Correlation effects in out-of-plane excitation-ionization collisions

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We present theoretical three-dimensional fully differential cross sections (FDCSs) for electron-impact excitation-ionization of helium when the ionized electron is found outside of the scattering plane. Using our first Born approximation model, we examine the effects of electron correlation in the initial state and show that it significantly affects the shape of the out-of-plane FDCS.

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I. INTRODUCTION

The effect of electron correlation has long been assumed to be crucial in charged particle collisions with helium. This is especially thought to be true for the various four-body collisions in which both atomic electrons change state during the collision. Here we focus on one of these four-body collisions: electron-impact excitation-ionization of helium. In the excitation-ionization process, an electron projectile collides with a helium atom. During the collision, one of the atomic electrons is ionized, and the other atomic electron is left in an excited state of the He^+ ion. Unlike the single-ionization process, which can be approximated as a three-body collision with the nonionized electron considered inactive [1–8], both electrons must be included in the excitation-ionization process, making it an excellent process in which to study correlation.

To study the effects of correlation, we examine fully differential cross sections (FDCSs) in which the momentum of each particle before and after the collision is known. Although this process has been widely studied in recent years [1–17], nearly all of these studies have focused on FDCSs with the ionized electron found in the scattering plane [18]. The scattering plane is defined to be the plane containing the initial and final momentum vectors of the projectile. Previous papers [19–22] have shown that for single ionization without excitation, correlation is not important in the scattering plane. Because excitation-ionization is a four-body process where correlation has been shown to be important in the scattering plane [19–22], the study of this process outside of the scattering plane is an ideal situation in which to further study correlation.

Also, in the past decade, much attention has been paid to FDCSs outside of the scattering plane in the single ionization of helium by heavy particle impact [23–28]. Surprising structures were observed in experimental results, and theory has struggled to fully explain the origin of these structures. The combination of excitation-ionization being a four-body process and the intense discussion of out-of-plane FDCSs in heavy particle single ionization motivates this study of out-of-plane FDCSs in excitation-ionization.

II. THEORY

The model we use is a first Born approximation (FBA) model [29] with the initial and final projectiles treated as plane waves, a reasonable assumption for the projectile energies studied here. Because the ionized electron has a smaller velocity, we treat it as a distorted wave with the distorting potential given by a spherically averaged He^+ potential. In the FBA model, the FDCS is proportional to the square of the transition matrix T_{fi},

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_2} = \mu_{pa}\mu_{ie}\frac{k_f k_e}{k_i}|T_{fi}|^2, \quad (1)$$

with

$$T_{fi} = \langle \Psi_f | V_i | \Psi_i \rangle. \quad (2)$$

Here μ_{pa} is the reduced mass of the projectile and target atom, μ_{ie} is the reduced mass of the He^+ ion and the ionized electron, k_f is the magnitude of the momentum of the scattered projectile, k_e is the magnitude of the momentum of the ionized electron, and k_i is the magnitude of the momentum of the incident projectile.

The initial-state wave function is a product of the incident projectile wave function $\beta_{\vec{k}_i}(\vec{r}_1)$ and the target helium atom wave function $\Phi_i(\vec{r}_2,\vec{r}_3)$,

$$\Psi_i = \beta_{\vec{k}_i}(\vec{r}_1)\,\Phi_i(\vec{r}_2,\vec{r}_3). \quad (3)$$

The final-state wave function is a product of the scattered projectile wave function $\beta_{\vec{k}_f}(\vec{r}_1)$, the ionized electron wave function $\chi_{\vec{k}_e}(\vec{r}_2)$, and the He^+ ion wave function $\varphi_{nlm}(\vec{r}_3)$,

$$\Psi_f = \beta_{\vec{k}_f}(\vec{r}_1)\,\chi_{\vec{k}_e}(\vec{r}_2)\,\varphi_{nlm}(\vec{r}_3). \quad (4)$$

