Final-state Φ_2 wave function in ion-helium collisions

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In this work we study the double-differential cross sections (DDCSs) of ejected electrons in single-ionization collisions of protons with helium atoms. The final state of the emitted electron is modeled by the correlated wave function Φ_2, a confluent hypergeometric function of two variables. We introduce a series representation of the Φ_2 wave function in terms of two-body Coulomb-like states, corresponding to the electron-projectile and electron-target relative motions. We consider undistorted and eikonal initial states that give rise to the Born Φ_2 and eikonal initial-state Φ_2 approximations, respectively. In both cases we obtain analytic series representations of the transition matrices, which exhibit a strong numerical convergence. We obtain DDCSs in ion-helium collisions in the intermediate- to high-energy regime with the Born Φ_2 approximation and show that it qualitatively agrees with the available experimental data. [S1050-2947(98)06610-4]

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I. INTRODUCTION

In this work we focus our attention on the ion-atom ionization problem, where a fully stripped ion collides with an atom and extracts one of its electrons to the continuum. The simplest ionizing collisions is the three-particle process $H^+ + H(1s) \rightarrow H^+ + H^+ + e^-$ since any other target will include at least one more particle in the system. Even in this collision the experimental as well as theoretical difficulties are far from being solved. From the theoretical point of view, these collisions generally involve three or more charged particles interacting through long-range Coulomb potentials. The calculation of the transition matrix $\langle \Psi_f^- | V_i | \psi_i \rangle = \langle \Psi_f | V_f | \psi_i^+ \rangle$ involves the exact solutions of the Schrödinger equation for the initial (Ψ_i^+) or final (Ψ_f^-) channels. The exact quantum-mechanical description of the wave function is not known and physically based approximations should be considered to describe these states. One of the most successful approximations to a three body continuum final state is the well-known $C3$ wave function [1]. This function can be written as a product of three two-body Coulombic wave functions, each of them representing the relative motion of each pair of particles. For the initial state, where the electron is bound in the atomic target, there are many approximated wave functions, ranging from the simple Born approximation (a product of a plane wave representing the incoming projectile and the atomic wave function) [2] to the impulse approximation [3], where the initial state is described as a convolution of the atomic wave and the Coulombic wave of the projectile-electron pair. The condition for a correct asymptotic behavior [4] in the initial channel gave rise to the successful distorted-wave theories where the projectile-electron interaction is taken as a pure Coulombic one (continuum distorted-wave approximations; see [5]) or asymptotically Coulombic [eikonal initial-states (EIS) approximation [6,7]]. The combination of both initial and final states and the related perturbations (V_i and V_f respectively) give rise to a set of theories that have been thoroughly used and have been very well described in the literature [8–10]. Calculations of differential and total cross sections with those theories that take into account all the interactions agree qualitatively with the experiments, although there are some quantitative discrepancies that remain unexplained. When the energy of the projectile decreases, the agreement becomes poor and other approaches to the collision process are required.

Recently, we have proposed an approximate wave function for the final channel of an ion-atom ionizing collision. The motion of the electron in the field of the projectile and the residual ionic target is described through the confluent hypergeometric function Φ_2 in two variables [11]. This wave function correlates both relative motions and goes beyond the simple product of two-body wave functions through the introduction of multivariable hypergeometric functions. It has been shown that this function correctly behaves asymptotically, while it resembles the molecularlike states when the two ions come close to each other. This last feature evidences the correlation in the motion of the electron with respect to the ions that is not included in the $C3$-like theories. These correlated wave functions also have been proposed for the two-electron and one-ion system [12].

We have presented recently some preliminary calculations of double-differential cross sections in a Born-like approximation using the Φ_2 wave function as a final state for H^+-H collisions [13]. We have shown that the calculation of the transition matrix involves the evaluation of the two-variable wave function F_3, a nonconfluent hypergeometric wave function of Appell and Kampé de Feriet with poorly known mathematical properties [14].

In this work we present the analytic derivation of the double-differential cross section in the Born Φ_2 and EIS Φ_2 approximations. This approach allows the application of the approximation to multielectronic atoms. We compare the results of the Born Φ_2 theory with experimental data for He

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targets in the intermediate- to high-energy regime. The plan of the paper is as follows. In Sec. II we make use of a series representation of the Φ_2 wave function to obtain analytical representations of the transition matrices. In Sec. III we show that this series is strongly convergent and that it is not necessary to compute any hypergeometric function within the Born Φ_2 approach. Furthermore, the analysis of the Φ_2 series give rise to a family of wave functions that are asymptotically well behaved. We discuss the comparison with the experiments on He targets in Sec. IV. Finally, we summarize the conclusions of our work. The Appendix shows some hints for the evaluation of the series presented and other topics related to the multivariable hypergeometric functions. Atomic units are used in this work unless otherwise stated.

II. Φ_2 APPROXIMATION

A. Series representation of the Φ_2 wave function

We consider a charged projectile with mass m_P and charge Z_P colliding with an atom (m_T, Z_T). In the process one of the electrons (m_e) of the atom is ionized. The final state can be viewed as a three-body Coulomb system with the Schrödinger equation

$$\left[-\frac{\nabla^2_{\mathbf{r}_j}}{2\mu_j} - \frac{\nabla^2_{\mathbf{R}_j}}{2\nu_j} + \sum_{j=T,P,PT} V_j \right] \overline{\Psi}(\mathbf{r}_i, \mathbf{R}_i) = E\overline{\Psi}(\mathbf{r}_i, \mathbf{R}_i), \tag{1}$$

where $\{\mathbf{r}_j, \mathbf{R}_j\}$ is a pair of Jacobi coordinates ($j=T$, P or PT), $\mu_j = m_i m_k/(m_i+m_k)$ and $\nu_j = m_j(m_i+m_k)/(m_i+m_j+m_k)$ are reduced masses, and V_j represents the Coulomb potential between interacting particles

$$V_T = -\frac{Z_T}{r_T}, \quad V_P = -\frac{Z_P}{r_P}, \quad V_{PT} = \frac{Z_P Z_T}{r_{PT}}.$$

