C^{6+}-impact ionization of helium in the perpendicular plane: Ionization to the ground state, excitation-ionization, and relativistic effects

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In search of the discrepancy between theory and experiment in perpendicular plane geometry for C^{6+} ionization of He at 100 MeV/amu, we have used the first and second Born approximations to examine whether ionization to an excited He^+ state could be significant, whether relativistic effects could be important, and whether there is substantive sensitivity to the He wave functions used in the calculations. We fail to find any explanation of the discrepancy. Of the three possibilities, only relativistic effects turn out to be significant but then only in changing the overall normalization of the cross section, not in changing its shape, which is a prerequisite to getting agreement with experiment. The second Born calculations are in excellent accord with previous impact parameter coupled pseudostate results [Phys. Rev. A **81**, 042704 (2010)] and confirm, yet again, that elastic scattering of the projectile by the target nucleus cannot explain the discrepancy. The calculations are extended to the lower impact energy of 2 MeV/amu. Here, in perpendicular plane geometry, ionization to excited He^+ states becomes significant and we find an interesting "oscillatory" structure in both the ground- and excited-state cross sections. Comparison is made with some relative experimental data and, although the agreement is poor, possibly because of the need to include experimental resolutions, there are nuances in the data that mirror the structures in the calculations.

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I. INTRODUCTION

The cold target recoil ion momentum spectroscopy technique [1,2] is one of the most powerful experimental methods for probing ionization mechanisms in atomic physics. Where it throws up a difference with theory it is therefore necessary to take the disageement very seriously. In pioneering work to measure the fully differential cross section for single ionization of He by C^{6+} [3–11], a substantial disagreement between theory and experiment for electron ejection into a plane (more or less) perpendicular to the momentum transfer $\mathbf{q}$ was revealed [6,11]. Fiol *et al.* [12] have claimed that this difference can be explained by experimental resolutions but, on examining this point in more detail, Dürr *et al.* [13] have concluded that, even after experimental resolutions are taken into account, there still remains a residual effect in substantial disagreement with theory.

Schulz *et al.* [6] have proposed that (virtual) elastic scattering of the projectile by the ion (essentially the atomic nucleus), after the ionization event, might explain the difference. In Ref. [14] a quantitative model incorporating this mechanism has been constructed and seems to give support to the idea. However, the model has a certain roughness about it, not least the assumption that ionization is necessarily followed by elastic scattering. In Ref. [15] a much more firmly grounded approximation based on impact parameter pseudostate close-coupling, and explicitly including the projectile-nucleus interaction, failed to confirm the elastic scattering explanation.

In the perpendicular plane the fully differential cross section takes on its smallest values [15]. Consequently, its behavior in this plane could be changed by effects that otherwise would be relatively insignificant. With this in mind, there are a number of theoretical issues which, therefore, still need to be addressed. First, it would be useful to have confirmation of the pseudostate results from a completely different approximation which blatantly includes the projectile-nucleus interaction. Second, since the pseudostate approximation used frozen core He wave functions, a check using more sophisticated wave functions should be made. Voitkiv *et al.* [16] have emphasized this as a general point. Third, in the theoretical work so far undertaken it has been assumed that the He^+ ion ends up in its $1s$ ground state. Could the observed structure in the perpendicular plane be due to events in which the He^+ is left in an excited state (i.e., excitation-ionization)? Finally, could relativistic effects be important? The most intensively studied case has been C^{6+} impacting at 100 MeV/amu. This corresponds to an incident (nonrelativistic) speed of 63.5 atomic units (a.u.), i.e., almost half of the speed of light ($c = 137$ a.u.)! In (e,2e) relativistic effects have been observed to rotate cross-section peaks [17] and so might move much larger cross sections toward the perpendicular plane.

We engage these points as follows. Since the impact energies are high, we adopt a perturbative approach, going up to the second Born approximation. Within this approximation we are able to use He wave functions that are much more sophisticated than the frozen core approximation. The employment of accurate wave functions is also necessary for a realistic evaluation of excitation-ionization which, being a double excitation process, cannot be treated in the frozen core approximation and is quite sensitive to the quality of the He wave functions [18]. In studying relativistic effects we go only as far as the first Born approximation but this should be adequate [17] in indicating whether they change the picture.

The structure of this article is as follows. In Sec. II we describe our theoretical approximations: the impact parameter coupled pseudostate approximation in Sec. II A; the second

Born approximation in Sec. II B; and the relativistic first Born approximation in Sec. II C. In Sec. III A we compare our theoretical results with the much studied case of ionization at 100 MeV/amu and in Sec. III B with perpendicular plane measurements at the much lower impact energy of 2 MeV/amu. Our assessment of the theoretical-experimental situation is presented in Sec. IV. Throughout we use atomic units (a.u.) in which $\hbar = m_e = e = 1$. All reported cross sections refer to the laboratory frame of reference [19].

II. THEORY

A. The impact parameter coupled pseudostate approximation (CP)

This approximation uses frozen core He wave functions and has been described in detail in Refs. [19,20]. The particulars of the calculations are set out in Ref. [15]. Following Ref. [15] we have assessed the convergence of our results by comparing two calculations, one with 165 states and the other with 75 states. We have made such a comparison for all of the cases reported here and are satisfied that the 165 state approximation has adequately converged, it is these numbers which are reported here.

