed}\quad r. \tag{24}$$

For ionization of atomic hydrogen by charged-particle impact, the final state consists of three charged particles in the continuum. Consequently, there are four asymptotic domains of momentum space (regions where at least two of the particles have large relative speed). We define these regions as follows:

$$\mathcal{R}_0:\ v_a\rightarrow\infty,\ v_b\rightarrow\infty,\ v_{ab}\rightarrow\infty,$$

$$\mathcal{R}_a:\ 0\leqslant v_a<\infty,\ v_b\rightarrow\infty,\ v_{ab}\rightarrow\infty,$$

$$\mathcal{R}_b:\ 0\leqslant v_b<\infty,\ v_a\rightarrow\infty,\ v_{ab}\rightarrow\infty,$$

$$\mathcal{R}_{ab}:\ 0\leqslant v_{ab}<\infty,\ v_a\rightarrow\infty,\ v_b\rightarrow\infty.$$

In order to investigate the validity of the 3C wave function in all these asymptotic domains, we consider the following high-energy ansatz for the exact scattering wave function developed from the final asymptotic state,

$$\Psi_f^- = \exp(i\mathbf{k}_a\cdot\mathbf{r}_a + i\mathbf{k}_b\cdot\mathbf{r}_b)A(\mathbf{r}_a)B(\mathbf{r}_b)C(\mathbf{r}_{ab}). \tag{25}$$

Substituting the ansatz (25) into the Schrödinger equation, $(H-E)\Psi_f^-=0$, we obtain the following equation for A, B, and C,

$$\frac{1}{A}\left[-\frac{1}{2\mu}\nabla^2_{\mathbf{r}_a} - i\mathbf{v}_a\cdot\boldsymbol{\nabla}_{\mathbf{r}_a} + \frac{Z_P}{r_a}\right]A + \frac{1}{B}\left[-\frac{1}{2}\nabla^2_{\mathbf{r}_b} - i\mathbf{v}_b\cdot\boldsymbol{\nabla}_{\mathbf{r}_b} - \frac{1}{r_b}\right]B + \frac{1}{C}\left[-\frac{1}{2\mu_{ab}}\nabla^2_{\mathbf{r}_{ab}} - i\mathbf{v}_{ab}\cdot\boldsymbol{\nabla}_{\mathbf{r}_{ab}} - \frac{Z_P}{r_{ab}}\right]C = \left[\frac{1}{\mu}\frac{\boldsymbol{\nabla}_{\mathbf{r}_a}A}{A} - \frac{\boldsymbol{\nabla}_{\mathbf{r}_b}B}{B}\right]\cdot\frac{\boldsymbol{\nabla}_{\mathbf{r}_{ab}}C}{C}. \tag{26}$$

Here μ_{ab} is the reduced mass of projectile and atomic electron. Since the confluent hypergeometric function satisfies the partial-differential equation

$$\left(-\frac{1}{2m}\nabla^2 - i\mathbf{v}\cdot\boldsymbol{\nabla} + \frac{\eta v}{r}\right)\,{}_1F_1(i\eta,1;-ikr-i\mathbf{k}\cdot\mathbf{r})=0, \tag{27}$$

where $\mathbf{k}=m\mathbf{v}$ (only the incoming-wave solution is shown), we can make the left-hand side of Eq. (26) vanish identically by choosing

$$A={}_1F_1(iZ_P/v_a,1;-ik_ar_a-i\mathbf{k}_a\cdot\mathbf{r}_a), \tag{28}$$

$$B={}_1F_1(-i/v_b,1;-ik_br_b-i\mathbf{k}_b\cdot\mathbf{r}_b), \tag{29}$$

$$C={}_1F_1(-iZ_P/v_{ab},1;-ik_{ab}r_{ab}-i\mathbf{k}_{ab}\cdot\mathbf{r}_{ab}). \tag{30}$$

The above choice for A, B, and C gives the CDW (3C) wave function (4). The problem now is to estimate the effect of neglecting the right-hand side of Eq. (26).

