Shifting of the electron-capture-to-the-continuum peak in proton-helium collisions at 10 and 20 keV

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A refined theoretical approach has been developed to study the double-differential cross sections (DDCS's) in proton-helium collisions as a function of the ratio of ionized electron velocity to the incident proton velocity. The refinement is done in the present coupled-channel calculation by introducing a continuum distorted wave in the final state coupled with discrete states including direct as well as charge transfer channels. It is confirmed that the electron-capture-to-the-continuum (ECC) peak is slightly shifted to a lower electron velocity than the equivelocity position. Comparing measurements and classical trajectory Monte Carlo (CTMC) calculations at 10 and 20 keV proton energies, excellent agreement of the ECC peak heights is achieved at both energies. However, a minor disagreement in the peak positions between the present calculation and the CTMC results is noted. A smooth behavior of the DDCS is found in the present calculation on both sides of the peak whereas the CTMC results show some oscillatory behavior particularly to the left of the peak, associated with the statistical nature of CTMC calculations.

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I. INTRODUCTION

In an ion-atom ionizing collision, one of the most interesting features is the so-called electron capture to the continuun (ECC) by the projectile ion. This essentially means that the electron after being ionized from the target atom moves like a continuum electron with respect to the projectile ion. Clearly, the electron velocity (v_e) will have to be very close to the projectile velocity (v_p) to enable them to move away together in convoy from the residual target ion. Theoretically, it can be shown that the velocity distribution of the outgoing electron contains a singular term $|v_p - v_e|^{-1}$ and is solely responsible for producing a cusp in the double differential cross section (DDCS). The existence of such a cusp in the forward direction ($\theta \sim 0^o$) in the ion-atom collision has been observed both theoretically and experimentally. The early predictions of cusp electrons were made nearly three decades back by Macek [1] and Salin [2] and were subsequently confirmed by Crooks and Rudd [3].

For some time the ECC cusp was known to be a high energy ($v_p \gg 1$ a.u.) phenomenon in an ion-atom collision. Theoretical and experimental investigations of ECC cuspology at intermediate and high incident energies have been reported since the pioneering work by Crooks and Rudd [3]. An excellent review was presented by Schultz *et al.* [4] containing all important work on ECC prior to the mid-1990s. All these found the ECC peak at the equivelocity position $v_e = v_p$ and asymmetry of the curve on the two sides of the peak was also noticed, particularly for the lower projectile velocities. Here we shall discuss only a few theoretical [5–11] and experimental [12–16] works. Chan and Eichler [5] suggested that the asymmetry could be derived by accurate evaluation of the first Born amplitude, which was ruled out by Breinig *et al.* [12]. Shakeshaft and Spruch [6] showed that the second Born calculation, which includes the distortion of the electronic state by the electron–residual-ion interaction, can reproduce the asymmetry desired. This was further supported by theoretical [7,8] and experimental [13] investigations. The classical trajectory Monte Carlo (CTMC) theory of Olson and co-workers [9,10] (and references therein) successfully reproduced both the peak position and the asymmetry. Measurements on ECC by highly charged ions were also reported [14,15]. Later Weber *et al.* [16] observed an abrupt rise in the longitudinal momentum distribution of recoil ions in p+He collisions, which was shown to be related to the ECC phenomenon. Very recently a combined measurement and CTMC calculation reported by Shah *et al.* [17] observed for in collisions of low-energy protons on the hydrogen molecule that the ECC peaks are slightly shifted toward lower electron velocity. A similar combined study was reported by McGrath *et al.* [18] for the same targets but at 100 keV projectile energy. No signature of any shifting of peak position is noticed in this work [18] while theory and measurement agreed extremely well. However, Illescas *et al.* [19] found a shifting in a CTMC calculation of the asymptotic longitudinal momentum distribution for 20, 100, and 400 keV protons colliding with He. The relative measurement of Shah *et al.* [17] was normalized with their CTMC calculation and good agreement was found in terms of the peak position and the asymmetry of the two halves of the curve. However, the CTMC double-differential cross sections for both targets (H_2 and He) and at both energies (10 and 20 keV) show some irregular behavior, particularly to the left of the peak. This motivated us to study the system using an independent theoretical model of validity in the low-energy region.