Exact solutions of Eq. (1) are not known and an approximate ansatz can be used instead. We can transform Eq. (1) from a Jacobi pair $\{\mathbf{r}_j, \mathbf{R}_j\}$ to the set of parabolic coordinates

$$\xi_j = r_j + \hat{\mathbf{k}}_j \cdot \mathbf{r}_j, \quad \eta_j = r_j - \hat{\mathbf{k}}_j \cdot \mathbf{r}_j \quad (j = T, P, PT), \tag{2}$$

where $\hat{\mathbf{k}}_j$ represents the unit vector in the direction of the relative momenta $\mathbf{k}_j$ for each pair of particles. In previous works we have shown different approximate solutions to the transformed equation. The full separable solution arises from neglecting all the coupling terms of the Schrödinger equation [15,16]. With this procedure we retrieve one of the most successful approximate solutions known as the $C3$ wave function, a product of three two-body Coulomb functions representing the independent interaction of each pair of particles

$$\Psi_{C3} = \varphi_{\mathbf{K}_f}(\mathbf{R}_T)\varphi_{\mathbf{k}_T}(\mathbf{r}_T)\prod_{l=1}^{3} f_l(\xi_l). \tag{3}$$

The functions $\varphi_{\mathbf{K}_f}(\mathbf{R}_T)$ and $\varphi_{\mathbf{k}_T}(\mathbf{r}_T)$ are the plane-wave eigenstates of the noninteracting Hamiltonian $\langle \mathbf{r}|\mathbf{k}\rangle = \varphi_{\mathbf{k}}(\mathbf{r}) = (2\pi)^{-3/2}\exp(i\mathbf{k}\cdot\mathbf{r})$. The solutions $f_l(\xi_l)$ are Coulomb waves

$$f_l(\xi_l) = N_{l1}F_1(ia_l, 1, -ik_l\xi_l), \tag{4}$$

where $N_l = \exp(-\pi a_l/2)\Gamma(1-ia_l)$ are the normalization factors and $a_l = -Z_l/k_l$ $(l=T,P)$ and $a_{TP} = Z_T Z_P/k_{PT}$ represent the Sommerfeld parameter for each interaction. As usual, ${}_1F_1(a,b,z)$ is the Kummer confluent hypegeometric function. One step beyond these approximation has been recently proposed by Gasaneo *et al.* [11,17]. There the coupling between the motion of the electron relative to the projectile and the residual ion is approximately introduced by the confluent hypergeometric function of two variables Φ_2 and the interaction between the heavy particles is represented by a two-body Coulomb wave function. The wave function reads

$$\begin{aligned}\Psi_1 = {} & N_{TP} N \varphi_{\mathbf{K}_f}(\mathbf{R}_T)\varphi_{\mathbf{k}_T}(\mathbf{r}_T) \\ & \times \Phi_2(ia_T, ia_P, 1, -ik_T\xi_T, -ik_P\xi_P) \\ & \times {}_1F_1(ia_{TP}, 1, -ik_{TP}\xi_{TP}),\end{aligned} \tag{5}$$

with

$$N = e^{(\pi/2)(a_T+a_P)}\Gamma(1-ia_T-ia_P). \tag{6}$$

The function Φ_2 has the double series representation

$$\Phi_2(b,b',c,x,y) = \sum_{m,n} \frac{(b)_m (b')_n}{(c)_{m+n}} \frac{x^m}{m!}\frac{y^n}{n!}, \tag{7}$$

where $(z)_n$ denotes the Pochhammer symbol. Even when this series mathematically converges for all finite values of x and y, it is not useful from a numerical point of view since it is necessary to calculate tenths of terms to achieve a relative precision of 1% in the calculation of the wave function near some particular values of the variables. This situation become worse when calculating the transition matrix and differential cross section.

Instead of Eq. (7) we make use of a one index series representation that has been found by Burchnall and Chaundy [18,19]:

$$\begin{aligned}\Phi_2(b,b',c,x,y) = {} & \sum_m a_m x^m y_1^m F_1(b+m, c+2m, x) \\ & \times {}_1F_1(b'+m, c+2m, y),\end{aligned} \tag{8}$$

where

$$a_m = \frac{(-1)^m (b)_m (b')_m}{(c+m-1)_m (c)_{2m} m!}. \tag{9}$$

We note that the lowest order of this series is the $C3$ wave function apart from a normalization factor.

B. Calculation of the transition matrices

We can now use the series (8) to obtain analytical expressions for the transition matrices in different approximations. We consider that the energy of the incident particle is high enough so that the heavy projectile follows a straight trajectory. In this case, using the impact parameter treatment, the internuclear potential and the wave function of the heavy

particles do not contribute to double-differential cross sections [20]. The transition matrix in the prior form in a Φ_2 approximation is

$$T^{\Phi_2}=\langle\Psi_f^{\Phi_2}|V_i|\Psi_i\rangle,$$

where V_i is the perturbation potential acting over the initial state Ψ_i. Taking into account the relation between $\mathbf{R}_T$ and the pair $(\mathbf{r}_P,\mathbf{r}_T)$ we can write $\varphi_{\mathbf{K}_f}(\mathbf{R}_T)\varphi_{\mathbf{k}_T}(\mathbf{r}_T)=\varphi_{\mathbf{q}_T}(\mathbf{r}_T)\varphi_{\mathbf{q}_P}(\mathbf{r}_P)$, with $\mathbf{q}_T=\mathbf{k}_T+\mathbf{K}_f$ and $\mathbf{q}_P=-\mathbf{K}_f$. The final-state wave function can be written as

$$|\Psi_f^{\Phi_2}\rangle=N\sum_m a_m|\chi_P^m\rangle|\chi_T^m\rangle, \tag{10}$$

with

$$\langle\mathbf{r}_j|\chi_j^m\rangle=\varphi_{\mathbf{q}_j}(\mathbf{r}_j)(-ik_j\xi_j)^m\mathcal{F}_m(\xi_j), \tag{11}$$

where $\mathcal{F}_m(\xi_j)={}_1F_1(ia_j+m,1+2m,-ik_j\xi_j)$ $(j=T,P)$.

