

Doubly differential cross sections for ionization in $\text{He}^{2+} + \text{He}$ collisions

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We study the $\text{He}^{2+} + \text{He}$ differential ionization problem using the two-electron wave-packet convergent close-coupling (WP-CCC) method. We present the results for doubly differential cross sections for ionization in terms of the angle and energy of the emitted electrons at intermediate collision energies. In this energy region, coupling between all reaction channels and electron-electron correlation effects are of considerable importance. These are fully accounted for in the WP-CCC approach. Overall, our results are in good agreement with the available experimental data and other theoretical calculations. We also discuss the saddle-point ionization mechanism for this collision system. It is concluded that this mechanism is not justified in the intermediate-energy region.

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I. INTRODUCTION

Electron production in collisions of protons and bare ions with helium has been intensively studied over the last several decades. In particular, ionization of He by He^{2+} ions has been a topic of discussion in a number of works (see, e.g., Refs. [1–8]). Most of the works for $\text{He}^{2+} + \text{He}$ collisions focused on providing integrated cross sections, however there are a few works available for differential ionization [9–15] and electron capture [16,17]. Although several attempts have been made to investigate two-electron processes such as double-ionization [2,4] and transfer-ionization [15,18], even the single-electron processes have not been completely understood, especially at the level of differential cross sections.

Barna *et al.* [6] applied a single-center atomic-orbital coupled-channel method to describe the ionization process in terms of total cross sections (TCSs) for $\text{He}^{2+} + \text{He}$ collisions above 600 keV/u, which showed good agreement with the experimental data available in this energy region. Moreover, two versions of the classical trajectory Monte Carlo (CTMC) method were tested. However, these approaches were not as successful as the close-coupling method. Another method applied was based on time-dependent density-functional theory (TDDFT) by Baxter and Kirchner [7] that uses two different models, the correlation-integral model of Wilken and Bauer (WB) and an independent-electron model (IEM). The TDDFT WB method showed better agreement than the TDDFT IEM one. The TCS for ionization were also studied by Terekhin *et al.* [8] using the three-body continuum distorted-wave (CDW) method with an eikonal initial state (EIS). Overall, all these theoretical approaches described the experimental data

of Refs. [1–5] on the integrated cross sections reasonably well (see, e.g., Ref. [19]).

In terms of the singly differential cross sections (SDCS), most of the works were devoted to studying electron-capture cross sections for $\text{He}^{2+} + \text{He}$ collisions rather than ionization. Several theoretical approaches have been applied to reproduce the experimental results of Schöffler *et al.* [17]. Zapukhlyak and Kirchner [20] employed the two-center basis generator method based on the IEM, Velayati *et al.* [21] applied the CDW approach using the EIS and eikonal final-state (EFS) descriptions, the three-body and four-body Coulomb-Born distorted-wave approximations were applied by Ghanbari-Adivi and Ghavaminia in Refs. [22] and [23], and Jana *et al.* [24] applied the distorted-wave approximation within the four-body formalism. The theoretical results showed different levels of agreement with the experimental data.

Bernardi *et al.* [10] presented the calculations based on the CDW and CTMC approaches along with the experimental results for the SDCS for ionization at 50 and 100 keV/u. The EIS approximation was employed within the CDW method. Both theoretical approaches described the measurements reasonably well.

Depending on the considered collision energies, various theoretical methods have been applied to the calculation of doubly differential cross sections (DDCS) for the $\text{He}^{2+} + \text{He}$ collision system. At high energies, where charge-transfer cross sections can be several orders of magnitude smaller than that for ionization [19], different forms of the Born approximation are applicable. Gayet and Salin [25] studied the amplitudes for ionization at high energies and showed that the Born approximation can be reliable starting from 0.75 MeV/u. The plane-wave first Born approximation (PWBA) was applied by Szabó *et al.* [26] to study the DDCS for 0.5 MeV/u $\text{He}^{2+} + \text{He}$ and $\text{He}^{2+} + \text{Ne}$ collisions at the backward ejection angles. For the helium target, their results showed good agreement with the available experimental data.

In the intermediate energy range, where the speed of the projectile is comparable to the orbital speed of electrons, more

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sophisticated theoretical approaches are needed to properly describe the underlying processes. Irby *et al.* [9] studied the DDCCS as a function of the speed and angle of the ejected electron at 100 keV/u both experimentally and theoretically. In their theoretical approach, they used the CTMC method. Although slight differences were seen between the predicted positions of the peak of the DDCCS at an ejection angle of 17° , the calculations agreed reasonably well with their own measurements.

Later, in the work of Bernardi *et al.* [10], the CDW-EIS approach was applied to calculate the DDCCS for ionization for the 100 keV/u $^3\text{He}^{2+} + \text{He}$ collision system as a function of the electron ejection energy at several ejection angles from 0° to 90° . For small ejection energies, considerable discrepancies were observed between the experimental data and the CDW-EIS results at ejection angles of 0° and 10° , where the theoretical results underestimated the experiment by a factor of 3. Furthermore, at large ejection energies, the CDW-EIS results overestimated the experiment at all angles.

Unlike the $p + \text{He}$ differential collision system, where experiments were well-described by theoretical approaches (see Refs. [27–29] and references therein), for the four-body differential problem of $\text{He}^{2+} + \text{He}$ collisions, there are some noticeable discrepancies even between the independent sets of experiments. Here we investigate the DDCCS using the wave-packet convergent close-coupling (WP-CCC) approach. One of the advantages of the approach in application to differential ionization processes is the possibility to investigate electrons ejected with arbitrary energy and into any angle. Moreover, in the process of ionization, we are able to distinguish the contributions of direct ionization and electron capture to the continuum, which can explain the emergence of some interesting features seen in the behavior of the differential ionization cross sections [30].

The WP-CCC approach has been employed to study collisions of fully stripped ions (such as protons, He^{2+} , C^{6+}) with helium for a wide-range of projectile energies. A single-center version of the approach applied to collisions of antiprotons and energetic protons with helium showed good agreement with the available experiments [31]. Later, a more comprehensive two-center WP-CCC approach, which takes into account the coupling between all possible reaction channels and electron-electron correlations, was developed and applied to the four-body $p + \text{He}$ scattering problem to calculate the integrated cross sections for all one-electron processes: electron capture, elastic scattering, target excitation and ionization, over a wide range of incident energies [32]. Very good agreement was observed in comparison with the available experiments and other theories for all considered processes. The WP-CCC method has also been applied to calculate singly and doubly differential cross sections for one-electron processes in $p + \text{He}$ collisions in Refs. [27–30,33]. Again, the calculated cross sections agreed with the experimental data very well. Overall, it was concluded that the WP-CCC approach can accurately describe the differential picture of all one-electron processes taking place in $p + \text{He}$ collisions at the levels of integrated, singly, and doubly differential cross sections.

The method was also extended to collisions of heavy projectiles with He. The integrated cross sections were presented in Ref. [19] for electron capture, elastic scattering, target

excitation, and ionization in $\text{He}^{2+} + \text{He}$ collisions for the incident energies from 10 keV/u to 5 MeV/u, with particular emphasis on the intermediate energies. The obtained results agreed well with the available experimental data for all considered processes. Very recently, the two-electron and effective one-electron WP-CCC approaches were employed to investigate the singly differential cross sections in the $\text{He}^{2+} + \text{He}$ collision system at intermediate projectile energies [34]. It was the first comprehensive calculation of the singly differential cross sections for all one-electron processes taking place in $\text{He}^{2+} + \text{He}$ collisions. Despite some discrepancies observed between the WP-CCC calculations and the experimental data for electron capture at 60 keV/u, the overall agreement was very good.