II. THEORETICAL METHOD

Proton impact ionization of an helium atom in its ground state is studied in the impact parameter formalism. The internuclear motion is treated classically and the vector distance between the nuclei is taken to be $\vec{R}=\vec{b}+\vec{v}t$, where $\vec{b}$ is the impact parameter, $\vec{v}$ is the velocity of the projectile relative to the target, and t is the time measured from the instant of the closest approach of the two nuclei. The Hamiltonian for the electron moving in the field of the projectile and the residual target nucleus is given by (atomic units are used throughout)

$$H_e = -\frac{\nabla_r^2}{2} - \frac{Z_T}{r_T} - \frac{Z_P}{r_P}. \tag{1}$$

Here $\vec{r}$, $\vec{r}_P$, and $\vec{r}_T$ denote the position vectors of the electron relative to the origin (assumed to be the midpoint of the two nuclei), projectile, and target, respectively. The initial state wave function used in the present calculation is of the form

$$\Psi_1 = \Phi_i(r_T)\exp\left(-\frac{i}{2}\vec{v}\cdot\vec{r}\right)\exp\left(i\epsilon_{\mathrm{He}} - \frac{i}{8}v^2\right)t, \tag{2}$$

where $\Phi_i(r_T)$, the ground state helium wave function, is taken to be the Roothan-Hartree-Fock function expressed as

$$\Phi_i(r_T) = \sum_{\lambda=1}^{5} \frac{Z_\lambda^{3/2} b_\lambda}{\sqrt{\pi}} \exp(-Z_\lambda r_T), \tag{3}$$

with binding energy ϵ_{He}.

The development in time t of the electron wave function Ψ is given by the time-dependent Schrödinger equation

$$\left(H_e - i\frac{\partial}{\partial t}\right)\Psi = 0, \tag{4}$$

together with the initial condition that the electron is attached to the target in its ground state at time $t=-\infty$. We can then write

$$\Psi = \int C_{k'}\psi_{k'_C}^{-} d\vec{k}'_C + \sum_i a_i\psi_{P_i} + \sum_j b_j\psi_{T_j}, \tag{5}$$

where the first term represents the integral over the continuum states followed by the summation over the discrete states in the direct and charge transfer channels. The coefficients $C_{k'}$, a_i, and b_j are functions of time. Substituting Ψ in Eq. (4), we get

$$i\int \dot{C}_{k'}\psi_{k'_C}^{-} d\vec{k}'_C = \left(H_e - i\frac{\partial}{\partial t}\right)\left[\sum_i a_i\psi_{P_i} + \sum_j b_j\psi_{T_j}\right] + \int C_{k'}\left(H_e - i\frac{\partial}{\partial t}\right)\psi_{k'_C}^{-} d\vec{k}'_C. \tag{6}$$

Since $\psi_{k'_C}^{-}$ is an asymptotic solution of

$$\left(H_e - i\frac{\partial}{\partial t}\right)\psi_{k'_C}^{-} = 0, \tag{7}$$

and $C_{k'}$ is small, we can neglect the last term in Eq. (6). Then multiplying both sides of Eq. (6) by $\psi_{k'_C}^{-*}$ and integrating over $\vec{r}$ space we arrive at

$$\frac{\partial}{\partial t}(C_k) = -i\int \psi_{k_C}^{-*}\left(H_e - i\frac{\partial}{\partial t}\right)\left[\sum_{i,j}(a_i\psi_{P_i} + b_j\psi_{T_j})\right]d\vec{r}. \tag{8}$$

The ionization amplitude $C_k(t=+\infty)$ is obtained by time integration utilizing the initial condition $C_k=0$ at $t=-\infty$. The continuum state wave function occurring in the final channel is represented by the product of two Coulomb wave functions, which takes into account the distortion due to the Coulomb fields of the target and projectile nuclei:

$$\psi_{k_C}^{-} = N_1 N_2 e^{i\vec{k}\cdot\vec{r}}\,{}_1F_1(i\alpha_P, 1; -i(k_P r_P + \vec{k_P}\cdot\vec{r_P})) \times {}_1F_1(i\alpha_T, 1; -i(k_T r_T + \vec{k_T}\cdot\vec{r_T}))e^{-ik^2t/2}, \tag{9}$$

$\vec{k}$ being the momentum of the ejected electron, $\alpha_P=-Z_P/k_P$, $\alpha_T=-Z_T/k_T$, $\vec{k}_P=\vec{k}-\vec{v}/2$, $\vec{k}_T=\vec{k}+\vec{v}/2$, $N_1=e^{-\pi\alpha P/2}\Gamma(1+i\alpha P)$, and $N_2=e^{-\pi\alpha T/2}\Gamma(1+i\alpha T)$.