The states χ_j^m are, apart from a plane-wave factor, the general solutions of a Schrödinger equation for a system of two particles interacting through Coulomb potentials. Furthermore, if we solve this problem within the oscillator representation we find that the two-charged-particle system can be described by two two-dimensional harmonic oscillators [21,22]. The wave function for each of these oscillators is represented by states similar to Eq. (11), where the angular momentum is related to the quantum number m. In the two-body case there exists further symmetries associated with the conservation of the Runge-Lenz vector and hence these quantum numbers m cannot be set independently. However, in the three-body case this symmetry does not exist. In that sense, the $|\Psi_f^{\Phi_2}\rangle$ state can be interpreted as a linear combination of all the eigenstates of the two-dimensional oscillators representing the electron-target and electron-projectile interactions. We would like to note that each product of the states $\chi_P^m\chi_T^m$ satisfies the correct asymptotic conditions in the region where all particles are far from each other and can be considered as a final wave function for an ionization process. Then a natural generalization of the function $\Psi_f^{\Phi_2}$ can be constructed upon a sum over all of these product states with different coefficients to Eq. (9).

The transition matrix will read

$$T^{\Phi_2}=N\sum_m a_m T_m, \tag{12}$$

$$T_m=\langle\chi_P^m\chi_T^m|V_i|\Psi_i\rangle. \tag{13}$$

To be able to obtain analytical expressions for the matrices T_m we observe that

$$x^m=\left.\frac{\partial^m}{\partial\tau^m}e^{\tau x}\right|_{\tau=0} \tag{14}$$

and then

$$\langle\mathbf{r}_j|\chi_j^m\rangle=\left.\frac{\partial^m}{\partial\tau_j^m}\varphi_{\mathbf{q}_j}(\mathbf{r}_j)e^{-i\tau_j k_j\xi_j}\mathcal{F}_m(\xi_j)\right|_{\tau_j=0}$$

$$=\left.\frac{\partial^m}{\partial\tau_j^m}\langle\mathbf{r}_j|\tilde{\chi}_j^m\rangle\right|_{\tau_j=0}, \tag{15}$$

where we defined $\langle\mathbf{r}_j|\tilde{\chi}_j^m\rangle=\varphi_{\mathbf{q}_j}(\mathbf{r}_j)e^{-i\tau_j k_j\xi_j}\mathcal{F}_m(\xi_j)$. In this way, the state $|\tilde{\chi}_j^m\rangle$ resembles the familiar expression that appears in the calculation of transition matrices in ionization theory [20]. Then we can write

$$T_m=\left.\frac{\partial^m}{\partial\tau_T^m}\frac{\partial^m}{\partial\tau_P^m}\langle\tilde{\chi}_P^m\tilde{\chi}_T^m|V_i|\Psi_i\rangle\right|_{\tau_T=\tau_P=0} \tag{16}$$

and we need to obtain

$$\tilde{T}_m=\langle\tilde{\chi}_P^m\tilde{\chi}_T^m|V_i|\Psi_i\rangle. \tag{17}$$

In the case of the Born Φ_2 approximation, the function Ψ_i^B is the undistorted initial state of the electron in a $1s$ state of an hydrogenic atom:

$$|\Psi_i^B\rangle=|\mathbf{K}_i,\psi_i\rangle,$$

$$\langle\mathbf{R}_T\mathbf{r}_T|\Psi_i^B\rangle=\varphi_{\mathbf{K}_i}(\mathbf{R}_T)\psi_i(\mathbf{r}_T)$$

$$=\varphi_{\mathbf{K}_i}(\mathbf{r}_T)\varphi_{-\mathbf{K}_i}(\mathbf{r}_P)\psi_i(\mathbf{r}_T),$$

where we have considered $m_P,m_T\gg m_e$, the electron mass. The ground state is

$$\psi_i(\mathbf{r}_T)=\sqrt{\frac{\lambda_T^3}{\pi}}\exp(-\lambda_T r_T)$$

and λ_T represents an effective charge useful for the calculation of ion-helium collisions. The perturbative potential is simply $V_i^B(r_P)=-Z_P/r_P$. Then the transition matrix $\tilde{T}_m$ reads

$$\tilde{T}^m=\langle\tilde{\chi}_P^m\tilde{\chi}_T^m|V_i^B(r_P)|\mathbf{K}_i,\psi_i\rangle.$$

It is easy to see that $\tilde{T}^m$ can be factored as $\tilde{T}_P^m\tilde{T}_T^m$, where

$$\tilde{T}_P^m=\langle\tilde{\chi}_P^m|V_i^B(r_P)|-\mathbf{K}_i\rangle,$$

$$\tilde{T}_T^m=\langle\tilde{\chi}_T^m|\mathbf{K}_i,\psi_i\rangle.$$

These are Nordsieck-like integrals where the second parameter of the hypergeometric functions $\mathcal{F}_m(\xi_j)$ is no longer one, but an integer number $1+2m$. We should use then the results of Ref. [23]. We note that to obtain $\tilde{T}_P^m$ we introduce an integrating factor $\exp(-\varepsilon r_P)$ with $\varepsilon>0$. The decorated variables will indicate a dependence on the parameters τ_i, while the undecorated ones correspond to the condition $\tau_i=0$. Upon defining

$$\tilde{\lambda}_P=\varepsilon-i\tau_P k_P,\quad \tilde{\lambda}_T=\lambda_T-i\tau_T k_T,$$

$$\tilde{\mathbf{Q}}_P=-\mathbf{P}+\tau_P\mathbf{k}_P,\quad \tilde{\mathbf{Q}}_T=\mathbf{P}+(\tau_T-1)\mathbf{k}_T$$