B. The second Born approximation (*B2*)

The second Born approximation to the scattering amplitude takes the form [18,21]

$$f^{\text{Born2}} = f^{B1} + f^{B2}, \tag{1}$$

where the first Born (*B1*) term is given by

$$f^{B1} = -\frac{1}{2\pi}\langle \mathbf{k}_f \psi_f | V | \mathbf{k}_0 \psi_0 \rangle \tag{2}$$

and the second Born term by

$$f^{B2} = -\frac{\mu}{8\pi^4} \lim_{\eta\to 0+} \sum_n \int d\mathbf{k} \langle \mathbf{k}_f \psi_f | V | \mathbf{k}\psi_n \rangle \frac{\langle \mathbf{k}\psi_n | V | \mathbf{k}_0 \psi_0 \rangle}{k_n^2 - k^2 + i\eta} \tag{3}$$

and where we use the compact notation

$$\langle \mathbf{k}_p \psi_p | V | \mathbf{k}_q \psi_q \rangle \equiv Z_P \langle e^{i\mathbf{k}_p\cdot\mathbf{R}} \psi_p(\mathbf{r}_1,\mathbf{r}_2) | \left(\frac{2}{R} - \frac{1}{|\mathbf{R}-\mathbf{r}_1|} - \frac{1}{|\mathbf{R}-\mathbf{r}_2|} \right) \times | e^{i\mathbf{k}_q\cdot\mathbf{R}} \psi_q(\mathbf{r}_1,\mathbf{r}_2) \rangle. \tag{4}$$

In (2) to (4), Z_P (=6) is the charge on the projectile; μ is the reduced mass of the projectile-atom system; $\mathbf{k}_0 = \mu\mathbf{v}_0$ and $\mathbf{k}_f = \mu\mathbf{v}_f$, where $\mathbf{v}_0(\mathbf{v}_f)$ is the initial (final) velocity of the projectile relative to the target; ψ_0 (ψ_f) is the initial (final ionized) state of the He atom; and $\mathbf{R}$ ($\mathbf{r}_i$) is the position vector of the projectile (ith electron) relative to the target nucleus. In (3) the sum is over all states ψ_n (energy ϵ_n) of the atom and

$$k_n^2 = k_0^2 + 2\mu(\epsilon_0 - \epsilon_n). \tag{5}$$

In the laboratory frame the fully differential cross section [we shall call it the triple differential cross section (TDCS)] in the second Born approximation is given by [19]

$$\frac{d^3\sigma^L}{dE d\Omega_e d\Omega_p} = \frac{v_f \kappa}{v_0} m_P^2 |f^{\text{Born2}}|^2, \tag{6}$$

where $\boldsymbol{\kappa}$ is the momentum of the ionized electron and m_P is the mass of the projectile. The cross section (6) corresponds to the projectile being scattered into the solid angle $d\Omega_p$ in the laboratory while the ionized electron is ejected into the solid angle $d\Omega_e$ with energy in the range E to $E + dE$. It is assumed that the target atom is initially at rest in the laboratory.

We note that the interaction $2Z_P/R$ between the projectile and the atomic nucleus, the key element of the elastic scattering explanation advanced in Refs. [6] and [14], survives in (4) only if $\psi_p = \psi_q$. This means that it does not contribute to the first Born term (2) but does contribute to the second Born term (3) for $\psi_n = \psi_0$ or ψ_f. The interpretation of (3) when $\psi_n = \psi_0$ is that the projectile elastically scatters (virtually) off the initial state of the atom and then ionizes it. When $\psi_n = \psi_f$, the projectile first ionizes the atom and then elastically scatters on the ionized state. It is the latter which is invoked in Refs. [6] and [14].

To evaluate the second Born term (3) we use the closure approximation [22] and set k_n^2 to an average value $\overline{k}^2$, where

$$\overline{k}^2 = k_0^2 + 2\mu(\epsilon_0 - \overline{\epsilon}) \tag{7}$$

and $\overline{\epsilon}$ is an average energy. The completeness of the atomic states ψ_n is then used to trivially perform the sum over n in (3) and leave a computationally feasible form as described in Ref. [21]. The closured second Born approximation is complementary to the impact parameter coupled pseudostate approximation (CP) in the following sense [23]. In the CP approximation the set of states is not complete but energy differences between states are respected. In the second Born approximation the completeness of the states is maintained but at the price of sacrificing energy differences. Another complementary element is that (2) and (3) come from a full wave treatment of the problem while CP resorts to a straight line impact parameter treatment, although, as argued in Ref. [19], at the impact energies studied here there should be neglegible difference between the two approaches.

A negative feature of the closure approximation is the need to choose an average energy $\overline{\epsilon}$. There is no rigorous procedure for making this choice. For low ejected energies, as here, a suitable choice seems to be the first ionization threshold [21,24,25], i.e.,

$$\overline{\epsilon} - \epsilon_0 = 0.9033 \text{ a.u.} \tag{8}$$

for both ionization to the ground state and excitation-ionization. To get some feeling for sensitivity to the value of $\overline{\epsilon}$, within reasonable limits, we have also evaluated the case

$$\overline{\epsilon} = \epsilon_0. \tag{9}$$

To calculate (2) and the closured version of (3) we need only to know the initial and final He wave functions. We consider two options.

Option 1. We adopt the frozen core approximation, taking ψ_0 to be the ground state wave function from the 165-state CP approximation and ψ_f to be the static exchange wave function, with ingoing scatted wave boundary conditions, for electron scattering by $He^+(1s)$, see Ref. [19].