In this paper, we present the results, obtained using the WP-CCC method, for the DDCCS for $^3\text{He}^{2+} + \text{He}$ collisions in comparison with experiments and other available theoretical calculations. Moreover, we discuss the so-called saddle-point (SP) mechanism in ionization proposed by Irby *et al.* [9] and Gay *et al.* [12], which suggests that ejected electrons of velocities around v_{SP} find themselves stranded on the potential saddle between the residual target ion and outgoing projectile, where

$$v_{\text{SP}} = \frac{v_p}{1 + (q_p/q_T)^{1/2}}, \quad (1)$$

with v_p being the projectile speed and q_p and q_T are the charges of the projectile and the residual target ion, respectively. Since for the collision system of interest we have $q_p = 2$ and $q_T = 1$, according to the saddle-point ionization theory, the electrons ejected with speeds $v_e \approx v_{\text{SP}} = 0.41v_p$ should give a dominant contribution to the doubly differential ionization cross section. We test this claim.

Unless specified otherwise, atomic units (a.u.) are used throughout this paper.

II. WAVE-PACKET CONVERGENT CLOSE-COUPPLING APPROACH

Within the WP-CCC approach, the total scattering wave function Ψ is investigated by solving the full Schrödinger equation

$$(H - E)\Psi = 0, \quad (2)$$

where H is the Hamiltonian corresponding to the four-body $\text{He}^{2+} + \text{He}$ system, and E is the total energy. We expand the scattering wave function in terms of N target-centered and M projectile-centered pseudostates in the form

$$\begin{aligned} \Psi \approx & \sum_{\alpha=1}^N \mathcal{F}_\alpha(\sigma) \psi_\alpha^T(\mathbf{r}_1, \mathbf{r}_2) e^{ik_\alpha \sigma} \\ & + \frac{1}{\sqrt{2}} \sum_{\beta=1}^M [\mathcal{G}_\beta(\rho_1) \psi_\beta^P(\mathbf{x}_1) \psi_0(\mathbf{r}_2) e^{ik_{1\beta} \rho_1} \\ & + \mathcal{G}_\beta(\rho_2) \psi_\beta^P(\mathbf{x}_2) \psi_0(\mathbf{r}_1) e^{ik_{2\beta} \rho_2}], \end{aligned} \quad (3)$$

where ψ_α^T is the helium wave function, ψ_β^P is the wave function of the He^+ ion, and $\psi_0 = \psi_1^P$ is the ground-state wave function of the residual target ion, He^+ . The indices α and

β denote the full set of quantum numbers representing the corresponding states in the $\text{He}^{2+} + \text{He}$ and $\text{He}^+ + \text{He}^+$ channels, respectively. The vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ (respectively, $\mathbf{x}_1$ and $\mathbf{x}_2$) are the position vectors of the helium electrons with respect to the target (respectively, projectile) center, $\boldsymbol{\sigma}$ is the position vector of the projectile relative to center of mass of the target atom, and $\boldsymbol{\rho}_1$ ($\boldsymbol{\rho}_2$) is position vector of the system of projectile and the first (second) electron relative to the residual helium ion (see Fig. 1 of Ref. [19] for the Jacobi coordinate system). Furthermore, $\mathbf{k}_\alpha$ is the momentum of the projectile relative to the target and $\mathbf{k}_{1\beta}$ (and $\mathbf{k}_{2\beta}$) is the momentum of the formed He^+ ion relative to the residual target ion in the corresponding channels. The expansion coefficients $\mathcal{F}_\alpha$ and $\mathcal{G}_\beta$ in the asymptotic region after the collision represent the transition-probability amplitudes.

The He wave functions are obtained by numerically solving the corresponding Schrödinger equation for the He atom within the frozen-core approximation, while analytic forms of the wave functions are used for the He^+ ion. The pseudostates representing the continuum are constructed using the wave-packet approach [35], where the continuum is discretized into a number of bins. In each bin, we integrate the target (or projectile) continuum wave functions to obtain the corresponding wave-packet pseudostates. The corresponding positive-energy pseudostates together with the negative-energy eigenstates form bases for the projectile and target centers used in expansion (3).

We note that in this expansion, unlike for the traditional atomic-orbital close-coupling methods, the total scattering wave function does not require the so-called electron-translation factors. The problem with these factors is that they can be chosen in infinitely many ways [36]. See Ref. [37] for more discussion.

We insert expansion (3) into Eq. (2), then we use the semiclassical approximation and neglect the terms that vary slowly with time because they are negligible. Prior to the collision, we have $t = -\infty$ and $t = 0$ corresponds to the closest approach of the projectile ion. This approximation allows us to write a temporal dependence $\mathcal{F}_\alpha(\boldsymbol{\sigma}) \approx F_\alpha(t, \mathbf{b})$ and $\mathcal{G}_\alpha(\boldsymbol{\rho}_1) \approx \mathcal{G}_\alpha(\boldsymbol{\rho}_2) \approx G_\alpha(t, \mathbf{b})$, where the impact-parameter vector $\mathbf{b}$ is chosen to be perpendicular to $\mathbf{v}_p$, the initial velocity of the projectile. Finally, successively multiplying all the terms first by

$$\psi_{\alpha'}^{T*}(\mathbf{r}_1, \mathbf{r}_2) e^{-i\mathbf{k}_{\alpha'} \cdot \boldsymbol{\sigma}},$$

and then by

$$\psi_{\beta'}^{P*}(\mathbf{x}_1) \psi_0(\mathbf{r}_2) e^{-i\mathbf{k}_{1\beta'} \cdot \boldsymbol{\rho}_1} + \psi_{\beta'}^{P*}(\mathbf{x}_2) \psi_0(\mathbf{r}_1) e^{-i\mathbf{k}_{2\beta'} \cdot \boldsymbol{\rho}_2}.$$

Integrating over the variables $\mathbf{r}_1$ and $\mathbf{r}_2$, we obtain a system of differential equations for the expansion coefficients:

$$\begin{aligned} i\dot{F}_{\alpha'} + i \sum_{\beta=1}^M \dot{G}_\beta K_{\alpha'\beta}^T &= \sum_{\alpha=1}^N F_\alpha D_{\alpha'\alpha}^T + \sum_{\beta=1}^M G_\beta Q_{\alpha'\beta}^T, \\ i \sum_{\alpha=1}^N \dot{F}_\alpha K_{\beta'\alpha}^P + i \sum_{\beta=1}^M \dot{G}_\beta L_{\beta'\beta}^P &= \sum_{\alpha=1}^N F_\alpha Q_{\beta'\alpha}^P + \sum_{\beta=1}^M G_\beta D_{\beta'\beta}^P, \\ \alpha' &= 1, 2, \dots, N, \quad \beta' = 1, 2, \dots, M, \end{aligned} \quad (4)$$

where dots over the coefficients denote their time derivatives. For the full details of the exchange matrix elements $K_{\alpha'\beta}^T$, $Q_{\alpha'\beta}^T$, $K_{\beta'\alpha}^P$, and $Q_{\beta'\alpha}^P$, and direct matrix elements $D_{\alpha'\alpha}^T$, $L_{\beta'\beta}^P$, and $D_{\beta'\beta}^P$, refer to Ref. [19].