and with $\mathbf{P}=\mathbf{K}_i-\mathbf{K}_f$ as the momentum transfer, we have

$$\tilde{T}_P^m=-\frac{4\pi Z_P}{(2\pi)^3}\frac{\tilde{A}_P^{ia_P-m}}{\tilde{D}_P}{}_2F_1(2m,-ia_P+m,1+2m,\tilde{z}_P), \tag{18}$$

$$\tilde{T}_T^m=\frac{4\pi}{(2\pi)^3}\sqrt{\frac{\tilde{\lambda}_T^3}{\pi}}\frac{\tilde{A}_T^{ia_T-m}}{\tilde{D}_T^2} \times\left(\tilde{L}_{T0}\,{}_2F_1+\frac{2m(-ia_T+m)}{1+2m}\tilde{L}_{T1}\,{}_2F_1^+\right), \tag{19}$$

where

$${}_2F_1={}_2F_1(2m,-ia_T+m,1+2m,\tilde{z}_T)$$

$${}_2F_1^+={}_2F_1(2m+1,-ia_T+m+1,2+2m,\tilde{z}_T)$$

are Gauss hypergeometric functions. We define

$$\tilde{U}_j=\frac{2\tilde{S}_j}{\tilde{D}_j},\quad \tilde{S}_j=S_j=\tilde{\mathbf{Q}}_j\mathbf{k}_j-i\tilde{\lambda}_j k_j,$$

$$\tilde{A}_j=\tilde{U}_j+1,\quad \tilde{z}_j=\frac{\tilde{U}_j}{\tilde{A}_j},\quad \tilde{D}_j=\tilde{\lambda}_j^2+\tilde{\mathbf{Q}}_j^2$$

and

$$\tilde{L}_{T0}=2\tilde{\lambda}_T-\frac{(-ia_T+m)\tilde{B}_T}{\tilde{A}_T},$$

$$\tilde{L}_{T1}=\frac{\tilde{B}_T}{\tilde{A}_T^2},\quad \tilde{B}_T=2(ik_T+\tilde{\lambda}_T\tilde{U}_T).$$

The first order ($m=0$) in the series representation (12), apart from a normalization factor, is the commonly known Born $C2$ approximation, where the final state of the electron is represented by the product of two outgoing Coulomb wave functions

$$T^{B-C2}=N_T N_P T_P^0 T_T^0,$$

where N_l are the normalization factors and T_l^0 are

$$T_P^0=-\frac{4\pi Z_P}{(2\pi)^3}\frac{A_P^{ia_P}}{D_P},\quad T_T^0=\frac{4\pi}{(2\pi)^3}\sqrt{\frac{\lambda_T^3}{\pi}}\frac{A_T^{ia_T}}{D_T^2}L_{T0}.$$

Furthermore, by setting $a_P=0$ and $m=0$ we recover the well-known first Born approximation (FBA) [2]:

$$T^{FBA}=N_T T_P^0(a_P=0)T_T^0.$$

We would like to note that even when the transition matrix is represented by a series, this representation does not constitute a sum over a perturbative series in the long-range potential of the electron-projectile interaction.

In the case of an eikonal initial state

$$\langle\mathbf{r}_T\mathbf{r}_P|\Psi_i^{EIS}\rangle=\varphi_{\mathbf{K}_i}(\mathbf{R}_T)\psi_i(\mathbf{r}_T)\mathcal{E}_{\mathbf{v}_i}(\mathbf{r}_P),$$

where $\mathcal{E}_{\mathbf{k}}(\mathbf{r})$ represents the asymptotic Coulomb interaction between the electron and the projectile

$$\mathcal{E}_{\mathbf{k}}(\mathbf{r})=\exp(ia_i\ln k\eta),$$

$$a_i=-Z_P/v_i$$

and the perturbation potential reads

$$V_i^{EIS}=-\frac{\nabla_{\mathbf{r}_P}^2}{2\mu_P}+\frac{1}{m_e}\nabla_{\mathbf{r}_P}\cdot\nabla_{\mathbf{r}_T},$$

where we again understand that the internuclear potential has been dropped based on an impact parameter approximation and is considered as an eikonal phase that do not affect the results for double-differential cross sections (DDCSs). The transition matrix is expressed in the same way as Eqs. (12) and (16), but since now the perturbation potential is itself a sum of two terms we have

$$\tilde{T}_m=\langle\tilde{\chi}_P^m\tilde{\chi}_T^m|V_i^{EIS}|\Psi_i^{EIS}\rangle \tag{20}$$

$$=\tilde{I}_m+\tilde{J}_m, \tag{21}$$

where

$$\tilde{I}_m=\tilde{I}_m^P\tilde{I}_m^T,\quad \tilde{J}_m=\tilde{\mathbf{J}}_m^P\cdot\tilde{\mathbf{J}}_m^T$$

and

$$\tilde{I}_m^P=\left\langle\tilde{\chi}_P^m\left|-\frac{\nabla_{\mathbf{r}_P}^2}{2\mu_P}\right|-\mathbf{K}_i,\mathcal{E}_{\mathbf{v}_i}\right\rangle,$$

$$\tilde{I}_m^T=\langle\tilde{\chi}_T^m|\mathbf{K}_i,\psi_i\rangle,$$

$$\tilde{\mathbf{J}}_m^P=\left\langle\tilde{\chi}_P^m\left|\frac{\nabla_{\mathbf{r}_P}}{m_e}\right|-\mathbf{K}_i,\mathcal{E}_{\mathbf{v}_i}\right\rangle,$$

$$\tilde{\mathbf{J}}_m^T=\langle\tilde{\chi}_T^m|\nabla_{\mathbf{r}_T}|\mathbf{K}_i,\psi_i\rangle.$$