Option 2. In calculating f^{B1} we take ψ_0 to be the highly accurate ground state wave function of Kinoshita [26] and ψ_f to be the wave function for electron scattering by $He^+(1s)$ in a 60-state coupled pseudostate approximation as described in Ref. [18]. For f^{B2} we take ψ_0 to be the wave function of Byron and Joachain [27] and ψ_f to be the three-state $1s$-$2s$-$2p$ close coupling wave function for $e^- + \mathrm{He}^+(1s)$ scattering, again as described in Refs. [18,21].

For excitation-ionization we consider only the case where He^+ is left in the $n = 2$ states and choose Option 2 where now ψ_f corresponds to electron scattering off the the $2s$ and $2p_{0,\pm 1}$ states of He^+ as appropriate, see Ref. [21]. For excitation-ionization it is essential that high-quality wave functions are used for the calculation of f^{B1} although, as argued in Ref. [18], lesser quality wave functions can be employed for f^{B2}. Details of how f^{B1} and f^{B2} are calculated are given in Refs. [18,21].

C. The relativistic first Born approximation

Following the derivation of Voitkiv *et al.* [28], the TDCS in the relativistic first Born approximation, and in the laboratory frame of reference, is given by

$$\frac{d^3\sigma_{\mathrm{rel}}^{L,B1}}{dE\,d\Omega_e\,d\Omega_p} = 4\alpha Z_P^2 m_P^2 \frac{k_f^L \kappa}{k_0^L}\frac{1}{q^4}|\langle\psi_f|e^{i\mathbf{q}\cdot\mathbf{r}_1} + e^{i\mathbf{q}\cdot\mathbf{r}_2}|\psi_0\rangle|^2, \tag{10}$$

where

$$\alpha \equiv \frac{\left(1+\frac{E_{\mathrm{kin}}}{m_P c^2}\right)^2}{\left[1-\left(\frac{\kappa^2+2I}{2cq}\right)^2\right]^2}. \tag{11}$$

In (10) and (11), $\mathbf{k}_0^L$ ($\mathbf{k}_f^L$) is the initial (final) momentum of the projectile in the laboratory, E_{kin} is the kinetic energy of the incident projectile, $\mathbf{q} \equiv \mathbf{k}_0^L - \mathbf{k}_f^L$ is the momentum transfer in the collision, and I is the ionization potential for the appropriate final ionic state of He^+, and we have taken the He wave functions to be nonrelativistic. Since, at the energies considered here, k_f^L/k_0^L and v_f/v_0 [see (6)] are effectively unity, we see that

$$\frac{d^3\sigma_{\mathrm{rel}}^{L,B1}}{dE\,d\Omega_e\,d\Omega_p} = \alpha \frac{d^3\sigma_{\mathrm{non-rel}}^{L,B1}}{dE\,d\Omega_e\,d\Omega_p}, \tag{12}$$

where $d^3\sigma_{\mathrm{non-rel}}^{L,B1}/dE\,d\Omega_e\,d\Omega_p$ is the nonrelativistic first Born cross section; see (6). Thus, for given κ and q, relativistic effects merely change the overall normalization of the nonrelativistic first Born TDCS, in particular there is no rotation of the binary and recoil peaks that might lead to structure in the perpendicular plane. At this level of approximation relativistic effects cannot explain the observed structure at 100 MeV/amu [6,11].

III. RESULTS

In displaying our results we adopt the following conventions. We take the z direction to be the direction of the incident projectile. The incident and scattered projectile define the x-z plane with the scattered projectile coming out on the negative x side. This Cartesian coordinate system is completed with a y axis to form a right-handed set. We study electron ejection in the x-z plane (coplanar geometry) and in the y-z plane (perpendicular plane geometry). In these geometries we adopt the convention that angles are measured from the z axis with those in the positive (negative) x or y half-plane lying in the range 0° to 180° (0° to −180°).

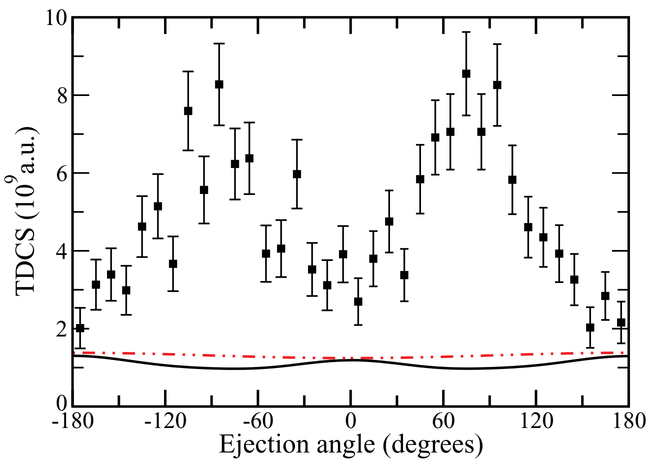

FIG. 1. (Color online) TDCS at 100 MeV/amu, $q = 0.75$ a.u., and an ejected electron energy of 6.5 eV in perpendicular plane geometry: (solid black curve) CP approximation and (dash-double-dot red curve) first Born approximation; experimental data from Ref. [6].

Where the He^+ ion is left in an excited state, e.g., $\mathrm{He}^+(2p_{\pm1})$, our convention is that the quantization axis for the ion state is taken in the direction of the outgoing electron [21].