This system of differential equations is solved for each impact parameter b , subject to the initial boundary conditions

$$\begin{aligned} F_\alpha(-\infty, \mathbf{b}) &= \delta_{\alpha,1s}, \quad \alpha = 1, \dots, N, \\ G_\beta(-\infty, \mathbf{b}) &= 0, \quad \beta = 1, \dots, M, \end{aligned} \quad (5)$$

because initially the He atom is in the ground state. The solutions $F_\alpha(t, \mathbf{b})$ and $G_\beta(t, \mathbf{b})$ represent the transition-probability amplitudes as $t \rightarrow +\infty$, i.e., the direct-scattering and electron-capture transition-probability amplitudes are $F_\alpha(+\infty, \mathbf{b})$ and $G_\beta(+\infty, \mathbf{b})$, respectively.

For the initial channel, we set $\mathbf{q}_i = \mathbf{k}_1$. For the final channel, $\mathbf{q}_f = \mathbf{k}_{\alpha'}$ for direct scattering, and $\mathbf{q}_f = \mathbf{k}_{\beta'}$ for electron capture. Then, using the impact-parameter transition-probability amplitudes, we find the amplitudes for direct scattering (DS), T_{fi}^{DS} , and electron-capture (EC), T_{fi}^{EC} , in momentum space as

$$T_{fi}^{\text{DS}}(\mathbf{q}_f, \mathbf{q}_i) = 2\pi i v_p e^{im\phi_f} \int_0^\infty db b [\tilde{F}_f(b) - \delta_{fi}] J_m(q_\perp b), \quad (6)$$

$$T_{fi}^{\text{EC}}(\mathbf{q}_f, \mathbf{q}_i) = 2\pi i v_p e^{im\phi_f} \int_0^\infty db b \tilde{G}_f(b) J_m(q_\perp b), \quad (7)$$

where m is the magnetic quantum number in the final channel, ϕ_f is the azimuthal angle of $\mathbf{q}_f$, $q_\perp$ is the magnitude of the perpendicular component of the momentum transfer $\mathbf{q} = \mathbf{q}_i - \mathbf{q}_f = (\mathbf{q}_i - \mathbf{q}_f)_\parallel + (\mathbf{q}_i - \mathbf{q}_f)_\perp$, J_m is the Bessel function of the m th order, and $\tilde{F}_f(b) = e^{im\phi_b} F_f(+\infty, \mathbf{b})$, $\tilde{G}_f(b) = e^{im\phi_b} G_f(+\infty, \mathbf{b})$, with ϕ_b being the azimuthal angle of $\mathbf{b}$. For more details refer to Ref. [36].

These are used to find the amplitudes for direct ionization (DI),

$$T_{fi}^{\text{DI}}(\boldsymbol{\kappa}, \mathbf{q}_f, \mathbf{q}_i) = \sum_{\ell m} \langle \varphi_\kappa | \psi_f^T \rangle T_{fi}^{\text{DS}}(\mathbf{q}_f, \mathbf{q}_i), \quad (8)$$

and electron capture into the continuum (ECC),

$$T_{fi}^{\text{ECC}}(\boldsymbol{\kappa}, \mathbf{q}_f, \mathbf{q}_i) = \sum_{\ell m} \langle \varphi_\kappa | \psi_f^P \rangle T_{fi}^{\text{EC}}(\mathbf{q}_f, \mathbf{q}_i). \quad (9)$$

Here ℓ and m are the orbital and magnetic quantum numbers of the wave packet corresponding to the final state f , $\boldsymbol{\kappa}$ ($\boldsymbol{\kappa}$) is the momentum of the ejected electron relative to the target (projectile) nucleus, φ_κ (φ_κ) is the corresponding true continuum state of He (the hydrogen-like He^+ ion).

As the DI and ECC amplitudes from the target and the projectile centers are defined in different frames of reference, they cannot be combined straightaway. To combine the amplitudes with the same projectile momentum, we first transform the ECC amplitude into the laboratory frame as $\boldsymbol{\kappa} = \boldsymbol{\kappa} - \mathbf{v}_p$. Then, the fully differential cross section (FDCS) is given as

$$\begin{aligned} \frac{d^3\sigma_{\text{ion}}}{dE_e d\Omega_e d\Omega_f} &= \frac{\mu^2}{(2\pi)^5} \frac{q_f \kappa}{k_i} (|T_{fi}^{\text{DI}}(\boldsymbol{\kappa}, \mathbf{q}_f, \mathbf{q}_i)|^2 \\ &\quad + |T_{fi}^{\text{ECC}}(\boldsymbol{\kappa} - \mathbf{v}_p, \mathbf{q}_f, \mathbf{q}_i)|^2), \end{aligned} \quad (10)$$

where μ is the reduced mass for the $\text{He}^{2+} + \text{He}$ channel, $E_e = \kappa^2/2$ is the energy of the ejected electron, $\Omega_e = (\theta_e, \phi_e)$ and $\Omega_f = (\theta_f, \phi_f)$ are the solid angles of the ejected electron and the scattered projectile, respectively. In the laboratory frame, the momentum transfer $\mathbf{q}$ is replaced by $\mathbf{q} - \boldsymbol{\kappa}$. Therefore, perpendicular component $q_\perp$ is substituted with $(\mathbf{q} - \boldsymbol{\kappa})_\perp$ in calculating the integral in Eq. (7). We note that this choice of the incoherent combination of the transition amplitudes is consistent with the definition of the total ionization cross section in the close-coupling formalism, where the ionization cross section is obtained by summing the integrated cross sections for target excitation into the positive-energy pseudostates and electron capture into the continuum of the projectile.

Then, we can define the DDCS for ionization in ejection angle and energy

$$\frac{d^2\sigma}{dE_e d\Omega_e} = \int \frac{d^3\sigma}{dE_e d\Omega_e d\Omega_f} d\Omega_f. \quad (11)$$

This is not the only way of presenting the angular distribution of emitted electrons. The doubly differential cross sections can also be presented in the forms

$$\frac{d^2\sigma}{dv_e d\Omega_e} = v_e \frac{d^2\sigma}{dE_e d\Omega_e} \quad (12)$$

and

$$\frac{d^2\sigma}{dv_e} = \frac{1}{v_e} \frac{d^2\sigma}{dE_e d\Omega_e}, \quad (13)$$

where v_e is the ejected electron velocity.

III. DETAILS OF CALCULATIONS AND CONVERGENCE STUDIES

The size of the target and projectile bases, as well as all other numerical parameters, were increased systematically until results converged. In the expansion shown in Eq. (3), the target and projectile centers are described by the corresponding N and M pseudostates, respectively. For simplicity, in calculations we set $N = M$. For the DDCS to converge, bound states up to principal quantum number $n_{\max} = 8$ and 35 wave-packet bins were used. Orbital angular momentum up to $\ell_{\max} = 6$ was used. The distribution for the discretization bins to form the wave packets was nonuniform, making the more sensitive energy region denser and using a smaller number of pseudostates in the remaining part.