The situation is not as simple as in the Born Φ_2 approximation because now the partial transition matrices are given in terms of the two variable F_1 hypergeometric functions and their derivatives. For brevity, we quote the results in terms of different integrals given in the Appendix:

$$\tilde{I}_m^P=-\frac{\nu_i v_i a_i^2}{\mu_p}I_1'(\tilde{\lambda}_P,\tilde{\mathbf{Q}}_P,\mathbf{v}_i,\mathbf{k}_P,1-ia_i,m-ia_P,1+2m), \tag{22}$$

$$\tilde{I}_m^T=\frac{1}{(2\pi)^3}\sqrt{\frac{\lambda_T^3}{\pi}}L_0'(\lambda_T',\mathbf{Q}_T,\mathbf{k}_T,m-ia_T,1+2m), \tag{23}$$

$$\tilde{\mathbf{J}}_m^P=\frac{1}{m_e}\mathbf{J}_9'(\lambda_P',\mathbf{Q}_P,\mathbf{v}_i,\mathbf{k}_P,-ia_i,m-ia_P,1+2m), \tag{24}$$

$$\tilde{\mathbf{J}}_m^T=\frac{1}{(2\pi)^3}\sqrt{\frac{\lambda_T}{\pi}}\lambda_T^2\mathbf{K}_{-1}'(\tilde{\lambda}_T,\tilde{\mathbf{Q}}_T,\mathbf{k}_T,m-ia_T,1+2m). \tag{25}$$

We note that when $m=0$ these expressions reduce to the usual continuum distorted wave–eikonal initial state (CDWEIS) approximation in prior form [24]. The integrals I_1' and $\mathbf{J}_9'$ are functions of the hypergeometric F_1. Numerical evaluation of this function is precluded for the moment due to the complexities of the poorly known analytical properties of the nonconfluent two-variable hypergeometric functions and hence we will restrict our attention to the Born-like theories. We note that the hypergeometric functions in Eqs. (18) and (19) are rational functions of the variables and can be easily evaluated (see the Appendix). In addition, it is easy to see that all decorated function have simple expressions for the respective derivatives of mth order. Then the evaluation of Eq. (16) is carried out by a recursive routine that implements the properties of products of derivatives (Leibniz's formula) and the chain rule [25]. This procedure enables us to obtain DDCSs with error less than 1%. Furthermore, the series that represents the transition matrix inheritates the strong numerical convergence of Eq. (8). Then, to achieve the mentioned relative error, it is necessary to sum only a few terms of the series (commonly no more than five), that is to say,

$$T^{\Phi_2} \approx T_M^{\Phi_2} = N \sum_{m=0}^{M} a_m T_m . \tag{26}$$

The DDCS in the electron energy and deflection angle is defined as

$$\sigma(E,\Omega) = \frac{d^2\sigma}{dE\,d\Omega} = (2\pi)^4 \nu_i \frac{k_T}{K_i} \int |T|^2 d\Omega_P ,$$

where the integration is carried out over the angular degrees of freedom Ω_P of the projectile. To represent the different contributions of the terms of the sum (26) we define

$$\sigma_M(E,\Omega) = (2\pi)^4 \nu_i \frac{k_T}{K_i} \int |T_M^{\Phi_2}|^2 d\Omega_P , \tag{27}$$

which represents the DDCS calculated in the Born Φ_2 approximation considering up to order M, and

$$\sigma_{mn}(E,\Omega) = \left(1 - \frac{\delta_{mn}}{2}\right)(2\pi)^4 \nu_i \frac{k_T}{K_i} \times \int (a_m T_m a_n^* T_n^* + a_m^* T_m^* a_n T_n) d\Omega_P , \tag{28}$$

which enables us to distinguish the different effects of each of the terms in the coherent sum (26). It is clear that

$$\sigma_M(E,\Omega) = \sum_{m,n=0}^{M} \sigma_{mn}(E,\Omega) \tag{29}$$

and $\sigma(E,\Omega) = \sigma_{M\to\infty}(E,\Omega)$.

In Fig. 1(a) we can see the contribution of the different orders to the DDCS at 0° of the ejected electron in a collision of protons with atomic hydrogen at 100-keV impact energy. The final distribution agrees with the values previously obtained [13]. A feature that this theory exhibits is an enhancement of the emission of ridge electrons. These electrons are emitted in the collision with velocities between 0 and the projectile velocity v_P. This enhancement has been

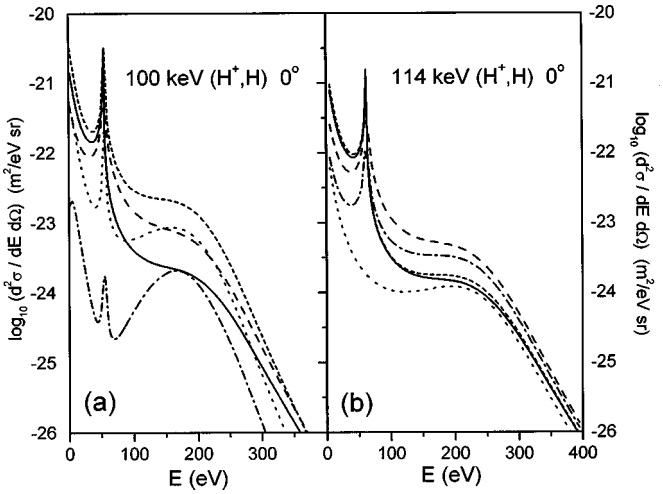

FIG. 1. (a) Different contributions of the coherent sum [Eq. (29)] in the double-differential cross section for an ionizing H^+-H collision in Born approximations. Solid line, Born Φ_2 approximation, i.e., $\sigma_{M\to\infty}(E,\Omega)$; long-dashed line, Born $C2$ approximation $[\sim\sigma_{00}(E,\Omega)]$; short-dashed line, $\sigma_{11}(E,\Omega)$; dotted line, $\sigma_{22}(E,\Omega)$; dash-dotted line, $\sigma_{33}(E,\Omega)$. (b) DDCS at 0° obtained with different orders of the Born Φ_2 approximation for a 114-keV H^+-H collision. Solid line, Born Φ_2 approximation $[\sigma_{M\to\infty}(E,\Omega)]$; long-dashed line, Born $C2$ approximation; dash-dotted line, $\sigma_{M=0}(E,\Omega)$; short-dashed line, $\sigma_{M=1}(E,\Omega)$, dotted line, FBA.