A. 100 MeV/amu impact energy

Figure 1 illustrates the problem addressed in this article. It shows the TDCS in the perpendicular plane (the y-z plane) for an electron ejection energy of 6.5 eV and a momentum transfer q of 0.75 a.u. Shown are the experimental data from Ref. [6] (see also Ref. [12]) together with the CP and first Born calculations from Ref. [15] in the frozen core approximation. There is a marked difference between experiment and theory. The experimental data indicate two large peaks near ±90° while, in complete contrast, the CP approximation shows two shallow dips at these positions. The first Born cross section is almost flat and close to the CP cross section. Dürr *et al.* have analyzed the resolutions in this experiment and conclude that they account for less than 50% of the structure seen in the experimental data, i.e., that experiment suggests a much larger cross section than theory with peaks, not dips, at ±90°.

First, let us lay to rest again the possibility that the difference can be explained by elastic scattering of the projectile by the ion [6,11,14]. In Fig. 2 we compare the CP approximation with the second Born approximation (*B2*). The agreement between CP and *B2* is very good. For *B2* we have used the same frozen core wave functions for ψ_0 and ψ_f as in CP, i.e., Option 1 of Sec. II B. We also show the *B2* results for the two different closure energies (8) and (9); there is little sensitivity to the choice. As explained in Sec. II B, the *B2* approximation is in many ways complementary to CP and clearly incoporates elastic scattering of the projectile by the nucleus through the terms $\psi_n = \psi_f$ and $\psi_n = \psi_0$ in (3). We conclude again [15] that elastic scattering of the projectile by the ion cannot explain the experimental data.

But, what about sensitivity to the choice of ψ_0 or ψ_f? Figure 3(a) compares the first and second Born approximations of Fig. 2, calculated using the frozen core wave functions

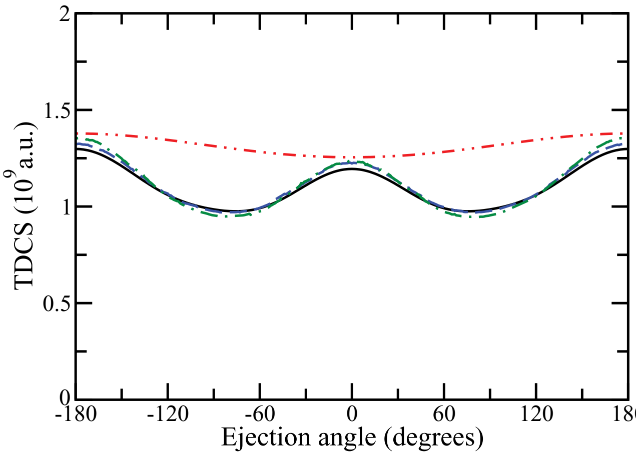

FIG. 2. (Color online) TDCS at 100 MeV/amu, $q = 0.75$ a.u., and an ejected electron energy of 6.5 eV in perpendicular plane geometry: (solid black curve) CP approximation, (dash-double-dot red curve) first Born approximation, (dashed blue curve) *B2* approximation with $\overline{\epsilon} - \epsilon_0 = 0.9033$ a.u., and (dash-dot green curve) *B2* approximation with $\overline{\epsilon} = \epsilon_0$.

(Option 1), with the same approximations evaluated using the more sophisticated wave functions of Option 2. In the *B2* calculations the average energy (8) has been used. For Option 2 the pedigree of the first Born term is excellent, as shown by the very good agreement between length and velocity forms in Ref. [18]. In the perpendicular plane the improved wave functions tend to reduce the cross section by about 3% but, more importantly, make no change to its shape. In coplanar geometry, Fig. 3(b), improving the wave functions reduces the binary peak by about 10%. The coplanar *B1* cross section calculated using Option 1 [not shown in Fig. 3(b)] almost coincides with the *B2* cross section of Option 2.

Figure 4 shows the cross sections for excitation-ionization to the $n = 2$ states of He^+. Let us look at perpendicular plane geometry first, Fig. 4(a). Here the first Born (*B1*) cross sections are quite flat but the *B2* cross sections display an "oscillatory" structure with peaks at 0°, $\pm 90^\circ$, and $\pm 180^\circ$. It is noteworthy that the first Born $He^+(2p_\pm)$ cross sections are symmetric about 0° but the *B2* cross sections are not, being mirror images of each other about this line. The full $He^+(n = 2)$ cross section, the sum of all the $n = 2$ cross sections, is, as it must be, symmetric about 0° for both *B1* and *B2*. Comparing figures 4(a) and 3(a), we see that excitation-ionization to $He^+(n = 2)$ amounts to about 5% of the TDCS in the perpendicular plane. Ionization to an excited He^+ state is therefore unlikely to account for the discrepancy between theory and experiment seen in Fig. 1.