Calculations were performed for impact parameters up to 10 a.u., which was found to be sufficient for the probabilities of all processes to fall off several orders of magnitude from their respective maxima (see Fig. 1). The projectile position along the z axis was incremented from $z_{\min} = -300$ a.u. to $z_{\max} = 300$ a.u. for all impact parameters, where 1000 exponentially distributed z points were used with the density being greatest at the origin. In Fig. 1, we present the weighted ionization probability $bP(b)$ as a function of the impact parameter b for 100 keV/u ${}^3\text{He}^{2+} + \text{He}$ collisions. The plotted data are the results in the impact-parameter range 0–10 a.u. for the values $\ell_{\max} = 0, \dots, 6$. The figure demonstrates the behavior of the ionization probability depending on the impact parameter,

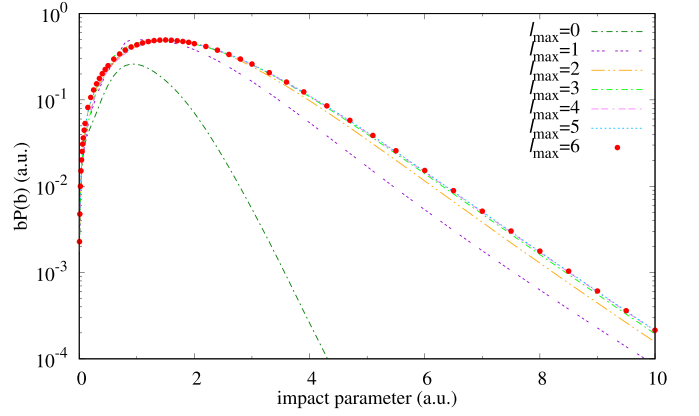


FIG. 1. Convergence of the weighted ionization probability $bP(b)$ for 100 keV/u ${}^3\text{He}^{2+} + \text{He}$ collisions as a function of impact parameter b with increasing $\ell_{\max}$, the maximum orbital angular-momentum quantum number of included states.

and it also shows the convergence of the probabilities in terms of $\ell_{\max}$. We can see that they converge very well. Furthermore, the probability declines sharply with the increase of the impact parameter, and it falls off more than three orders of magnitude already at 10 a.u. Increasing $b_{\max}$, the maximum of the impact parameters, further (up to 20) did not show any differences for the generated DDCS. This allows us to conclude that, at this collision energy, setting $b_{\max} = 10$ is reasonable. Similar conclusions were drawn for 250 keV/u.

Convergence of the results was checked in terms of all basis parameters such as the maximum principal quantum number and number of discretization bins, however here we demonstrate the convergence only with respect to the maximum orbital angular momentum because it appeared to be the most challenging one to establish. The DDCS differential in ejected-electron energy and angle, calculated using Eq. (11), for single ionization (SI) in 100 keV/u ${}^3\text{He}^{2+} + {}^4\text{He}(1s^2) \rightarrow {}^3\text{He}^{2+} + {}^4\text{He}^+(1s) + e^-$ collisions are presented in Fig. 2 for ejection angles of 10° , 30° , and 70° , where $\ell_{\max}$ is increased from 0 to 6. We observe varying levels of convergence depending on the ejection angle considered. For the ejection angles of 10° and 30° , the results converge very well and the difference between the $\ell_{\max} = 5$ and $\ell_{\max} = 6$ results is negligible. In the ejection angle of 70° , the results are also convergent up to 200 eV. For the other angles not shown in Fig. 2, the convergence pattern is similar. Even in the worst case, the deviation between the $\ell_{\max} = 5$ and $\ell_{\max} = 6$ results is within 30% for all ejection angles and energies. The data, which we are going to compare our results with, are all available in regions where WP-CCC results have demonstrated very good convergence. Therefore, we present the $\ell_{\max} = 6$ results as our final ones.

IV. DOUBLY DIFFERENTIAL CROSS SECTIONS FOR IONIZATION

Figure 3 presents the DDCS results for ionization in 100 keV/u ${}^3\text{He}^{2+} + \text{He}$ collisions as a function of ejected-electron energy in comparison with the corresponding experimental [9–12,14,15] and theoretical data [9,10] at several

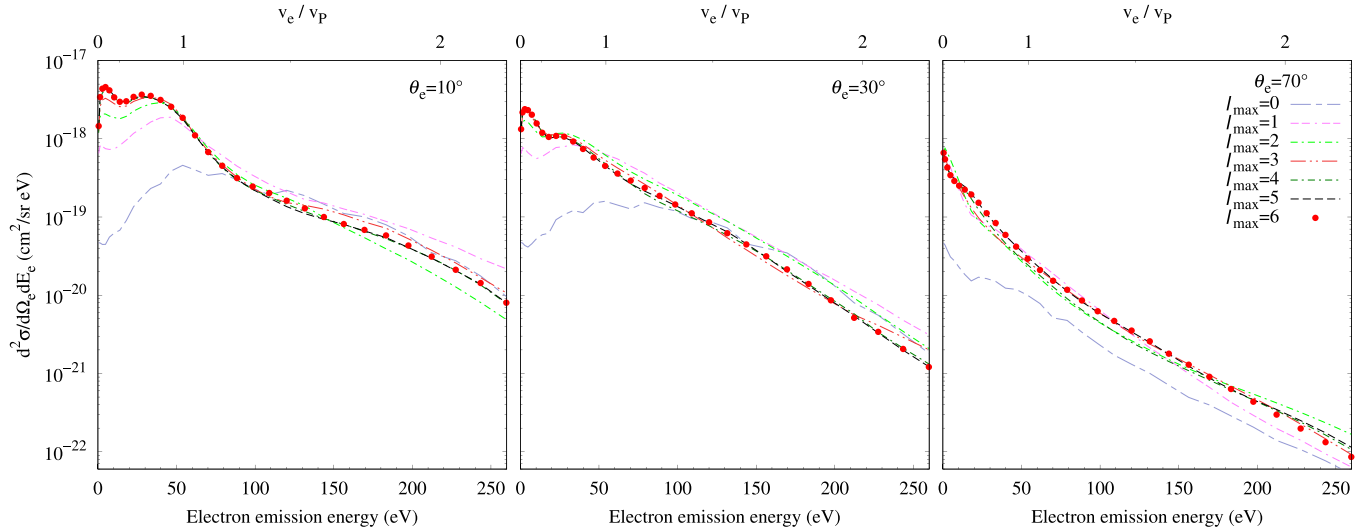


FIG. 2. Convergence of the doubly differential cross section for ionization in 100 keV/u ${}^3\text{He}^{2+} + \text{He}$ collisions as a function of the ejected electron energy with increasing ℓ_{max} at various emission angles.

fixed electron ejection angles from 10° to 90° . We note that, at some angles, the experimental results are provided for the total electron emission (TEE), which includes cross sections for all emission processes, such as single and double ionization, as well as transfer ionization and excitation ionization. They are denoted with stars (*) after the experiment name. The present results are expected to slightly underestimate these data. We notice an overall good agreement between the results. At the ejection angles of 20° and 45° , agreement between the WP-CCC results and the experimental data of Martínez *et al.* [15] is very good for SI of the target. Also, from that set of experimental data, we can see the difference between the SI cross sections and the TEE ones. It shows that, for this collision energy, SI is the dominant electron emission process, which is especially true for smaller ejection angles. We note that the difference in the shape of the WP-CCC results and the experimental TEE measurements of the Bariloche group at other angles is of a similar nature. In comparison with the other theoretical results, our results are in good agreement with the CDW-EIS calculations [10] for emission angles of 30° and 50° . However, for 10° and 17° some discrepancies are seen. They are especially noticeable at the smallest emission energies, where the CDW-EIS results underestimate all other results.