Considering first the asymptotic domains $\mathcal{R}_0$, $\mathcal{R}_a$, and $\mathcal{R}_b$, where $v_{ab}\to\infty$, we write Eq. (26) as a partial-differential equation for C. That is, we take A to be given by Eq. (28) and B to be given by Eq. (29), but leave C arbitrary for the moment. Then we obtain the following equation for C,

$$\left[-\frac{1}{2\mu_{ab}}\nabla^2_{\mathbf{r}_{ab}} - (i\mathbf{v}_{ab}+\mathbf{V}_a-\mathbf{V}_b)\cdot\boldsymbol{\nabla}_{\mathbf{r}_{ab}} - \frac{Z_P}{r_{ab}}\right]C=0, \tag{31}$$

where $\mathbf{V}_a$ is given by Eq. (10) and $\mathbf{V}_b$ is given by Eq. (11). The 3C eigenequation is obtained by neglecting $\mathbf{V}_a$ and $\mathbf{V}_b$. Now V_a and V_b are negligible relative to $v_{ab}\to\infty$, since both are bounded in the entire coordinate space, see Eq. (21). Thus the Schrödinger equation reduces to the eigenequation for the 3C wave function in the asymptotic domains where $v_{ab}\to\infty(\mathcal{R}_0,\mathcal{R}_a,\mathcal{R}_b)$.

More precisely, in $\mathcal{R}_0$, we can use Eq. (24) to estimate the magnitudes of $\mathbf{V}_a$ and $\mathbf{V}_b$, since both v_a and v_b go to infinity in $\mathcal{R}_0$. Thus, $V_a=O(|Z_P/\mu|/v_i)$ and $V_b=O(1/v_i)$. Now $|Z_P|$ can be greater than 1 only for a *heavy* projectile (a multiply charged ion) and then μ is at least of the order of a thousand atomic units (much larger than any physically realizable $|Z_P|$). For a light projectile (electron or positron), $|Z_P/\mu|=1$. Thus the parameter $|Z_P/\mu|$ is never larger than unity for any real charged particle colliding with a real atom (we exclude, for example, a target "atom" of positronium). As a result, V_a vanishes at least as fast as V_b, so the relevant quantity is the magnitude $V_b=O(1/v_i)$ *relative to* $v_{ab}=O(v_i)$. Thus the Schrödinger equation reduces, to leading order in $1/v_i^2$, to the 3C eigenequation in $\mathcal{R}_0$.

In $\mathcal{R}_a$, v_a can be small, so we have to use Eq. (21) to estimate the magnitude of $\mathbf{V}_a$. We obtain $V_a=O(|Z_P|)$. Since $V_b=O(1/v_i)$ is smaller than V_a, the validity of the 3C wave function is determined by the magnitude $V_a=O(|Z_P|)$ relative to $v_{ab}=O(v_i)$. Thus the Schrödinger equation reduces, to leading order in $|Z_P/v_i|$, to the 3C eigenequation in $\mathcal{R}_a$.

Since the vast majority of ionizing collisions involve small momentum transfer to the target, the most important asymptotic region of momentum space is $\mathcal{R}_b$. Here $v_a\to\infty$, so we use Eq. (24) to obtain $V_a=O(|Z_P/\mu|/v_i)$. Since v_b can be small, we use Eq. (21) to estimate the magnitude of $\mathbf{V}_b$, obtaining $V_b=O(1)$. Since V_a is smaller than V_b, the validity of the 3C wave function is determined by the magnitude $V_b=O(1)$ relative to $v_{ab}=O(v_i)$. Thus the Schrödinger equation reduces, to leading order in $1/v_i$, to the 3C eigenequation in $\mathcal{R}_b$.

Finally, in the asymptotic domain $\mathcal{R}_{ab}$, where v_{ab} can be small, we return to the ansatz (25), take C to be given by Eq. (30), and write Eq. (26) as a partial-differential equation for A and B,

$$\frac{1}{A}\left[-\frac{1}{2\mu}\nabla^2_{\mathbf{r}_a} - (i\mathbf{v}_a+\mathbf{K}_{ab}/\mu)\cdot\boldsymbol{\nabla}_{\mathbf{r}_a} + \frac{Z_P}{r_a}\right]A + \frac{1}{B}\left[-\frac{1}{2}\nabla^2_{\mathbf{r}_b} - (i\mathbf{v}_b-\mathbf{K}_{ab})\cdot\boldsymbol{\nabla}_{\mathbf{r}_b} - \frac{1}{r_b}\right]B=0, \tag{32}$$

where $\mathbf{K}_{ab}$ is given by Eq. (12). The 3C eigenequation is obtained by neglecting $\mathbf{K}_{ab}$. In $\mathcal{R}_{ab}$, K_{ab} is $O(|Z_P|)$ while both v_a and v_b are $O(v_i)$. The contribution from the largest neglected term is thus $O(|Z_P/v_i|)$ and, therefore, the Schrödinger equation reduces, to leading order in $|Z_P/v_i|$, to the 3C eigenequation in $\mathcal{R}_{ab}$.