The "oscillatory" structure seen in Fig. 4(a) is worthy of comment. It obviously comes from higher-order interactions implicit in the second Born term f^{B2}. We shall see this structure developing in the ground state $He^+(1s)$ CP cross section of Figs. 5(a) and 7 at the lower impact energy of 2 MeV/amu and persisting in the $He^+(n = 2)$ cross section of Figs. 6(a) and 7 at this energy. We note that it is also present in the Glauber and CDW-EIS cross sections calculated by Voitkiv *et al.* [16] for a projectile with $Z_P = 30$ incident on H at $v_0 = 60$ a.u.. It is clear that under the right circumstances there

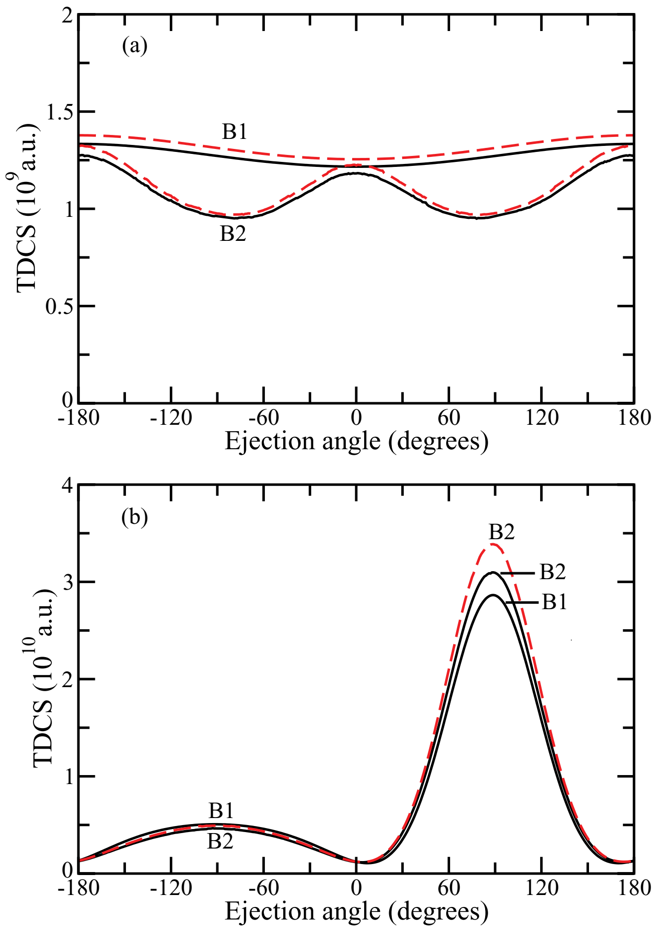

FIG. 3. (Color online) TDCS at 100 MeV/amu, $q = 0.75$ a.u., and an ejected electron energy of 6.5 eV in (a) perpendicular plane geometry, (b) coplanar geometry: (dashed red curves) calculated with frozen core wave functions (Option 1) and (solid black curves) calculated with improved (Option 2) wave functions. *B1* (*B2*) = first (second) Born approximation.

is pronounced structure in the perpendicular plane. However, for C^{6+} incident on He at 100 MeV/amu that structure has largely disappeared and we are left with only a vestige of its former prominence, as seen in the CP cross section of Fig. 1.

Figure 4(b) shows the $He^+(n = 2)$ cross sections in coplanar geometry. Apart from $He^+(2p_{\pm 1})$, the *B1* cross sections are larger in the recoil region (around -90°) than in the binary region (around $+90^\circ$); the reverse is true in the *B2* approximation. The *B1* and *B2* cross sections for $He^+(2p_{\pm 1})$ are very similar, peaking near 0° and $\pm 180^\circ$, and the $2p_{-1}$ and $2p_{+1}$ cross sections in each approximation are identical, as they must be in coplanar geometry. It is also noteworthy that, unlike ionization to $He^+(1s)$, Fig. 3, the $He^+(n = 2)$ cross section is of similar size in the perpendicular and coplanar geometries. Comparing Figs. 4(b) and 3(b), it is clear that excitation-ionization has even less impact in coplanar geometry.

Finally, we come to relativistic effects. From (11) and (12) we calculate that the first Born cross sections will be raised by 22% due to relativitic effects, this is not insubstantial but is an overall normalization effect, not a change in shape.

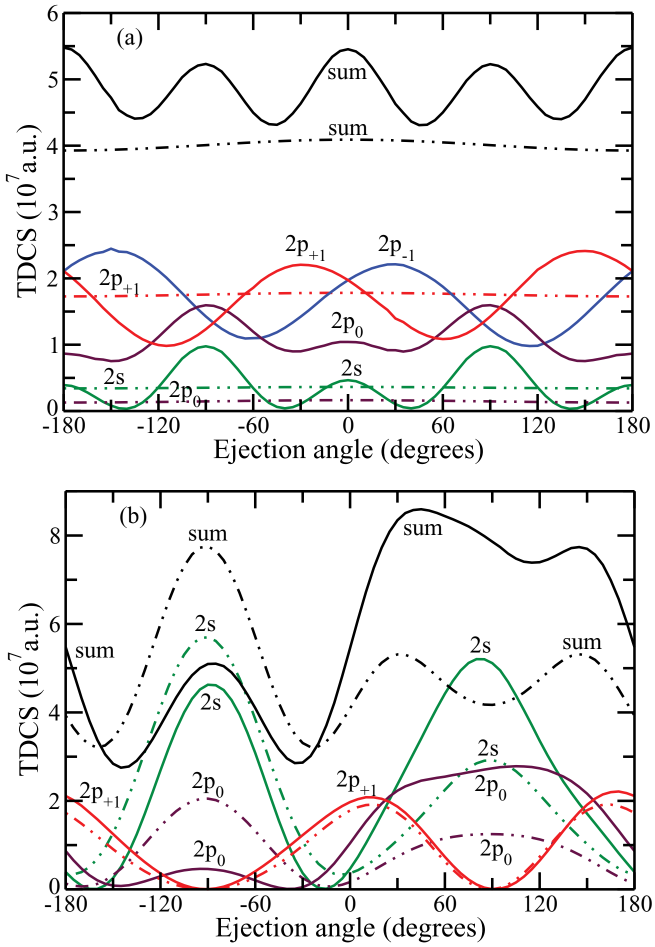

FIG. 4. (Color online) TDCS for excitation-ionization to $He^+(n=2)$ at 100 MeV/amu, $q=0.75$ a.u., and an ejected electron energy of 6.5 eV in (a) perpendicular plane geometry and (b) coplanar geometry: (solid curves) second Born approximation and (dash-double-dot curves) first Born approximation. Note that for $2p_{+1}$ and $2p_{-1}$ the first Born cross sections are identical in all geometries while the second Born cross sections are only identical in coplanar geometry.