We also observe that there are some discrepancies between the two sets of experimental data by Gay *et al.* [12] and Bernardi *et al.* [10] at 10° and 20° , and between the data of Irby *et al.* [9] and Bernardi *et al.* [10] at 17° . The WP-CCC data align more closely with the data of Bernardi in terms of shape than those of Gay and Irby. Bernardi *et al.* [13], in their response to Ref. [12], mentioned that the measurements of Gay *et al.* [12] were not sufficiently reliable to make direct comparison with their data in Ref. [10]. Later, DuBois [14] reported the results that are consistent with those of Bernardi. They proposed that the data of Gay *et al.* [12] might be affected by the possible contamination of the He^{2+} beam by H_2^+ ions. They also showed the difference between the DDCS results obtained by the 100 keV/u H_2^+ and 100 keV/u He^{2+}

beams, which was considerable. Overall, it was concluded that the measurements of Irby *et al.* [9] and Gay *et al.* [12] were in error. For electron emission into 80° and 90° only the WP-CCC results are shown because there are no experimental or theoretical data to compare with for ejection angles larger than 70° .

The WP-CCC cross sections and typical contributions from the DI and ECC components are shown in Fig. 4 for 10° , 30° , and 70° . The cross sections show a local minimum for the angles up to 30° . It emerges due to combination of the ECC and DI components, according to the definition of the FDCS in Eq. (10), and reflects the fact that the two components peak at slightly different electron emission energies. This minimum could, to a certain extent, be an artifact of the incoherent combination of amplitudes used in this work. Note, however, the magnitude of the local minimum is comparable with, if not smaller than, the difference between the independent measurements (see the 10° , 17° , and 20° panels in Fig. 3). Starting from 45° , the DI component peaks in the forward direction, and the ECC one has a maximum at around 30 eV, and this remains reasonably consistent across all ejection angles. An example is shown for 70° ejection angle. As the electron ejection angle increases, the second maximum first takes the shape of a shoulder and then disappears. We can see that this is due to the falloff in the ratio of the ECC and DI peaks, which is almost 1 at 10° and is very small at 70° .

In Fig. 5, we present DDCS for SI at the collision energies of 250 keV/u for the electron ejection angles from 0° to 20° as a function of ejected-electron speed in three different formats. The results are compared with the experimental results of DuBois [14] available only at 15° . The experimental data are for the TEE, however, as we mentioned above, this comparison is justified by the fact that SI is the dominant process in electron emission at intermediate energies. The left column presents the ionization cross section differential in the speed and angle of the ejected electron using the form shown in Eq. (12), the middle column is differential in the energy and angle by Eq. (11), and the right column is differential in the

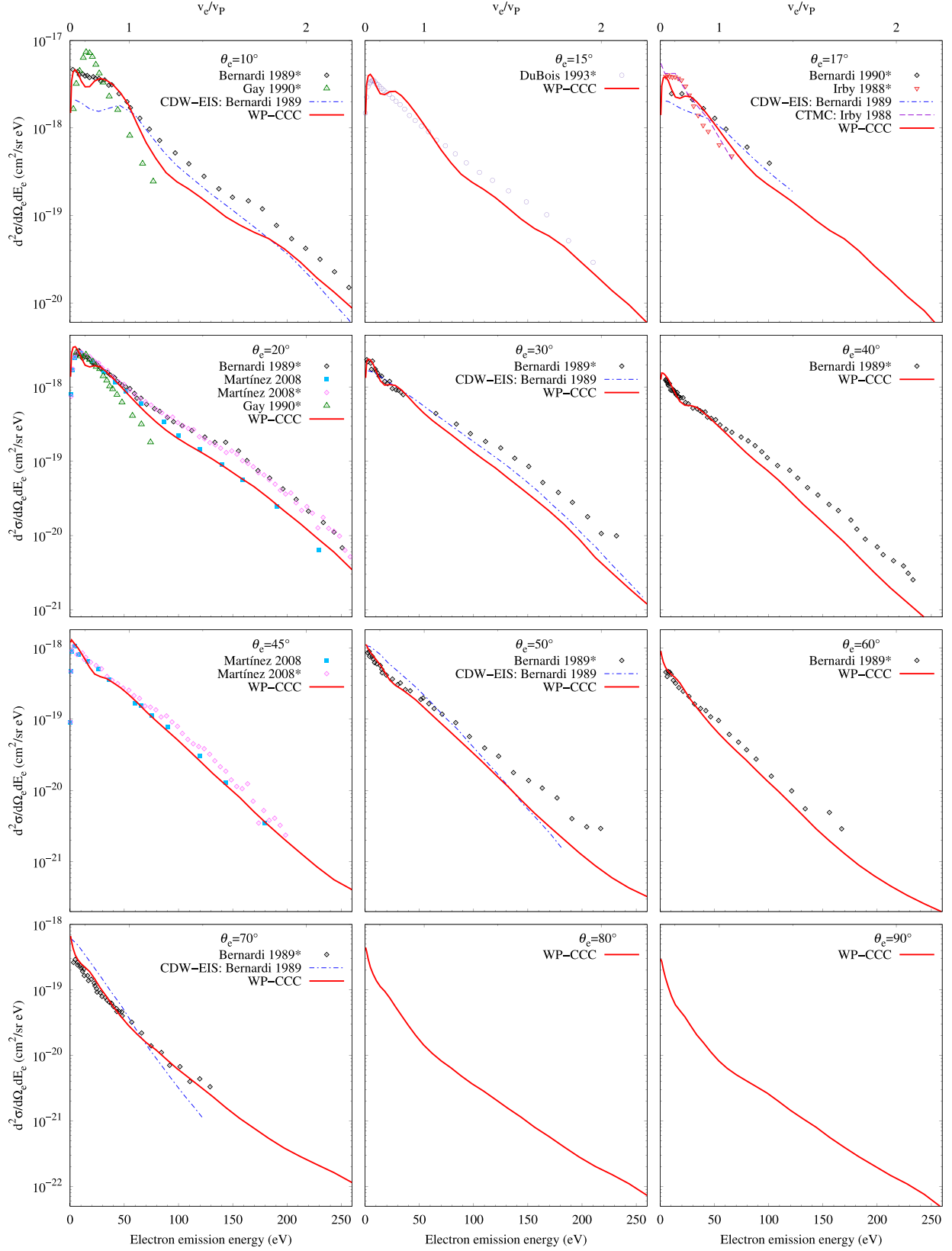


FIG. 3. Doubly differential cross section for ionization in 100 keV/u ${}^3\text{He}^{2+} + \text{He}$ collisions as a function of ejected-electron energy at various emission angles. The present WP-CCC results are represented by the red solid lines. The experimental data are from Bernardi *et al.* [10,11], Gay *et al.* [12], DuBois [14], Martínez *et al.* [15], Irby *et al.* [9], and the CDW-EIS calculations are from Bernardi *et al.* [10]. A star (*) stands for the data for total electron emission (including all emission processes).