Summarizing the above results, we investigated the validity of the CDW (3C) final-state wave function (4) for large total energy E. We found that the Schrödinger equation re duces, to leading order in $|Z_P/v_i|$ in the full coordinate space, to the eigenequation for the 3C wave function if the projectile of charge Z_P with an initial speed v_i becomes slow relative to either the ionized electron or the residual target ion. On the other hand, if the projectile remains fast relative to both target fragments, the neglected contribution is just $O(1/v_i)$ and if, in addition, the target fragments are fast relative to *each other*, the neglected contribution is only $O(1/v_i^2)$. Thus the 3C wave function is asymptotically correct in all asymptotic domains of momentum space for all configurations of the three particles in coordinate space.

III. RESULTS

We evaluate the scattering amplitude (1) by direct six-dimensional numerical (Gauss-Legendre) quadrature [17]. 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 $\mathbf{q}$. We estimate that our numerical uncertainty is 2% at the peak values in the fully differential cross sections (FDCS).

A. Preliminary considerations

In the case of electron-impact ionization of atomic hydrogen, the projectile is indistinguishable from the atomic electron and, therefore, an exchange amplitude should be included when calculating the cross section. However, test calculations revealed that the exchange contribution is less than 2% at the higher energies (150 and 250 eV). At 54.4 eV, exchange reduces the FDCS uniformly by about 10%. In the preceding section, we showed that the 3C wave function is correct to leading order in $1/v_i$, regardless of how close the three particles are. For 54.4-eV impact energy, $v_i=2$, so the 3C wave function is not accurate if all three particles are close together. In the case of direct ionization, this should not be a major problem, since most of the contribution to the direct amplitude comes from large separations between the projectile and the target. On the other hand, most of the contribution to the exchange amplitude comes from small separations between projectile and target and, therefore, at 54.4 eV, the 3C and CDW-EIS exchange amplitudes are probably just order-of-magnitude estimates of the exact exchange amplitude. Finally, our numerical method is not well suited to the calculation of the exchange amplitude, since the ejection of a fast electron means a highly oscillatory integrand, necessitating a huge increase in computation time. Since the exchange amplitude is small, hard to calculate, and may not even improve the theory, we neglect it.

It is also of interest to discuss the relative importance of the two terms in Eq. (1). Although the sum of these two terms is the direct amplitude for ionization, neither term individually has strong physical meaning, since the sole purpose of the second term is to remove the double counting of interactions that occurs in the first term. Nevertheless, we find it interesting that the squared modulus of either term is typically an order of magnitude larger than the squared modulus of their sum.