The discrete part of the wave function in Eq. (8) is obtained by solving the time-dependent Schrödinger equation

$$H_e\Psi_d = i\frac{\partial\Psi_d}{\partial t} \tag{10}$$

using the variational technique developed by Sil [20]. For this purpose we consider the integral

$$I = \frac{1}{2}\int\left[\Psi_d^*\left(i\frac{\partial}{\partial t} - H_e\right)\Psi_d + \Psi_d\left(-i\frac{\partial}{\partial t} - H_e\right)\Psi_d^*\right]d\vec{r}\,\mathrm{d}t \tag{11}$$

to be stationary with respect to small arbitrary variation of Ψ_d and its complex conjugate Ψ_d^*. The trial wave function Ψ_d here is a linear combination of two ground state wave functions 1 on the target and 2 on the projectile nucleus:

$$\Psi_d = A(t)\Psi_1 + B(t)\Psi_2, \tag{12}$$

where A and B are functions of time only, with

$$\Psi_1 = \phi_i(r_T)e^{i\epsilon_{\mathrm{He}}t-(i/8)v^2t}, \quad \Psi_2 = \frac{1}{\sqrt{\pi}}e^{-r_p}e^{i\epsilon_{\mathrm{H}}t-(i/8)v^2t}. \tag{13}$$

As above ϵ_{He} and ϵ_{H} are the binding energies of the helium and hydrogen atoms. The electron translational factor $e^{i\vec{v}\cdot\vec{r}}$ has been neglected here as we are interested in low-projectile-velocity impact. Ψ_1 and Ψ_2 are the normalized ground state wave functions of the helium and hydrogen atoms, respectively. Substituting the trial function $\Psi_d=A\Psi_1+B\Psi_2$ in Eq. (8) we get

$$C_K(t=+\infty)=\int_{-\infty}^{+\infty}dt\int\Psi_{k_c}^{-*}\left(H-i\frac{\partial}{\partial t}\right)(A\Psi_1+B\Psi_2)d\vec{r}$$
$$=-\int_{-\infty}^{+\infty}dt\int\Psi_{k_c}^{-*}\left[A\frac{Z_P}{r_P}\Psi_1+B\frac{Z_T}{r_T}\Psi_2+i(\dot{A}\Psi_1+\dot{B}\Psi_2)\right]d\vec{r}, \quad (14)$$

and rearranging the terms we finally get

$$C_k(t=+\infty)=-\int_{-\infty}^{+\infty}dt[Z_PAT_1+Z_TBT_2+i(\dot{A}S_1+\dot{B}S_2)] \quad (15)$$

where

$$T_1=\int\frac{\Psi_{k_c}^{-*}\Psi_1}{r_P}d\vec{r},\quad T_2=\int\frac{\Psi_{k_c}^{-*}\Psi_2}{r_T}d\vec{r},$$
$$S_1=\int\Psi_{k_c}^{-*}\Psi_1d\vec{r},\quad S_2=\int\Psi_{k_c}^{-*}\Psi_2d\vec{r},$$

which are functions of time. The evaluation of T_1, T_2, S_1, and S_2 is not straightforward and needs special attention. We shall describe their evaluation in the next section. In order to calculate the amplitudes $A(t)$,$B(t)$ and their time derivatives we first evaluate the space integration in Eq. (11) and write

$$I=\int L\,dt, \quad (16)$$

where

$$L=\frac{1}{2}[i\{g_{11}(A^*\dot{A}-A\dot{A}^*)+g_{12}(A^*\dot{B}-B\dot{A}^*)+g_{21}(B^*\dot{A}-A\dot{B}^*)$$
$$+g_{22}(B^*\dot{B}-B\dot{B}^*)\}-2A^*AF_{11}^B-A^*B(F_{12}^A+F_{12}^B)$$
$$-AB^*(F_{12}^{B*}+F_{12}^{A*})-2BB^*F_{22}^A] \quad (17)$$

and

$$F_{11}^P=\int\Psi_1^*V_P\Psi_1d\vec{r},\quad F_{12}^T=\int\Psi_1^*V_T\Psi_2d\vec{r},$$
$$F_{12}^P=\int\Psi_1^*V_P\Psi_2d\vec{r},\quad F_{22}^T=\int\Psi_2^*V_T\Psi_2d\vec{r},$$
$$g_{12}=\int\Psi_1^*\Psi_2d\vec{r},\quad g_{21}=g_{12}^*,\quad g_{11}=g_{22}=1,$$

where $V_P=-Z_P/r_P$ and $V_T=-Z_T/r_T$.