widely observed experimentally for different collisions systems and energies. To study this effect we have also plotted in Fig. 1(a) the contribution of the different orders $\sigma_{mm}(E,\Omega)$ in the transition matrix for a collision of 100-keV protons with hydrogen. We observe that the first order $\sigma_{11}(E,\Omega)$ is responsible for the enhancement of the structures in the ridge region, while higher terms are orders of magnitude smaller than the first one. We note that the contribution of σ_{mn} $(m\neq n)$ gives a destructive interference. These facts clearly show that the series convergence is mainly driven by the parameter a_m that include several factorials in the denominator.

Different DDCSs $\sigma_M(E,\Omega)$ calculated with $M=0,\ldots,2$ are shown in Fig. 1(b). We observe that the main correction is provided by the first order of the series $(M=1)$ and the higher orders introduce only small changes in the shape of the DDCSs. This is a general feature of this calculation reproducible for different angles and impact energies. Even in the case of a complex target this characteristic remains and the first partial sum gives a rough idea of the full DDCSs.

III. IONIZATION OF HELIUM

Three main characteristics arise in the ejected electron spectra: the soft electron (SE) peak [26], a structure in the region where the electrons are ejected with small velocities; the electrons captured to the continuum (ECC) of the projectile Coulomb potential described by a sharp peak centered in the projectile velocity [27]; and the binary sphere, a smooth structure where the electrons would lie after a head-on collision with the projectile [29]. The expression of the transition matrices of the preceding section enables us to calculate double-differential cross sections considering a target of helium. We represent the ground state of helium by a one-

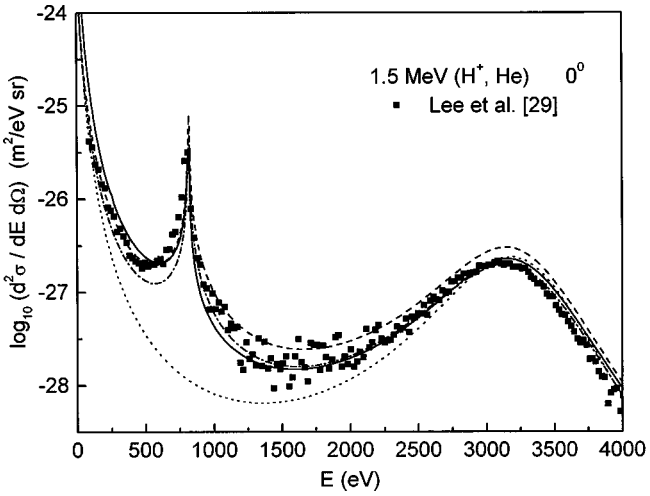

FIG. 2. DDCS at 0° for a 1.5-MeV H^+-He collision. Solid line, Born Φ_2 approximation; dashed line, Born C2 approximation; dotted line, FBA; dash-dotted line, CDW EIS approximation. Experimental data are from Lee *et al.* [29].

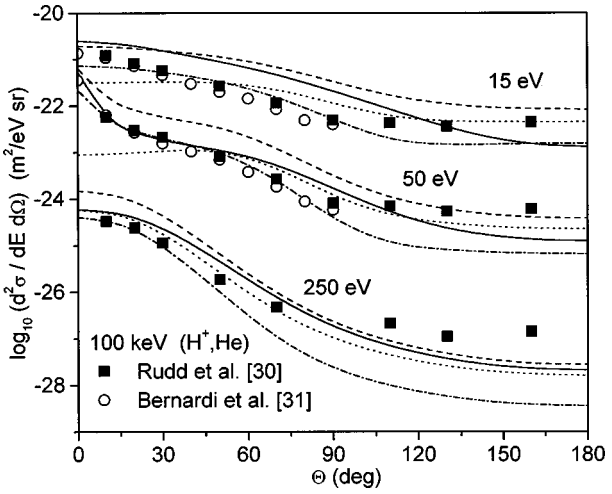

FIG. 3. Angular distribution of ejected electrons for a 100-keV H^+-He collision. Energies correspond to soft electrons (15 eV), ECC electrons (50 eV), and binary electrons (250 eV). Experimental data were obtained by Rudd *et al.* [30] (■) and Bernardi *et al.* [31] (○). The theories are similar to those in Fig. 2.

electron model with a five-term Roothan-Hartree-Fock orbital defined as

$$\varphi_i(r_T)=\sum_{j=1}^{5}\frac{(2\lambda_j)^{3/2}}{(8\pi)^{1/2}}a_j\exp(-\lambda_j r_T), \tag{30}$$

where a_j and λ_j are given by Ref. [28]. The state of the electron in the final channel is modeled by a Φ_2 continuum wave function with an effective charge of $Z_T=1.6875$. We should point out that this is a very approximate way to include the effect of the passive electron of helium in the final state; however, a Φ_2-correlated final state with passive electrons is not available yet.

In Fig. 2 we compare the theoretical DDCS in the forward direction for the collision $H^+ + He \rightarrow H^+ + He^+ + e^-$ with the experimental data of Lee *et al.* [29]. The impact energy of the collision is 1.5 MeV/amu. We plot the results of undistorted calculations (the FBA and the Born $C2$ and Born Φ_2 approximations) and the CDW EIS calculations. The Born Φ_2 theory qualitatively agrees with experimental data, giving all the main features of the forward ejected electrons. However, it overestimates the asymmetry of the SE cusp and enhances the ridge electrons yield. On the contrary, the Born $C2$ and CDW EIS approximation give similar results in the soft region, even when they differ in the representation of the initial channel. Therefore, we could think that the correlation in the Φ_2 final state is responsible for this high asymmetry. We have to recall that the Φ_2 wave function exhibits a high probability of finding the electrons in the spatial region between the two heavy centers [11,17]. Furthermore, we should note that in the present approximation, the initial and final states are not orthogonal. Since the Φ_2 final wave function is correlated, an equivalent correlated initial channel should be considered instead the simple Born initial one. However, such an initial state is not known yet.