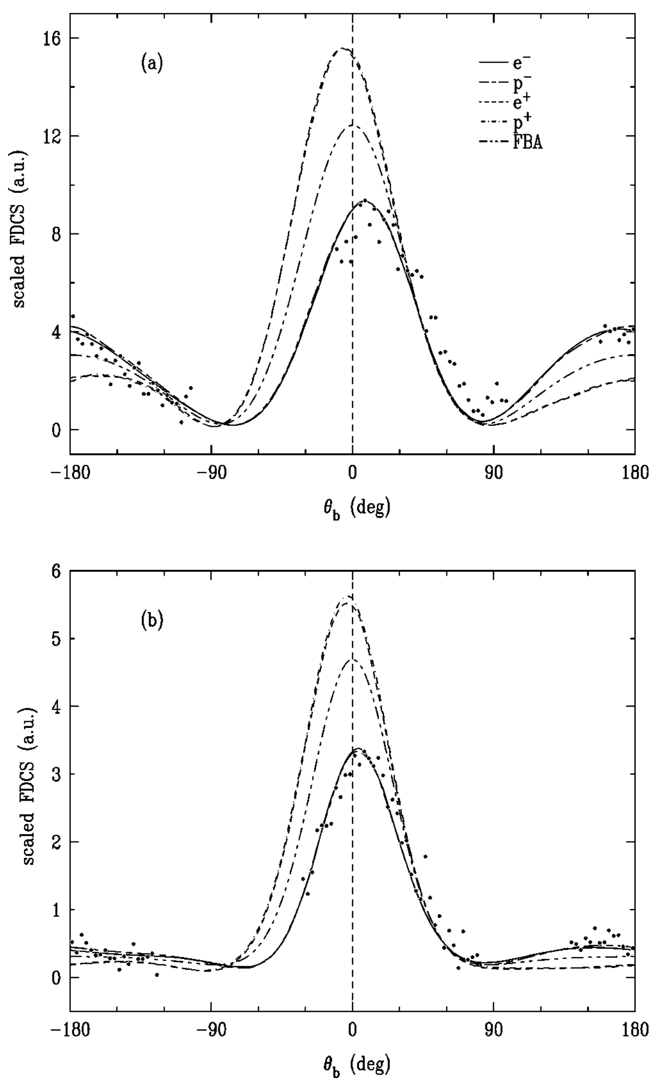

FIG. 1. Scattering-plane fully differential cross sections (FDCS) in the center-of-mass (c.m.) coordinate system for ionization of H(1s) by the impact of electrons (e^-), protons (p^+), and their antiparticles in the CDW-EIS approximation. For the heavy projectiles ($p^\pm$), the FDCS are scaled using Eq. (18). The (c.m.) collision energy is 250 eV (212 keV) for $e^\pm$ ($p^\pm$) and all projectiles have the same *final* speed. The energy of the ionized electron is 5 eV and θ_b is the polar angle of the ionized electron relative to the momentum-transfer direction (θ_b negative corresponds to both the projectile and the ionized electron emerging in the same half plane). The c.m. scattering angle of the projectile is: (a) 3° for $e^\pm$ (3.29×10^{-3} deg for $p^\pm$) and (b) 8° (8.86×10^{-3} deg). Also shown is the first Born approximation (FBA), which yields the same scaled FDCS for all projectile impacts, and absolute electron-impact measurements (solid circles) from Ehrhardt *et al.* [8], multiplied by a factor of 0.88.

B. Fully differential cross sections

FDCS measurements for electron impact [8] characteristically have two maxima with the one near 0° (relative to the direction of momentum transfer) being referred to as the binary peak since 0° is the angle that a stationary atomic electron would emerge after a single collision with the projectile. The peak near 180° is called the recoil peak since it results