Making the integral $I=\int L\,dt$ stationary with respect to small arbitrary variations of A^* and B^*, we get coupled differential equations as follows:

$$2AF_{11}^P+B(F_{12}^T+F_{12}^P-i\dot{g}_{12})=2i(\dot{A}+\dot{B}_{g12}), \quad (18)$$

$$A(F_{12}^{P*}+F_{12}^{T*}-i\dot{g}_{12}^*)+2BF_{22}^T=2i(\dot{A}g_{12}^*+\dot{B}). \quad (19)$$

These coupled differential equations are then solved numerically using the Runge–Kutta method to obtain $A(t)$,$B(t)$ and their time derivatives as a function of time and the time integration in Eq. (15) is then performed to obtain $C_K(t=+\infty)$. In solving the differential equations numerically, we ensure unitarity of the integral $\int\Psi_T^*\Psi_T d\vec{r}$ throughout the time interval and we make use of the initial condition that at $t=-\infty$, $A=1$, and $B=0$. Finally the double-differential cross section is given by

$$\frac{d^2\sigma}{dE_e d\Omega_e}=\int d\vec{b}|C_K(t=+\infty)|^2. \quad (20)$$

III. EVALUATION OF T_1, T_2, S_1, AND S_2

The integrals T_1, T_2, S_1, and S_2 can be generated from a parent integral

$$J=\int\Psi_{k_c}^{-*}\frac{e^{-\lambda r_T-\mu r_P}}{r_Pr_T}d\vec{r} \quad (21)$$

by noting that

$$T_1=\lim_{\mu\to0}\left(\frac{\partial J}{\partial\lambda}\right),\qquad T_2=\lim_{\lambda\to0}\left(\frac{\partial J}{\partial\mu}\right),$$
$$S_1=\lim_{\mu\to0}\left(\frac{\partial^2 J}{\partial\lambda\,\partial\mu}\right),\quad S_2=\lim_{\lambda\to0}\left(\frac{\partial^2 J}{\partial\lambda\,\partial\mu}\right). \quad (22)$$

Using $\Psi_{k_c}^{-*}$ from Eq. (9) we can recast the integral in Eq. (16) as

$$J=\frac{2}{\pi}\int e^{i\vec{Q}\cdot\vec{R}}(E)^{-1-i\alpha_P}(E-F)^{i\alpha_P}(G)^{-1-i\alpha_T}(G-H)^{i\alpha_T}d\vec{Q}, \quad (23)$$

where

$$E=(\vec{Q}-\vec{k}/2)^2+\mu^2,\quad F=2[-\vec{k}_P\cdot(\vec{Q}-\vec{k}/2)+i\mu k_p], \quad (24)$$

$$G=(\vec{Q}+\vec{k}/2)^2+\lambda^2,\quad H=2[\vec{k}_T\cdot(\vec{Q}+\vec{k}/2)+i\lambda k_T]. \quad (25)$$

At this stage we perform the derivatives shown in Eq. (22) with respect to λ and μ to get T_1, T_2, S_1, and S_2. On introducing the limits some of these integrals can be performed numerically. Others behave as $(\vec{Q}\pm\vec{k}/2)^{-4}$ and possess serious numerical difficulty. Having realized that the dominating contributions to the $\vec{Q}$ integrand for these integrals come from the neighborhood of $\vec{Q}=\pm\vec{k}/2$, we use the substitution $\vec{Q}\pm\vec{k}/2=\epsilon\vec{r}$. This makes the angular integration easy to perform. The remaining radial part is then done analytically by choosing a suitable contour around the real axis.

IV. RESULTS AND DISCUSSION

Using the above theoretical method we have calculated the double-differential cross sections for ionization of He by

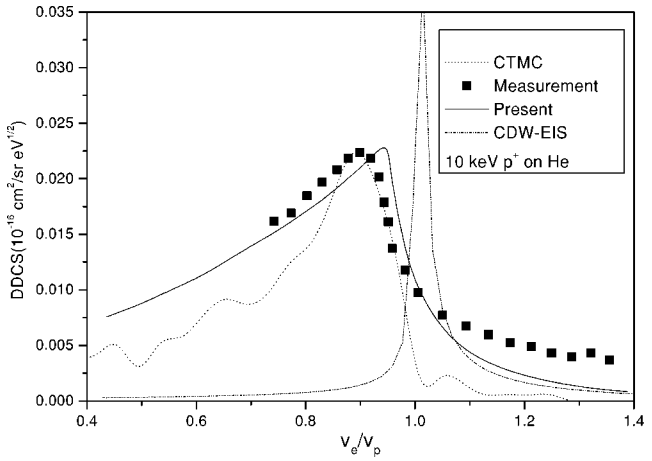

FIG. 1. Double-differential cross sections as a function of v_e/v_p for 10 keV protons colliding with He. Filled squares and dotted line are the results of Shah *et al.* [17] and solid line is the present result. Dash-dot-dotted line is the CDW-EIS result calculated using the computer code of McSherry *et al.* [23].