In the region of the ECC, the theory reproduces the shape of the peak and gives the right asymmetry, i.e., an enhancement of the electronic emission for velocities lower than the projectile one. On the other hand, the Born $C2$ approximation gives a symmetric peak around v_i. This general feature of the Born Φ_2 approximation can be related to the shape of the high-order terms ($m \geqslant 1$) that contribute to the final state. As we pointed out before, the enhancement in the ridge region is clearly related to the first order of the series representation of the transition matrix and hence to the first order of the Φ_2 series (Fig. 1). Furthermore, the asymmetries shown by this theory can be traced in the interference terms in $|T|^2$, when T is represented as a coherent sum. We note that both the CDW EIS and Born $C2$ approximations agree well with the data, but do not predict the right asymmetry in the peak. Of course, the FBA does not have this cusp structure since the interaction between the projectile and the electron is only accounted for perturbatively in the evaluation of the transition matrix. Meanwhile, for energies greater than the projectile one and up to the binary peak, all theories agree well with the experimental data.

Now we can turn our attention to the angular structure of the DDCS. In Fig. 3 we plot the DDCS as a function of the emission angle for 100-keV protons colliding with helium. The energies considered for the emitted electrons correspond to velocities near the SE peak ($v \sim 0$), near the ECC peak ($v \sim v_P$), and above the binary electrons ($v > 2v_P$). Experimental data correspond to works of Rudd *et al.* [30] and Bernardi *et al.* [31]. General agreement with the data can be seen. In the low-energy region, the Born Φ_2 theory overestimates the data for small angles giving rise to a higher angular asymmetry in the SE peak than expected. The dynamical correlation introduced by the Φ_2 wave function in the final state seems to give the electron-projectile interaction effects required to produce asymmetric SE and ECC cusps.

A similar picture can be seen for a collision of 1-MeV protons with helium (Fig. 4). The data correspond to the works of Rudd *et al.* [30] and Pedersen *et al.* [32]. Here again the angular asymmetry in the SE region is overestimated, while the agreement with the data for other energies is good. Furthermore, we can trace the right asymptotic limit for high impact energies by a simple comparison between the Born Φ_2 and FBA theories in both Figs. 3 and 4.

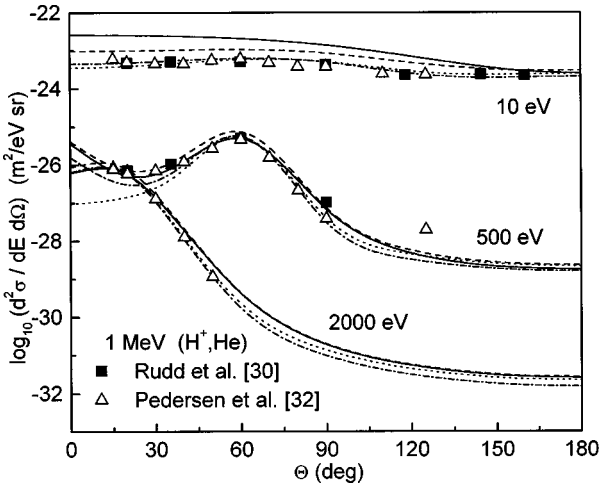

FIG. 4. Same as Fig. 3, for a 1-MeV H^+-He collision. Energies correspond to soft electrons (10 eV), ECC electrons (500 eV) and binary electrons (2000 eV). Data (■) from Rudd *et al.* [30] and (△) from Pedersen *et al.* [32].

IV. CONCLUSIONS AND OUTLOOK

In this work we have calculated double-differential cross sections for ionizing collisions of helium for different projectiles and energies. We used as the final three-body state the correlated Φ_2 wave function recently introduced [11]. We obtained analytical expressions of the transition matrices for the Born Φ_2 and EIS Φ_2 approximations through a series representation of the Φ_2 wave function, where each term is a product of two confluent hypergeometric functions, each representing the interaction of the electron with the projectile and target, respectively. We have shown that the lowest order of this series gives the common Born $C2$ and CDW EIS approximations when we use an undistorted or distorted initial state and perturbations, respectively. The main contribution to the DDCS comes from this order, but significant differences arise from the first-order term, while higher orders only incorporate small modifications into the shape of the structures. The calculation in the EIS Φ_2 approximation is precluded for the moment due to the complexities of the analytical properties of the two-variable hypergeometric function.

The calculation of the DDCS in the Born Φ_2 approximation with a series representation is strongly convergent for all energies and angles of the ejected electron. The overall agreement with experimental data is qualitatively good. The theory overestimates the DDCS in the region of the SE peak, but predicts the asymmetries of the SE and ECC peaks in the right way. Furthermore, the angular structure for backward angles is very well described by the Born Φ_2 approximation, even better than the CDW EIS theory.

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APPENDIX

1. Computation of the transition matrix in the Born Φ_2 approximation

The calculation of expressions (18) and (19) and their corresponding derivatives can be carried out by noting that the hypergeometric functions can be reduced to rational expressions. We note that we should obtain the functions ${}_2F_1(n,b,n+1,z)$ where n is an integer. It is easy to see that

$$ {}_2F_1(n,b,n+1,z)=\frac{n!}{(1-b)_{n-1}}\frac{1-(1-z)^{1-b}p_n(z)}{(-z)^n}, $$

with

$$ p_n(z)=\sum_{j=0}^{n-1}(1-b)_{n-1}\frac{z^j}{j!}. $$

In this way, the function can be evaluated for any value of the parameters and the variable.