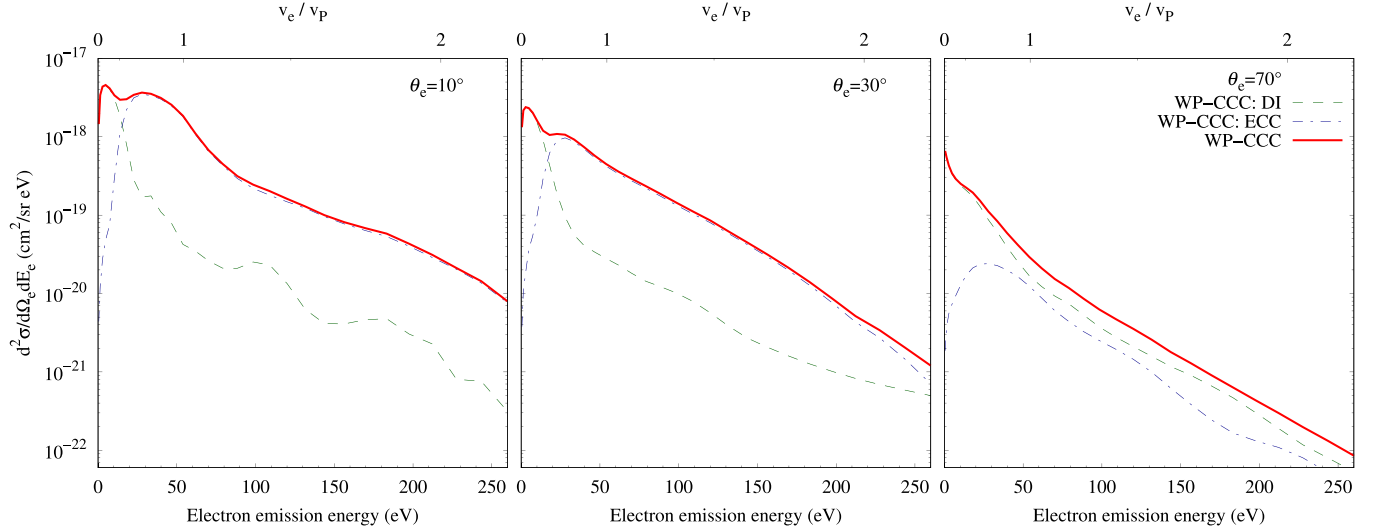


FIG. 4. Doubly differential cross section for ionization in 100 keV/u ${}^3\text{He}^{2+} + \text{He}$ collisions as a function of ejected-electron energy at various emission angles. The present WP-CCC results are shown together with their DI and ECC components.

velocity of the ejected electron by Eq. (13). In all panels the DI and ECC components of the WP-CCC cross sections are also shown. We note that, at 15° , as published in the original paper [14], at low electron velocity the data points are very congested making accurate extraction of the original values impossible. This may have affected the quality of the digitized data below $v_e/v_P = 0.2$. We observe very good agreement with the experimental data across the whole range of electron emission energies. Not surprisingly, agreement is good for all three representations of the DDCS, as the agreement in one should be reflected in the other formats as well. The purpose of comparing the results with the experiment in three ways is to show that the choice of the format is immaterial, and it is demonstrated in Fig. 5. However, depending on the way the DDCS is presented, certain parts of the space may be enhanced or, alternatively, suppressed. From the right panels, we can see that the third format of the DDCS ($d^2\sigma/dv_e$) is not very convenient for presenting physical results because it blows up in the part of the kinematic region corresponding to the emission of low-energy electrons, obscuring the rest of the collision space. This is due to the $1/v_e$ factor in its definition [see Eq. (13)].

Irby *et al.* [9] performed measurements and CTMC calculations of the DDCS at ejection angle of 17° and collision energies of 60, 100, and 120 keV/u. They observed that $d^2\sigma/dv_e d\Omega_e$ for the fixed ejection angle has a maximum when plotted as a function of the ejected-electron speed. They proposed that the peak is formed because of the denser electron distribution in the so-called saddle point of the heavy-particle interaction potential in the postcollisional system. It was also stated that, for $p + \text{He}$ collisions, the saddle-point speed is $v_{\text{SP}} = 0.5v_P$, and for $\text{He}^{2+} + \text{He}$ collisions it shifts to $v_{\text{SP}} = 0.41v_P$. This point is shown in Fig. 5 using a vertical line. Later, Gay *et al.* [12] supported this idea by providing the results of their further measurements and calculations. However, this topic has remained controversial [13–15]. Bernardi *et al.* [13] suggested that the results presented by Gay *et al.* [12] were insufficient to allow a

reliable comparison with their experiments and with the theoretical models. This view was supported by DuBois [14] based on experimental data for differential electron emission in H^+ and He^{2+} collisions with helium, who suggested that the He^{2+} measurements by Gay *et al.* [12] were in error. For detailed justification of this claim, see Ref. [14]. However, the idea of saddle-point ionization persisted [38] (see also Refs. [39,40]).

Figure 5 shows that the saddle-point ionization theory is not justified. If the electron is ejected in the forward direction, all three representations of the DDCS have a maximum at $v_e/v_P = 1$, which is due to ECC. In addition, $d^2\sigma/dv_e$ peaks at $v_e = 0$ as well. As the emission angle increases, the magnitude of the ECC peak sharply reduces while its position moves to the left away from the $v_e/v_P = 1$ point in all three representations. At the same time, the magnitude of the DI peak in $d^2\sigma/dv_e d\Omega_e$ and $d^2\sigma/dE_e d\Omega_e$ slightly reduces while its position does not change. As a result, the relative contribution of the DI component grows as the angle increases. At 5° the DI and ECC components become comparable leading to a double-peak structure. The DI component starts to dominate and becomes responsible for the single-peak structure starting from 10° . At 25° and above, the ECC component falls so much that even the shoulder seen in $d^2\sigma/dv_e d\Omega_e$ and $d^2\sigma/dE_e d\Omega_e$ at 10° , 15° , and 20° becomes hardly noticeable (not shown). Thus, the position of the peak in the net DDCS shifts to the DI peak position because the ECC component of the ionization cross sections quickly drops in magnitude as a function of the emission angle. We conclude that the peak in $d^2\sigma/dv_e d\Omega_e$ and $d^2\sigma/dE_e d\Omega_e$ for ejection angles above 10° is purely due to direct ionization. Thus, our calculations confirm the picture of differential ionization of helium induced by He^{2+} impact that is based on the experimental measurements by Bernardi *et al.* [10,11], Martínez *et al.* [15], and DuBois [14]. In the recent work of Spicer *et al.* [30], a similar conclusion was drawn based on the results provided for the $p + \text{He}$ system. The saddle-point mechanism of ionization was thoroughly studied for intermediate-energy collisions. The doubly differential cross sections for ionization for 52 and 103 keV