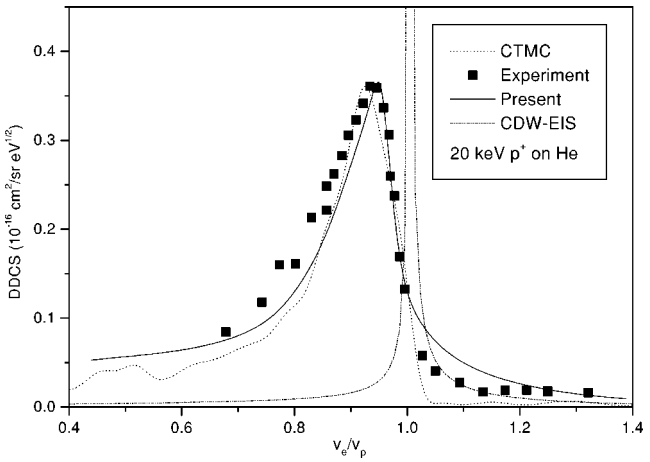

FIG. 2. Same as in Fig. 1 but for 20 keV protons on He.

proton impact. The present model takes into account the charge transfer channel, the effect of which is very important particularly at lower impact energies. In the ionization of helium atom by proton impact, the electron ejected from the target is carried along by the projectile for a short period. This indicates that an electron capture event, forming atomic hydrogen, has taken place before the electron is actually ionized and moves into the projectile continuum. We have incorporated this effect in our calculation. The results of 10 and 20 keV impact energies are presented in Figs. 1 and 2, respectively. The present results are compared with the combined theoretical (CTMC) and experimental work of Shah *et al.* [17]. In their work the relative measurement was normalized with the CTMC calculation. We are grateful to Shah and Illescas [21] for these data. The irregular behavior of the CTMC curve may be partly due to the statistical nature of CTMC calculations.

It is clear from Fig. 1 that the general behavior of our DDCS curve is very similar to the experimental data except that the position of the peak is slightly shifted toward a higher electron velocity in our case, but well below the $v_e = v_p$ position. Another important feature reproduced is the asymmetry about the peak. In Fig. 2, however, both the peak position and the asymmetry are in excellent agreement with the measurement. We note that the peak position moves slowly toward $v_e = v_p$ as the projectile velocity increases and the asymmetry about the peak is stronger at 10 than at 20 keV. This asymmetry was also noted [22] even for 191 keV protons on He. These are well-understood features: as the projectile velocity decreases, the effect of the residual target ion on the outgoing electron becomes even more prominent. It is of some concern that the peak position in our calculation at 10 keV (Fig. 1) does not quite agree with the CTMC calculation and the relative measurement [17]. The present calculation should be working at this energy where $v_p \sim 0.63$ a.u. The convergence of the different numerical integrations was checked by increasing the number of Gaussian points. The reason for any disagreement of the peak position at 10 keV incident energy is not very clear. We may presume that the influence of excited states of the hydrogen atom in the capture channel may improve the situation. An absolute measurement and further calculations at this energy are needed to draw a conclusion.

Finally, we have also used the CDW-EIS code [23] to calculate the double-differential cross sections for the same system and included these results in both Figs. 1 and 2. Clearly, at these low energies the CDW-EIS results give poor agreement both qualitatively and quantitatively. This is not surprising. The CDW-EIS code is a very successful approximation for ionization calculations but it is not expected to be valid when $Z_P/v_P < 1$ which is precisely the case in the present calculations at 10 and 20 keV. Besides, for such low projectile energies ($Z_P/v_P < 1$) the inclusion of an explicit capture channel is very important. Unfortunately, the CDW-EIS approximation does not account for such an explicit capture channel.

It is imperative that the present theoretical method be used in many ionization, charge transfer, and transfer ionization problems. In principle, it would be more useful for low-energy ionization of atoms by ionic projectiles of charge $Z_P > 1$ when capture into the excited states of the projectile followed by ionization would be important.

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