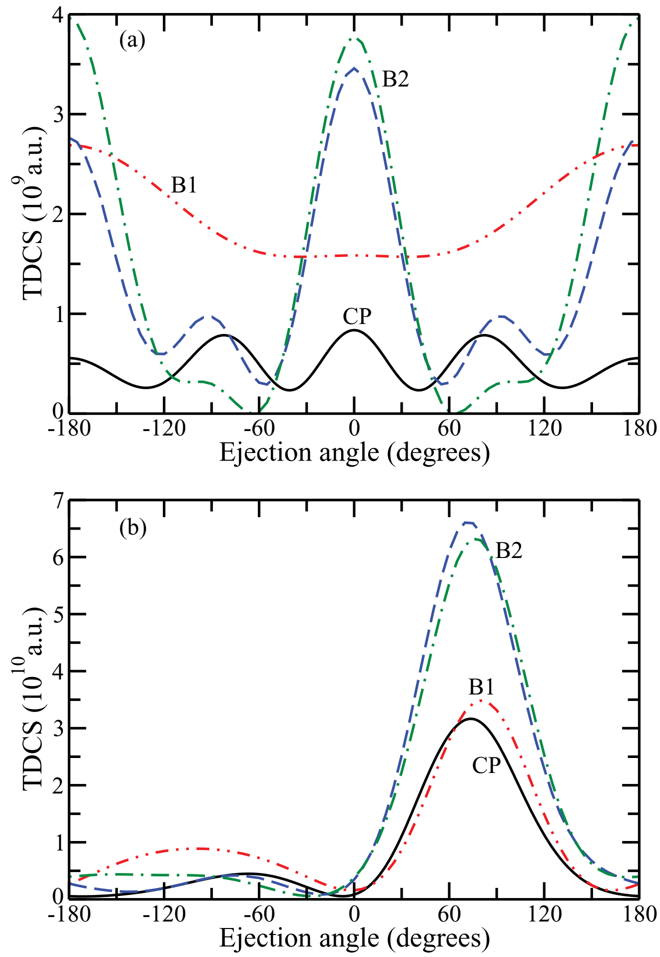

FIG. 5. (Color online) TDCS at 2 MeV/amu, $q=0.70$ a.u., and an ejected electron energy of 4 eV in (a) perpendicular plane geometry and (b) coplanar geometry: (solid black curve) CP approximation, (dash-double-dot red curve) first Born approximation, (dashed blue curve) *B2* approximation with $\bar{\epsilon}-\epsilon_0=0.9033$ a.u., and (dash-dot green curve) *B2* approximation with $\bar{\epsilon}=\epsilon_0$.

To summarize, we have reconfirmed the CP result that elastic scattering of the projectile by the nucleus is not the explanation of the discrepancy between theory and experiment seen in Fig. 1. We have shown that neither improving the He wave functions nor allowing for excitation-ionization should have any substantive effect in resolving the discrepancy. We have also shown that relativistic effects are important but only in changing the overall normalization of the TDCS, not in altering its shape. While this is a first Born result, the first Born term is so dominant at 100 MeV/amu that it is unlikely to be changed in relativistic higher-order approximations.

B. 2 MeV/amu impact energy

At this impact energy there are relative experimental data in the perpendicular plane for ejected electron energies of 1 and 4 eV at momentum transfers, q, of 1.5 a.u. and 0.70 a.u., respectively [6]. Here, as (11) confirms, we can immediately eliminate relativistic effects as being significant.

Figure 5 shows the first Born, second Born and CP approximations for the 4-eV case, all calculated in the frozen core approximation (Option 1). Although the details differ, the general pattern is the same for 1-eV ejection. We see that the second Born approximation differs substantially from the first Born approximation. For coplanar geometry, Fig. 5(b), the CP approximation is close to the first Born approximation, a closeness which in Ref. [15] led us to the erroneous conclusion that we were near the perturbative regime; Fig. 5 destroys that illusion. Unlike the case of 100 MeV/amu, the second Born approximation now clearly shows sensitivity to the choice of the closure energy $\bar{\epsilon}$. It should be noted, however, that, while the details are sensitive, the pattern remains the same. The "oscillatory" structure that was noted in the second Born excitation-ionization cross section of Fig. 4(a) for $He^+(n=2)$ is now also appearing in the ground state CP cross section of Fig. 5(a). As at 100 MeV/amu, improving the He wave functions (Option 2) only changes the first and second Born results by a few per cent in the direction of reducing the cross section.