On the other hand, the decorated functions $\tilde{A}_j$, $\tilde{U}_j$, $\tilde{z}_j$, etc., as a function of the parameters τ_j can be cast in the form

$$ \tilde{f}(\lambda)=\frac{a}{b+c\lambda}, $$

where λ represents the parameter τ_j and a, b, and c are functions of the dynamic variables. Then the derivatives of mth order can be obtained:

$$ \frac{d^m\tilde{f}}{d\lambda^m}=m!\left(-\frac{c}{a}\right)^m[\tilde{f}(\lambda)]^{m+1} \tag{A1} $$

and since $\tilde{f}(\lambda=0)=f$ we have

$$ \left.\frac{d^m\tilde{f}}{d\lambda^m}\right|_{\lambda=0}=m!\left(-\frac{c}{a}\right)^m[f]^{m+1}. $$

For example, it is easy to see that

$$ \tilde{z}_j=\frac{U_j}{A_j+\tau_jU_j}. $$

Applying Eq. (A1) we have

$$ \left.\frac{d^m\tilde{z}_j}{d^m\tau_j}\right|_{\tau_j=0}=-m!\tilde{z}_j^{m+1}. $$

This procedure enable us to recursively obtain the derivatives of all decorated functions evaluated for $\tau_j=0$. Combining the chain rule and the Leibniz rule, all the derivatives in Eq. (16) can be obtained analytically.

2. Integrals in the EIS Φ_2 approximation

The integral in the EIS Φ_2 approximation is similar to the table of Nordsieck integrals compiled by Gravielle and Miraglia. In our case the second parameter in the confluent hypergeometric functions is no longer one, but any integer number. Then we can use the results of Colavecchia, Gasaneo, and Garibotti [23]. We quote here the final results:

$$I_1'(z,\mathbf{q},\mathbf{p}_1,\mathbf{p}_2,ia_1,ia_2,b_2)=\int d\mathbf{r}\,\exp(-zr+i\mathbf{q}\cdot\mathbf{r})\frac{1}{r}\mathcal{F}_2'\mathcal{E}_1$$
$$=\gamma_1\lim_{p_1\to\infty}J_1'(b_1=1)$$
$$=4\pi\gamma_1\frac{U_1^{-ia_1}A_2^{-ia_2}}{D}F_1,$$

$$L_0'(z,\mathbf{q},\mathbf{p}_1,ia_1,b_1)$$
$$=\int d\mathbf{r}\cdot e^{-zr+i\mathbf{q}\cdot\mathbf{r}}\mathcal{F}_1'=-\frac{\partial}{\partial z}J_1'(a_2=0)$$
$$=\frac{4\pi A_1^{-ia_1}}{D^2}\left[L_{012}F_1+\frac{(b_1-1)ia_1}{b_1}L_{02}^1{}_2F_1^+\right],\qquad\text{(A2)}$$

with

$$L_{01}=2z-\frac{ia_1B_1}{A_1},\quad L_{02}^1=-\frac{A_2B_1}{A_1},$$

$$\mathbf{J}_9'(z,\mathbf{q},\mathbf{p}_1,\mathbf{p}_2,ia_1,ia_2,b_2)$$
$$=\int d\mathbf{r}\,\exp(-zr+i\mathbf{q}\cdot\mathbf{r})\mathcal{F}_2'\nabla_{\mathbf{r}}\mathcal{E}_1$$
$$=\gamma_1'\lim_{p_1\to\infty}\mathbf{J}_3'=\gamma_1\lim_{p_1\to\infty}\mathbf{J}_3'(b_1=1)$$
$$=8\pi ia_i\gamma_1\frac{U_1^{-ia_1-1}A_2^{-ia_2}}{D^2}[J_{91}'\mathbf{p}_1+J_{92}'\mathbf{p}_2+J_{93}'\mathbf{q}],$$

with

$$J_{91}'=izF_1+\frac{ia_2}{b_2A_2}\left(p_2+iz\frac{A_3}{U_1}\right)F_1^+,$$

$$J_{92}'=-\frac{ia_2p_1}{b_2}F_1^+,$$

$$J_{91}'=-p_1F_1-\frac{ia_2p_1}{b_2A_2}\left(\frac{A_3}{U_1}\right)F_1^+.$$

Finally,

$$\mathbf{K}_{-1}'(z,\mathbf{q},\mathbf{p}_1,ia_1,b_1)$$
$$=\int d\mathbf{r}\,\exp(-zr+i\mathbf{q}\cdot\mathbf{r})\frac{\mathbf{r}}{r}\mathcal{F}_1'$$
$$=-4\pi i\nabla_{\mathbf{q}}L_{-1}'$$
$$=8\pi i\frac{A_1^{-ia_1}}{D^2}\left\{\left[\frac{ia_1}{A_1}\mathbf{p}_1+\mathbf{q}\left(1-ia_i+\frac{ia_1}{A_1}\right)\right]{}_2F_1\right.$$
$$\left.+\frac{ia_1(b_1-1)}{b_1A_1^2D}(U_1\mathbf{q}-\mathbf{p}_1){}_2F_1^+\right\},$$

where the hypergeometric functions are defined as

$$\mathcal{F}_i'={}_1F_1(ia_i,b_1,i\mathbf{p}_j\cdot\mathbf{r}+ip_jr),$$

$$F_1=F_1(ia_2,b_2-1,ia_1,b_2,z_2,x_1),$$

$$F_1^+=F_1(ia_2+1,b_2-1,ia_1+1,b_2+1,z_2,x_1),$$

$${}_2F_1={}_2F_1(b_1-1,ia_1,b_1,z_1),$$

$${}_2F_1^+={}_2F_1(b_1,ia_1+1,b_1+1,z_1)$$

and F_1 and F_1^+ represent Appell's two-variables hypergeometric functions [14]. The other variables are defined in [23] and [33].

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