In this first-order perturbative model, the perturbation V_i is simply the Coulomb interaction between the projectile and the target helium atom,

$$V_i = \frac{-2}{r_1} + \frac{1}{r_{12}} + \frac{1}{r_{13}}. \quad (5)$$

To study the effects of initial-state correlation, we perform two FBA calculations. The FBA-HY (Hylleraas) calculation uses a 20-parameter Hylleraas wave function that includes both radial and angular correlations to describe the target helium atom [30]. The FBA-VAR (variational) calculation uses a product variational wave function that does not include correlation and is akin to an independent electron model. According to momentum conservation, one would expect the ionized electron to be ejected primarily in the direction of the momentum transferred from the projectile to the target. This momentum-transfer direction $\vec{q} = \vec{k}_i - \vec{k}_f$ lies in the scattering plane by definition. Therefore, the largest FDCS should be observed in the scattering plane, and not much out-of-plane

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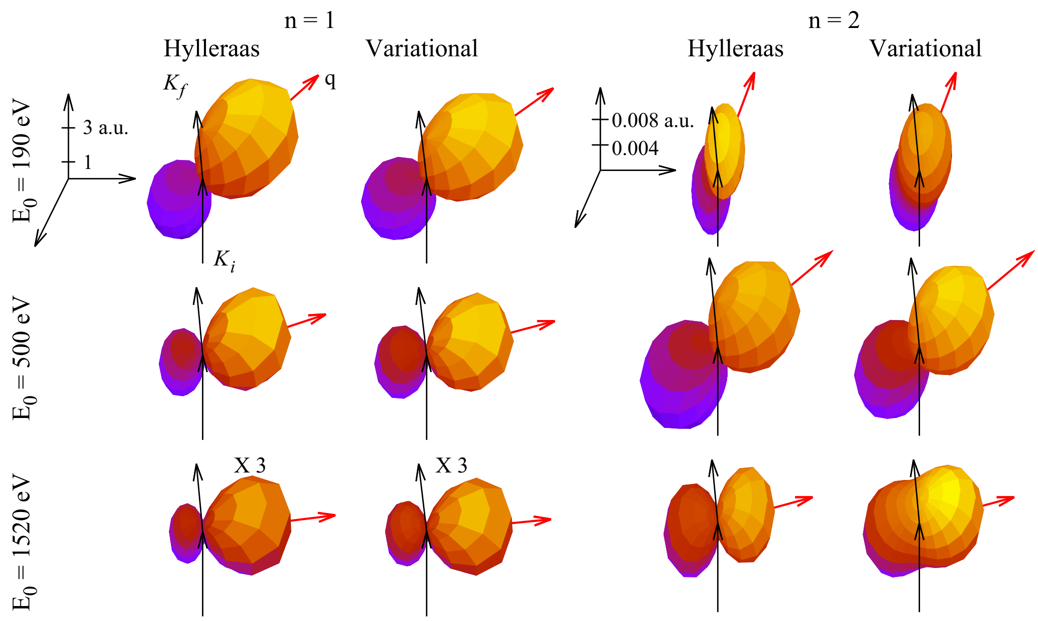

FIG. 1. (Color online) Three-dimensional FDCS for electron-impact excitation-ionization of helium using the FBA-HY and FBA-VAR. Results are shown for an ionized electron energy of 3 eV and a projectile scattering angle of 4.1°. The incident projectile energy and final state of the He^+ ion are labeled in the figure as are the incident projectile (k_i), scattered projectile (k_f), and momentum-transfer (q) directions.

structure is expected. This would be particularly true for the FBA-VAR model where the two atomic electrons move independently of each other. When correlation is included, it is reasonable to expect that there could be an increased likelihood of finding the ionized electron outside of the scattering plane.

III. RESULTS

In Figs. 1 and 2, we show three-dimensional FDCSs as a function of the ionized electron angle with and without correlation for different incident projectile and ionized electron energies [31]. These particular kinematics were chosen because the range of incident projectile energies probes different parts of the initial-state wave function, which contains information about electron correlation effects. In particular, one can calculate a classical impact parameter associated with a given projectile energy and scattering angle for potential scattering. The incident projectile energies presented here (190, 500, and 1520 eV) correspond to impact parameters of 4, 1.5, and 0.5 a.u. for electrons scattering from a helium nucleus. By examining the radial charge distribution of the Hylleraas and variational wave functions, the approximate