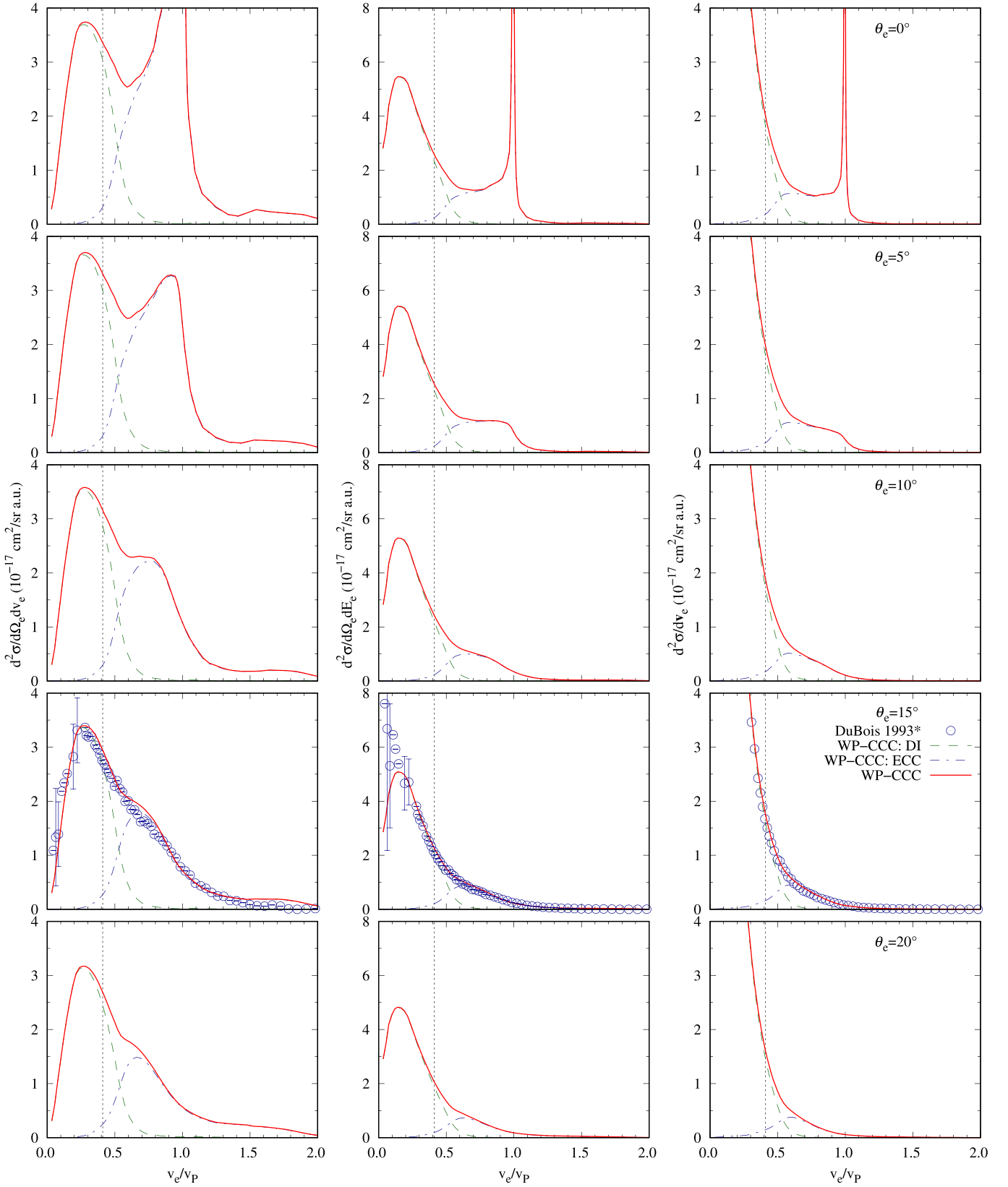


FIG. 5. Doubly differential cross section for ionization in 250 keV/u ${}^3\text{He}^{2+} + \text{He}$ collisions in three different forms given by Eqs. (12), (11), and (13) (the left, middle, and right columns, respectively). The electron ejection angles are $0^\circ, 5^\circ, 10^\circ, 15^\circ$, and 20° . The present WP-CCC results are represented by the red solid lines. The experimental TEE data are from DuBois [14]. The vertical line in each panel corresponds to $v_e/v_P = v_{SP} = 0.41$, the position of a saddle point expected according to Irby *et al.* [9].

collisions showed no sign of the saddle-point mechanism. It was concluded that the saddle-point ionization proposition at intermediate energies was not justified. The results presented here fully support this conclusion.

V. SUMMARY AND CONCLUSIONS

To summarize, we investigated the ionization cross sections differential in ejection energy and angle for the intermediate-energy ${}^3\text{He}^{2+} + \text{He}$ collisions using the four-body WP-CCC method. At 100 keV/u, the energy distribution of electrons were presented for ejection angles from 10° to 90° and were compared with the available experimental measurements. There are discrepancies in the experimental data presented by Gay *et al.* [12], Irby *et al.* [9], and Bernardi *et al.* [10] at small ejection angles. Our results showed better agreement with the latter ones. Overall, at other ejection angles the WP-CCC calculations agreed well with experiment, especially with the data of Martínez *et al.* [15], where agreement was very good. We also presented the DI and ECC components of the cross sections and found that at small ejection angles the ECC peak is responsible for the appearance of the second maximum. As the ejection angle increases, the contribution from the ECC component diminishes and becomes negligible. We also presented the doubly differential cross sections for 250 keV/u at the ejection angles between 0° and 20° . The results at 15° were compared with the corresponding

experimental measurements of DuBois [14], and they showed excellent agreement. We presented the results in three different forms which enabled us to analyze the saddle-point theory of ionization for the ${}^3\text{He}^{2+} + \text{He}$ system proposed by Irby *et al.* [9] and Gay *et al.* [12]. According to this proposition, the peak of ionization cross sections should be located at $v_e = 0.41 v_p$, independent of the ejection angle. However, as in the case of $p + \text{He}$ collisions [30], our results showed that it does not hold. The position of the ECC peak gradually moves to the left from $v_e = v_p$ and its magnitude drops with increasing ejection angle until it becomes negligible in comparison with the DI peak.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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- [1] L. J. Puckett, G. O. Taylor, and D. W. Martin, Cross sections for ion and electron production in gases by 0.15–1.00-MeV hydrogen and helium ions and atoms, *Phys. Rev.* **178**, 271 (1969).
 - [2] H. Knudsen, L. H. Andersen, P. Hvelplund, G. Astner, H. Cederquist, H. Danared, L. Liljeby, and K. G. Rensfelt, An experimental investigation of double ionisation of helium atoms in collisions with fast, fully stripped ions, *J. Phys. B: At. Mol. Phys.* **17**, 3545 (1984).
 - [3] R. D. DuBois, Ionization and charge transfer in He^{2+} -rare-gas collisions. II, *Phys. Rev. A* **36**, 2585 (1987).
 - [4] M. B. Shah and H. B. Gilbody, Single and double ionisation of helium by H^+ , He^{2+} and Li^{3+} ions, *J. Phys. B: At. Mol. Phys.* **18**, 899 (1985).
 - [5] M. B. Shah, P. McCallion, and H. B. Gilbody, Electron capture and ionisation in collisions of slow H^+ and He^{2+} ions with helium, *J. Phys. B: At. Mol. Opt. Phys.* **22**, 3037 (1989).
 - [6] I. F. Barna, K. Tokési, and J. Burgdörfer, Single and double ionization of helium in heavy-ion impact, *J. Phys. B: At. Mol. Opt. Phys.* **38**, 1001 (2005).
 - [7] M. Baxter and T. Kirchner, Time-dependent density-functional-theory studies of collisions involving He atoms: Extension of an adiabatic correlation-integral model, *Phys. Rev. A* **93**, 012502 (2016).
 - [8] P. Terekhin, P. Montenegro, M. Quinto, J. Monti, O. Fojón, and R. Rivarola, A critical study on electronic processes involving electron capture and ionization of He targets by interaction with multiply charged ion beams, *Nucl. Instrum. Methods Phys. Res. Sect. B* **408**, 150 (2017).
 - [9] V. D. Irby, T. J. Gay, J. W. Edwards, E. B. Hale, M. L. McKenzie, and R. E. Olson, Projectile-charge dependence of ejected-electron spectra, *Phys. Rev. A* **37**, 3612 (1988).
 - [10] G. C. Bernardi, S. Suárez, P. D. Fainstein, C. R. Garibotti, W. Meckbach, and P. Focke, Two-center effects in electron emission in ${}^3\text{He}^{2+}$ -He and H^+ -He collisions at intermediate energies, *Phys. Rev. A* **40**, 6863 (1989).
 - [11] G. Bernardi, P. Fainstein, C. R. Garibotti, and S. Suarez, Projectile charge dependence of the ionisation spectra for H^+ and ${}^3\text{He}^{2+}$ ions on He and Ne atoms, *J. Phys. B: At. Mol. Opt. Phys.* **23**, L139 (1990).
 - [12] T. J. Gay, M. W. Gealy, and M. E. Rudd, Projectile- and target-charge dependent effects in ionizing collisions of H^+ and He^{2+} with He, Ne and Ar atoms, *J. Phys. B: At. Mol. Opt. Phys.* **23**, L823 (1990).
 - [13] G. Bernardi, S. Suarez, P. Fainstein, C. Garibotti, W. Meckbach, and P. Fock, Reply to projectile- and target-charge dependent effects in ionizing collisions of H^+ and He^{2+} with He, Ne and Ar atoms, *J. Phys. B: At. Mol. Opt. Phys.* **23**, L829 (1990).
 - [14] R. D. DuBois, Differential electron emission for isotachic H^+ and He^{2+} impact on helium, *Phys. Rev. A* **48**, 1123 (1993).
 - [15] S. Martínez, G. Bernardi, P. Focke, S. Suárez, and D. Fregenal, Transfer ionization and total electron emission for 100 keV/amu He^{2+} colliding on He and H_2 , *J. Phys. B: At. Mol. Opt. Phys.* **41**, 145204 (2008).