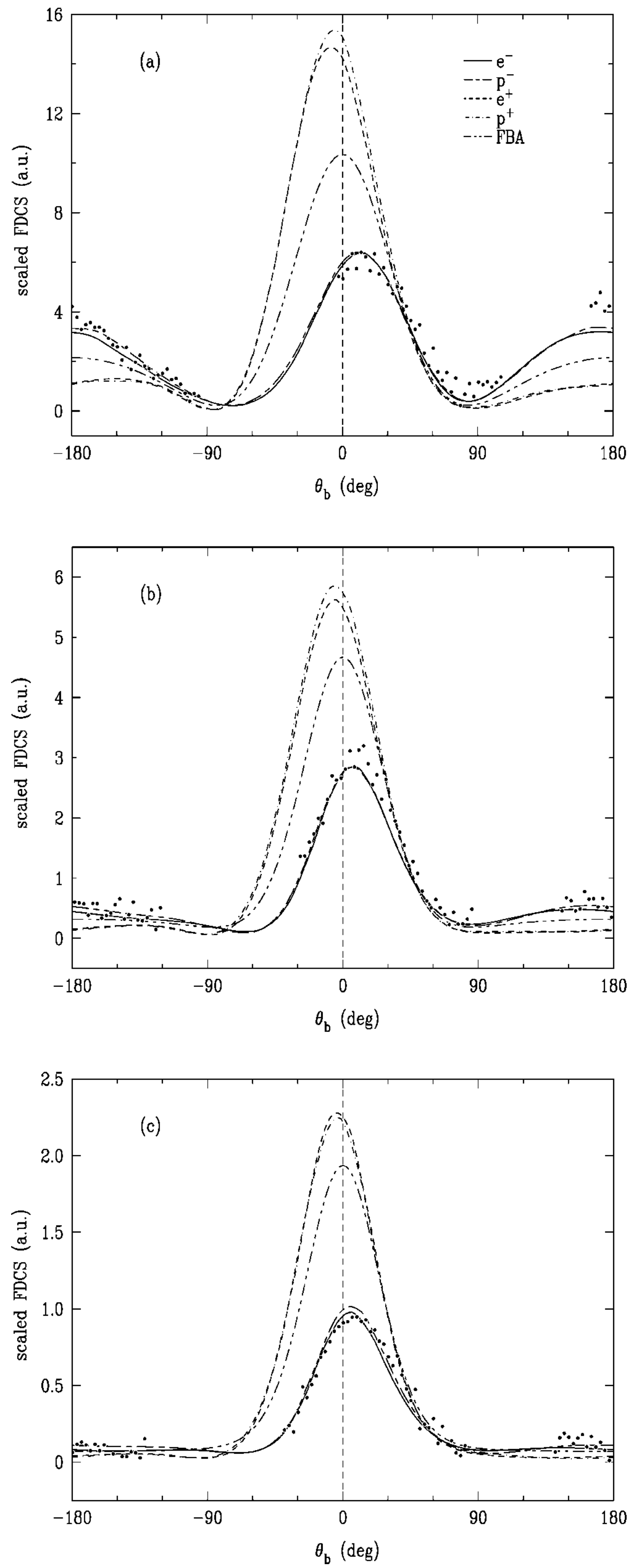

FIG. 2. Same as Fig. 1 for a c.m. collision energy of 150 eV (121 keV) for $e^{\pm}$ ($p^{\pm}$) and projectile scattering angles of (a) 4° (3.09×10^{-3} deg), (b) 10° (11.2×10^{-3} deg), and (c) 16° (17.9×10^{-3} deg). Here the absolute electron-impact measurements from Ehrhardt *et al.* [8] have been multiplied by a factor of 0.86.