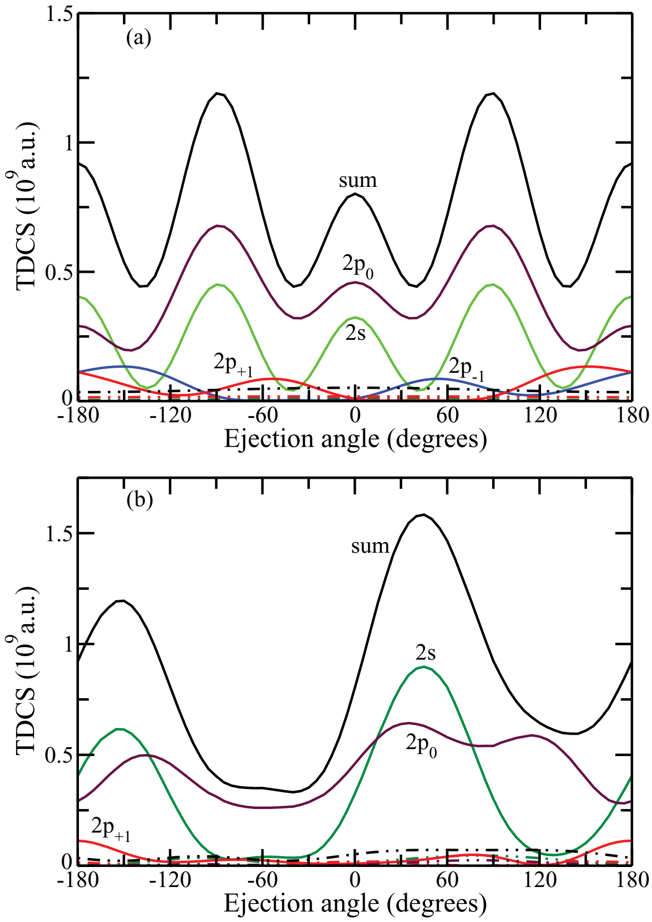

FIG. 6. (Color online) TDCS for excitation-ionization to $He^+(n=2)$ at 2 MeV/amu, $q = 0.70$ a.u., and an ejected electron energy of 4 eV in (a) perpendicular plane geometry and (b) coplanar geometry: (solid curves) second Born approximation and (dash-double-dot curves) first Born approximation. Note that for $2p_{+1}$ and $2p_{-1}$ the first Born cross sections are identical in all geometries while the second Born cross sections are only identical in coplanar geometry.

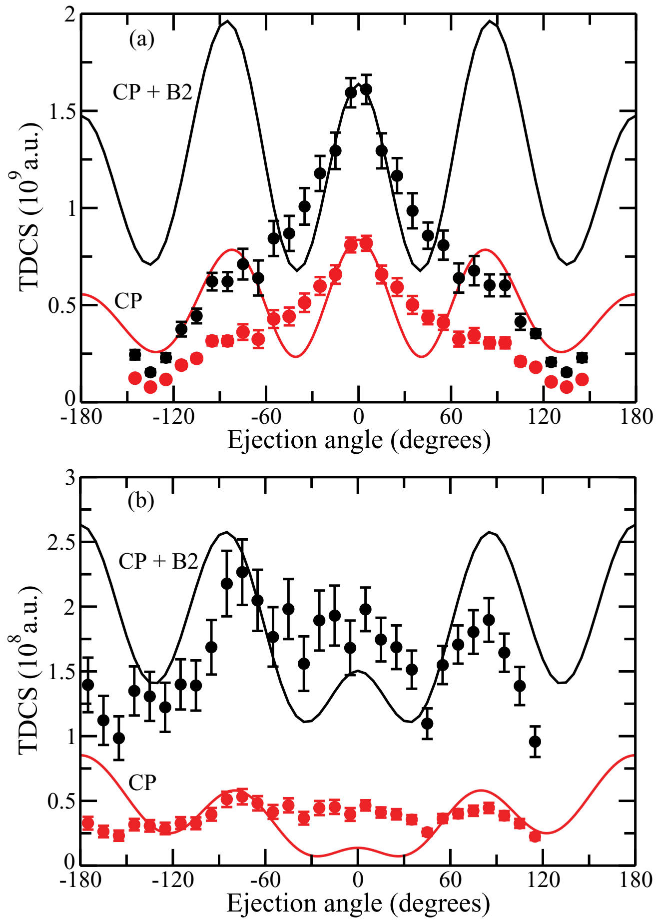

FIG. 7. (Color online) TDCS in perpendicular plane geometry at 2 MeV/amu for (a) 4-eV electron ejection at $q = 0.70$ a.u. and (b) 1-eV electron ejection at $q = 1.5$ a.u.. As explained in the text, the theoretical curves correspond to ionization to $He^+(1s)$ (CP) and ionization to $He^+(n = 1 + n = 2)$ (CP + $B2$). The relative experimental data from Ref. [6] have been separately normalized to each curve to give the best visual fit.

Figure 6 shows first and second Born cross sections for excitation-ionization to $He^+(n = 2)$ for an ejected electron energy of 4 eV and $q = 0.70$ a.u.. Results for 1-eV ejection at $q = 1.5$ a.u. are similar but a factor of 10 smaller. Here we see that the first Born term is completely dominated by the second Born contribution. This is not unexpected since, as shown in Ref. [21], in an uncorrelated model of the He atom the first Born term for double excitation processes is identically zero and the second Born term becomes the leading term in the perturbative expansion. While correlation leads to a nonzero first Born term, we would expect the second Born term to play a much more dominant role in excitation-ionization than it does in ionization to the ionic ground state. Again, we note the "oscillatory" structure in the perpendicular plane cross sections, Fig. 6(a), and the comparable sizes of the coplanar and perpendicular plane results.