- [16] V. Mergel, R. Dörner, J. Ullrich, O. Jagutzki, S. Lencinas, S. Nüttgens, L. Spielberger, M. Unverzagt, C. L. Cocke, R. E. Olson, M. Schulz, U. Buck, E. Zanger, W. Theisinger, M. Isser, S. Geis, and H. Schmidt-Böcking, State selective scattering angle dependent capture cross sections measured by cold target recoil ion momentum spectroscopy, *Phys. Rev. Lett.* **74**, 2200 (1995).
- [17] M. S. Schöffler, J. Titze, L. P. H. Schmidt, T. Jahnke, N. Neumann, O. Jagutzki, H. Schmidt-Böcking, R. Dörner, and I. Mančev, State-selective differential cross sections for single and double electron capture in $\text{He}^{+,2+}$ -He and p -He collisions, *Phys. Rev. A* **79**, 064701 (2009).
- [18] A. L. Godunov, J. H. McGuire, V. S. Schipakov, H. R. J. Walters, and C. T. Whelan, Total cross sections for transfer ionization in fast ion-helium collisions, *J. Phys. B: At. Mol. Opt. Phys.* **39**, 987 (2006).
- [19] S. U. Alladustov, C. T. Plowman, I. B. Abdurakhmanov, I. Bray, and A. S. Kadyrov, Wave-packet continuum discretization approach to He^{2+} -He collisions, *Phys. Rev. A* **106**, 062819 (2022).
- [20] M. Zapukhlyak and T. Kirchner, Projectile angular-differential cross sections for electron transfer processes in ion-helium collisions: Evidence for the applicability of the independent electron model, *Phys. Rev. A* **80**, 062705 (2009).
- [21] A. Velayati, E. Ghanbari-Adivi, and O. Ghorbani, Classical and semiclassical simulations of differential single charge exchange in fast alpha-helium collisions, *J. Phys. B: At. Mol. Opt. Phys.* **51**, 185201 (2018).
- [22] E. Ghanbari-Adivi and H. Ghavaminia, Electron capture by alpha particles from helium atoms in a Coulomb-Born distorted-wave approximation, *J. Phys. B: At. Mol. Opt. Phys.* **45**, 235202 (2012).
- [23] E. Ghanbari-Adivi and H. Ghavaminia, Differential single-capture cross sections for fast alpha-helium collisions, *Few-Body Syst.* **55**, 1109 (2014).
- [24] S. Jana, C. R. Mandal, and M. Purkait, Four-body charge transfer processes in collisions of bare projectile ions with helium atoms, *J. Phys. B: At. Mol. Opt. Phys.* **48**, 045203 (2015).
- [25] R. Gayet and A. Salin, Simultaneous capture and ionisation by fast ion impact on helium, *J. Phys. B: At. Mol. Phys.* **20**, L571 (1987).
- [26] G. Szabó, A. Kövér, and L. Gulyás, Ejected electrons at backward angles from He and Ne by He^{2+} impact, *Acta Phys. Hung.* **65**, 195 (1989).
- [27] K. H. Spicer, C. T. Plowman, I. B. Abdurakhmanov, A. S. Kadyrov, I. Bray, and S. U. Alladustov, Differential study of proton-helium collisions at intermediate energies: Elastic scattering, excitation, and electron capture, *Phys. Rev. A* **104**, 032818 (2021).
- [28] K. H. Spicer, C. T. Plowman, I. B. Abdurakhmanov, S. U. Alladustov, I. Bray, and A. S. Kadyrov, Proton-helium collisions at intermediate energies: Singly differential ionization cross sections, *Phys. Rev. A* **104**, 052815 (2021).
- [29] K. H. Spicer, C. T. Plowman, S. U. Alladustov, I. B. Abdurakhmanov, I. Bray, and A. S. Kadyrov, Doubly differential cross sections for ionisation in proton-helium collisions at intermediate energies: energy and angular distribution of emitted electrons, *Eur. Phys. J. D* **77**, 131 (2023).
- [30] K. H. Spicer, C. T. Plowman, N. W. Antonio, M. S. Schöffler, M. Schulz, and A. S. Kadyrov, Ruling out a saddle-point mechanism of ionization in intermediate-energy ion-atom collisions, *Phys. Rev. A* **109**, 062805 (2024).
- [31] I. B. Abdurakhmanov, A. S. Kadyrov, I. Bray, and K. Bartschat, Wave-packet continuum-discretization approach to single ionization of helium by antiprotons and energetic protons, *Phys. Rev. A* **96**, 022702 (2017).
- [32] S. U. Alladustov, I. B. Abdurakhmanov, A. S. Kadyrov, I. Bray, and K. Bartschat, Wave-packet continuum-discretization approach to proton collisions with helium, *Phys. Rev. A* **99**, 052706 (2019).
- [33] K. H. Spicer, C. T. Plowman, M. Schulz, and A. S. Kadyrov, Doubly differential ionization in proton-helium collisions at intermediate energies: Energy distribution of emitted electrons as a function of scattered-projectile angle, *Phys. Rev. A* **108**, 022803 (2023).
- [34] S. U. Alladustov, C. T. Plowman, M. S. Schöffler, I. Bray, and A. S. Kadyrov, Singly differential studies of one-electron processes in He^{2+} -He collisions, *Phys. Rev. A* **109**, 022805 (2024).
- [35] I. B. Abdurakhmanov, A. S. Kadyrov, and I. Bray, Wave-packet continuum-discretization approach to ion-atom collisions: Non-rearrangement scattering, *Phys. Rev. A* **94**, 022703 (2016).
- [36] B. H. Bransden and M. R. C. McDowell, *Charge Exchange and the Theory of Ion-Atom Collisions* (Clarendon, Oxford, 1992).
- [37] I. B. Abdurakhmanov, J. J. Bailey, A. S. Kadyrov, and I. Bray, Wave-packet continuum-discretization approach to ion-atom collisions including rearrangement: Application to differential ionization in proton-hydrogen scattering, *Phys. Rev. A* **97**, 032707 (2018).
- [38] V. D. Irby, Importance of electron time-of-flight measurements in momentum imaging of saddle-point electron emission, *Phys. Rev. A* **60**, 1135 (1999).
- [39] M. A. Abdallah and C. L. Cocke, Comment on “Importance of electron time-of-flight measurements in momentum imaging of saddle-point electron emission”, *Phys. Rev. A* **63**, 056701 (2001).
- [40] V. D. Irby, Reply to “Comment on ‘Importance of electron time-of-flight measurements in momentum imaging of saddle-point electron emission’”, *Phys. Rev. A* **63**, 056702 (2001).