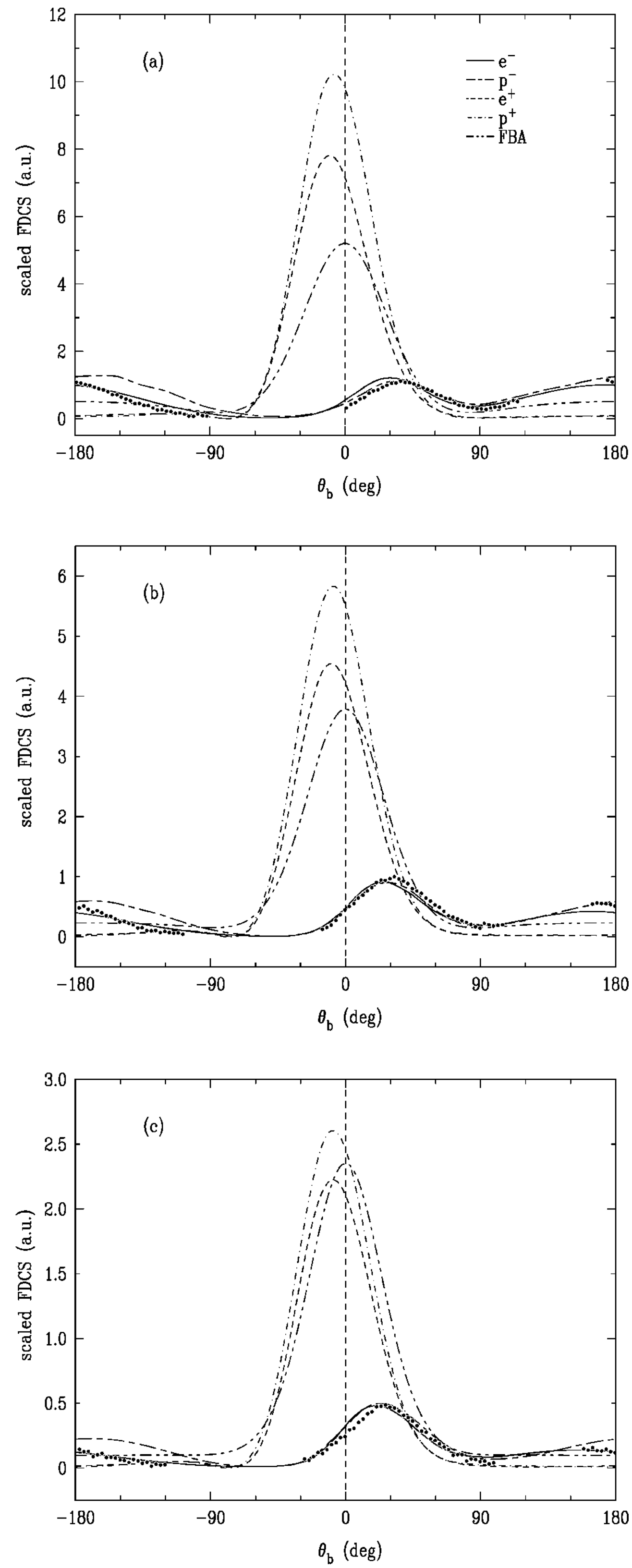

FIG. 3. Same as Fig. 1 for a c.m. collision energy of 54.4 eV (32.9 keV) for $e^{\pm}$ ($p^{\pm}$) and projectile scattering angles of (a) 10° (9.69×10^{-3} deg), (b)16° (17.9×10^{-3} deg), and (c) 23° (26.7×10^{-3} deg). Here the solid circles are absolute electron-impact measurements from Ehrhardt and Röder [9], multiplied by a factor of 0.92.

from the atomic electron colliding with the projectile and then backscattering off the ion.

Our FDCS results are shown in Figs. 1–3. In the FBA, the FDCS is symmetric about the momentum transfer direction, is maximum at 0°, and the scaled cross section is the same for all projectile charges and masses. For better theories that include the interaction of the projectile with the nucleus and the interaction of the projectile with the atomic electron in the system wave function (such as CDW-EIS), one would expect to see a projectile charge dependence (that is, beyond the simple Z_P^2 dependence predicted by FBA). From the figures, it is seen that the CDW-EIS scaled cross sections for opposite projectile charges are very different. On the other hand, scaled cross sections for the same projectile charge and different masses are very similar—in fact, almost indistinguishable for the higher energies (the larger binary cross section indistinguishable curves correspond to e^+ and p^+ while the smaller binary cross section indistinguishable curves correspond to e^- and p^-). We note that in the CDW-EIS, relative to the FBA, both binary and recoil peaks shift to larger (smaller) angles between the two outgoing particles for negatively (positively) charged projectiles as one would expect intuitively. Interestingly, in the case of the binary peak, this shift is reproduced by a distorted-wave Born approximation (DWBA—not shown) that includes the projectile–target-ion interaction exactly, but neglects the projectile-electron interaction in the formation of the final-state wave function (see Whelan *et al.* [18], and references therein). It has been suggested (contrary to intuition) that the shift in the position of the binary peak is caused by the final-state interaction between projectile and target ion alone [12], a supposition that is supported by calculations more sophisticated than DWBA including those in Ref. [12] and the present work (see Fig. 4). Relative to the FBA, the magnitude at the maximum of the binary (recoil) peak decreases (increases) for negatively charged projectiles and increases (decreases) for positively charged projectiles. Test calculations revealed that interference between final-state projectile–target-ion and projectile-electron interactions is important in determining the magnitude of both peaks.

For a c.m. impact energy of 250 eV (212 keV) and a c.m. scattering angle of 3° (3.29×10^{-3} deg) in the case of $e^\pm$ ($p^\pm$), the scaled FDCS for p^+ coincides with the FDCS for e^+ [Fig. 1(a)]. The curves for negatively charged projectiles nearly coincide except for a slight difference in the recoil peak region. When the scattering angle is increased to 8° for $e^\pm$ (8.86×10^{-3} deg for $p^\pm$), small differences appear at the maximum in the binary peak between light and heavy projectiles with the same charge and, in the case of negatively charged projectiles, very small differences also occur over nearly the entire range of the recoil peak [Fig. 1(b)]. In the case of electron-impact ionization, where absolute measurements are available [8], there is quantitative agreement between the CDW-EIS theory and experiment. (The measurements at 250 and 150 eV have an overall normalization uncertainty of 15% and an internormalization, or relative, uncertainty of 10%.) Here we have multiplied the absolute measurements for 250-eV electron-impact ionization by a factor of 0.88 (which is clearly permissible since the overall uncertainty is 15%) so that the shapes of the theoretical and experimental cross sections can be easily compared. Note that this scaling factor of 0.88 only takes into account the *overall* uncertainty in the measurements. There is still the 10% relative uncertainty. This means that experiment should now be within ±10% of the theoretical curve for quantitative agreement to be claimed. It is seen from Fig. 1 that CDW-EIS is indeed in quantitative agreement with the absolute measurements for 250-eV electron impact.