What are we to make of this? The CP results in coplanar geometry are in accord with the three-body distorted wave-eikonal initial state (3DW-EIS) calculations of Foster *et al.* [10,15] and with the continuum distorted wave (CDW) and classical trajectory Monte Carlo (CTMC) calculations of Otranto *et al.* [29]. These approximations are nonperturbative and also include the projectile-nucleus interaction to vaying degrees. The CP results are also in good, although not perfect agreement [15] with the coplanar measurements of Fischer *et al.* [7]. In addition, we have already noted in Sec. II A the convergence of the CP approximation with the number of states included. All of this leads us to have considerable confidence in the coplanar CP cross section and so we must conclude from Fig. 5(b) that the second Born approximation for ionization to the He^+ ground state is, in absolute terms, unreliable. But, maybe, the relative sizes of the second Born approximations for ground state ionization and excitation-ionization could give a reasonable estimate of the importance of excitation-ionization. On this basis, we would estimate from Figs. 5 and 6 that $He^+(n = 2)$ excitation-ionization could account for about 30% of the total 4-eV perpendicular plane cross section and 3% of the total coplanar cross section. For 1-eV ejection (not shown here), we would estimate 30 and 10%, respectively. On the other hand, if the second Born approximation for excitation-ionization is giving the correct size then, comparing with CP, these numbers would be 60 and 5%, respectively, for 4-eV ejection, and 75 and 25% respectively for 1-eV ejection.

Figure 7 compares our theoretical results with the experimental data from Ref. [6]. In this figure we show the CP approximation for ionization to $He^+(1s)$ and the sum of the CP cross section and the second Born cross section ($B2$) for excitation-ionization to $He^+(n=2)$. The experimental data, which are relative, have been separately normalized to each curve to give the best visual fit. We again remark on the "oscillatory" structure in the theoretical results. Allowance for excitation-ionization does not greatly alter the shape of the CP cross section. The measurements cannot be said to be in agreement with the theory, although imagination may permit some correlation of dips, bumps, and plateaus with features in the theoretical curves. To make a proper assessment experimental resolutions need to be taken into account. This is beyond the scope of the present work.

IV. CONCLUSIONS

We have made a detailed study of C^{6+} ionization of He in the perpendicular plane. We have shown that a second Born treatment of ionization to $He^+(1s)$ at 100 MeV/amu is in almost perfect agreement with our previous CP calculations [15]. Apart from using the same initial and final state He wave functions, these two approximations are completely independent and, as explained in Sec. II B, complementary. Both include the interaction between the projectile and the He nucleus, the second Born approximation most obviously so. This result confirms beyond reasonable doubt that elastic scattering of the projectile by the target nucleus [6,11,14] cannot explain the discrepancy between theory and experiment highlighted in Refs. [6,14].

The question of sensitivity to the quality of the He wave functions [16] has been addressed within the context of the first and second Born approximations. In the closured version of the second Born approximation the intermediate He states ψ_n are, by default, exact and the accuracy of the second Born term (3), as of the first Born term (2), depends only on the accuracy of the initial and final He states. We have shown, for ionization to $He^+(1s)$, that our results have only little sensitivity to the quality of the He wave functions beyond the frozen core approximation used in the CP calculations, most particularly so for ionization in the perpendicular plane at 100 MeV/amu where the second Born approximation is valid.

We have examined whether ionization to an excited state of He^+ could be important in understanding the perpendicular plane measurements. We have studied only ionization to the $He^+(n=2)$ level which should be the dominant contribution. We find that it has little effect at 100 MeV/amu but could be quite significant, at least in the perpendicular plane, at 2 MeV/amu. At this lower energy we have also made comparison with relative experimental measurements in perpendicular plane geometry [6] and, while we do not get agreement, there are nuances in the data which mirror the structure in the calculations. Indeed, one of the interesting results to come out of the present work is the "oscillatory" structure in the perpendicular plane cross sections that can be seen both in the $He^+(1s)$ and $He^+(n=2)$ channels. As the first Born cross section is unstructured in these cases, the structure obviously comes from higher-order effects.

At 100 MeV/amu the velocity of the C^{6+} is almost half the speed of light. We have used the first Born approximation to investigate relativistic effects and find that they are significant at this energy but only in increasing the magnitude of the cross section, by 22%, not in changing its shape. The rotation of the TDCS, that, from our experience with (e,2e) [17], we thought might have been a possibility, did not materialize. Obviously, the two situations are not parallel. The difference is that the bound and ejected electrons in Ref. [17] are also relativistic, unlike here. So, although important, relativistic effects cannot explain the difference between theory and experiment seen in the perpendicular plane at 100 MeV/amu. At 2 MeV/amu they are neglegible. It might be objected that relativistic effects could exert a more profound influence at higher than first order. We think this unlikely since, nonrelativistically, the 100 MeV/amu cross section is dominated by the first Born contribution; see Fig. 2.

All of the calculations reported here are single center, the target nucleus being the center. At such high impact energies, and such low ejection energies relative to the target, this should be satisfactory. In support of this statement we note that our CP and second Born results at 100 MeV/amu are in accord with the calculations of Fiol *et al.* [12] who used the two-center, projectile and target nucleus, CDW approximation.

To conclude, we have failed to find any effect which can explain the discrepancy with experiment in the perpendicular plane seen in Refs. [6,14].

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