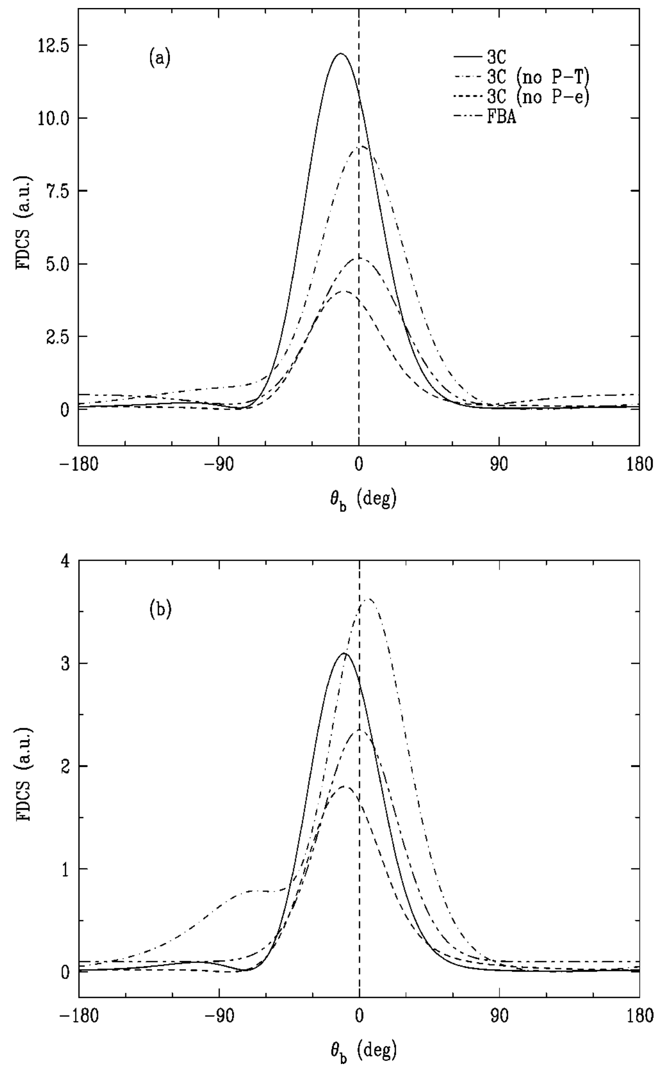

FIG. 4. Scattering-plane fully differential cross section (FDCS) for positron-impact ionization of H(1*s*) in the center-of-mass coordinate system. The collision energy is 54.4 eV and the ionized electron has an energy of 5 eV as in Fig. 3. The curve labeled 3C is the full 3C result including all final-state interactions. The curve labeled 3C (no *P-T*) is the result of a 3C calculation but with the projectile–target-ion interaction switched off in the final-state wave function and the curve labeled 3C (no *P-e*) is the result of a 3C calculation but with the projectile-electron interaction switched off in the final-state wave function. The positron scattering angle is (a) 10° and (b) 23°.

For a c.m. impact energy of 150 eV (121 keV) and c.m. scattering angles of 4°, 10°, and 16° (3.09×10^{-3},

11.2×10^{-3}, and 17.9×10^{-3} deg) in the case of $e^{\pm}$ ($p^{\pm}$), differences remain small for projectiles differing only in mass (Fig. 2). Interestingly, as the scattering angle is increased, the magnitude of the CDW-EIS binary peak for positively charged projectiles approaches that of the FBA, while for negatively charged projectiles the CDW-EIS and experimental (available for electron impact) binary peaks move farther away (in magnitude) from the FBA. The absolute measurements for 150-eV electron-impact ionization [8] have been multiplied by a factor of 0.86. It is seen from Fig. 2 that CDW-EIS is in quantitative agreement with the absolute measurements for 150-eV electron impact except for a slight underestimation of the recoil peak for a scattering angle of 4°. For 150-eV electron impact, measurements also exist for $E_b=3$ and 10 eV; however, these cases revealed no new physics and are therefore not shown.

For the much lower impact energy of 54.4 eV (32.9 keV) in the case of $e^{\pm}$ ($p^{\pm}$), projectile-mass differences remain small for the binary peak in the case of negatively charged projectiles and for the recoil peak in the case of positively charged projectiles (Fig. 3). However, the scaling law clearly breaks down for the recoil (binary) peak for projectiles with a negative (positive) charge. The c.m. scattering angles are 10°, 16°, and 23° for $e^{\pm}$ and 9.69×10^{-3}, 17.9×10^{-3}, and 26.7×10^{-3} deg, respectively, for $p^{\pm}$. In the case of electron-impact ionization, the absolute measurements [9] have been multiplied by a factor of 0.92 (the experimental uncertainty is 35% for the overall normalization and 10% for internormalization) and it is seen that CDW-EIS is in near quantitative agreement with experiment. As observed at the higher energies, the magnitude of the binary peak for positively charged projectiles approaches that of the FBA as the scattering angle is increased; in fact, for a scattering angle of 23° for e^{+}, the magnitude of the binary-peak maximum for positron impact actually becomes *smaller* than that predicted by FBA.

To explore this further we repeated the positron-impact calculations at 54.4 eV, but this time omitting initial-state correlation (3C approximation). The magnitude of the 3C binary-peak maximum approaches that of the FBA with increasing scattering angle just as rapidly as CDW-EIS (Fig. 4). Thus, the above-observed effect is due to *final-state* interactions. Further investigations revealed that neither the projectile–target-ion nor the projectile-electron interaction alone is responsible for this effect, since neglecting *either* interaction causes the above-observed behavior to disappear. (Neglecting the projectile–target-ion interaction leads to a binary peak larger than that predicted by the FBA for all scattering angles, while neglecting the projectile-electron interaction leads to a smaller binary peak than FBA; in neither case does the binary peak approach that of the FBA with increasing scattering angle.) For a scattering angle of 10°, the binary peak that results from including all final-state interactions is larger than both the binary peak neglecting the projectile–target-ion interaction and the binary peak neglecting the projectile-electron interaction. As the scattering angle is increased, however, the binary peak that includes all final-state interactions becomes smaller than the binary peak neglecting the projectile–target-ion interaction. This is a signature of destructive interference between final-state projectile-electron and projectile–target-ion interactions. Thus the apparent success of the FBA for positively charged projectiles at larger scattering angles is fortuitous and can be traced to destructive interference between *individually strong* projectile–target-ion and projectile-electron final-state interactions neglected in the FBA.

IV. SUMMARY AND CONCLUSION

In this paper, we studied the fully differential cross section (FDCS) for ionization of atomic hydrogen by the impact of electrons, protons, and their antiparticles in the CDW-EIS approximation. Although CDW-EIS has been used successfully for many years for less differential cross sections, these results, to our knowledge, represent the first reported *fully differential* CDW-EIS cross sections for ion impact.

We investigated the validity of the CDW (3C) final-state wave function for large total energy E. We found that the Schrödinger equation reduces, to leading order in $|Z_P/v_i|$ in the full coordinate space, to the eigenequation for the 3C wave function if the projectile of charge Z_P and initial speed v_i becomes slow relative to either the ionized electron or the residual target ion. If the projectile remains fast relative to both target fragments, the neglected contribution is just $O(1/v_i)$ and if, in addition, the target fragments are fast relative to *each other*, the neglected contribution is only $O(1/v_i^2)$. Thus the 3C wave function is asymptotically correct in all asymptotic domains of momentum space for all configurations of the three particles in coordinate space.

We have presented CDW-EIS scaled FDCS. In the FBA, the scaled cross sections would be the same for all projectile charges and masses. The scaled CDW-EIS cross sections exhibited a strong charge dependence but almost no mass dependence for final projectile speeds greater than 2–3 a.u. for the dominant case of small momentum transfer to the atom $(q<1)$. With decreasing projectile energy, positive projectiles exhibit a stronger mass dependence than negative projectiles (an attractive projectile-electron interaction brings the two outgoing particles closer together in the final state, hence their mutual interaction is stronger). Interestingly, the magnitude of the binary peak for positive projectiles approaches that of the FBA with increasing scattering angle. This apparent "success" of the FBA for positive projectiles was traced to a fortuitous destructive interference between two very strong final-state interactions neglected in the FBA.

ACKNOWLEDGMENT

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