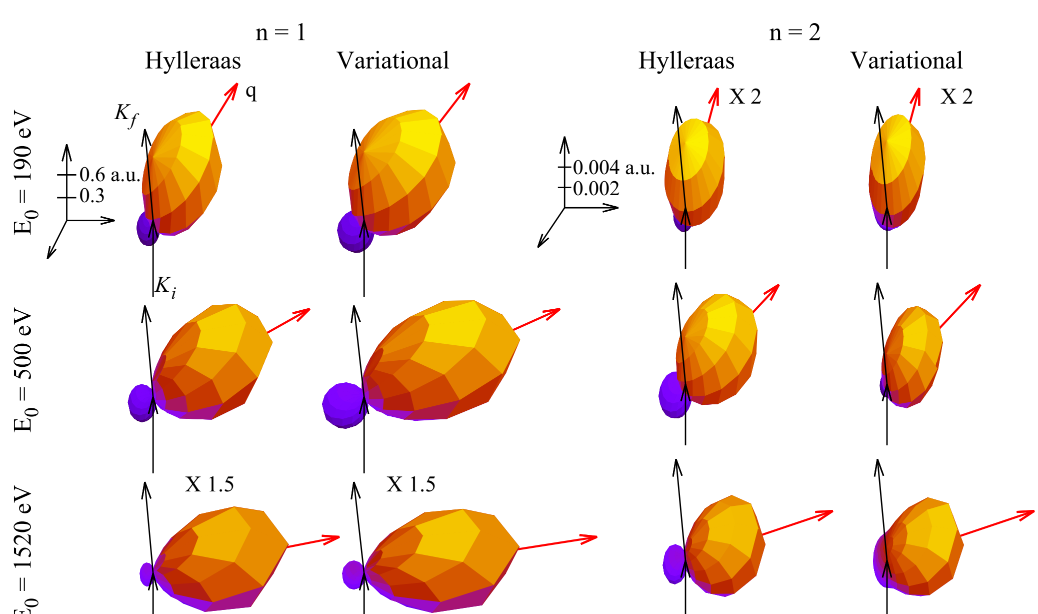

FIG. 2. (Color online) The same as Fig. 1 but with an ionized electron energy of 20 eV.

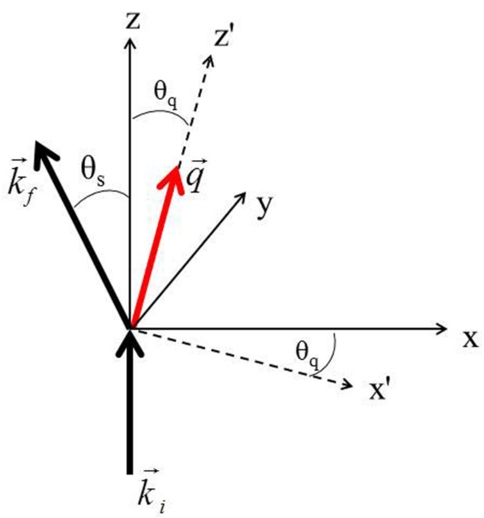

FIG. 3. (Color online) Coordinate system showing the incident projectile momentum (k_i), scattered projectile momentum (k_f), and momentum-transfer vectors (q). The incident projectile momentum is in the z direction; the scattered projectile momentum and momentum transfer both lie in the x-z plane. The perpendicular plane is defined as the x'-z' plane where a rotation about the y axis by an angle θ_q has been performed to find the x' and z' axes.

size of the target helium atom is found to be about 3 a.u. with the most observable differences between the charge distribution appearing at larger radial distances. Therefore, the three incident energies studied here probe a small radial distance where the charge distributions are similar, a large radial distance where the charge distributions are different, and a radial distance in the middle. Our previous papers on this process have shown that the models perform poorly for large scattering angles [10,19,29], and so we restrict this study to a small scattering angle of 4.1°.

In the three-dimensional plots, the FDCS for a particular ionized electron is shown as the radial distance from the origin where the collision occurs. The initial and final projectile momentum directions are shown in the figures along with the momentum-transfer direction. The final-state He^+ ion is left in either the ground $n = 1$ state or the first $n = 2$ excited state. Note that to get the FDCS for $n = 2$, the individual FDCS for $2s$, $2p0$, and $2p \pm 1$ have been summed. In all $n = 2$ cases, the $2s$ FDCS is the dominant contribution to the sum by about one order of magnitude and is the primary cross section that influences the overall shape.

The $n = 1$ results show well-known and expected features. There is a large binary lobe in the direction of momentum transfer as one would expect from momentum conservation. A small recoil lobe in the direction opposite of momentum transfer is also observed and is larger for an ionized electron

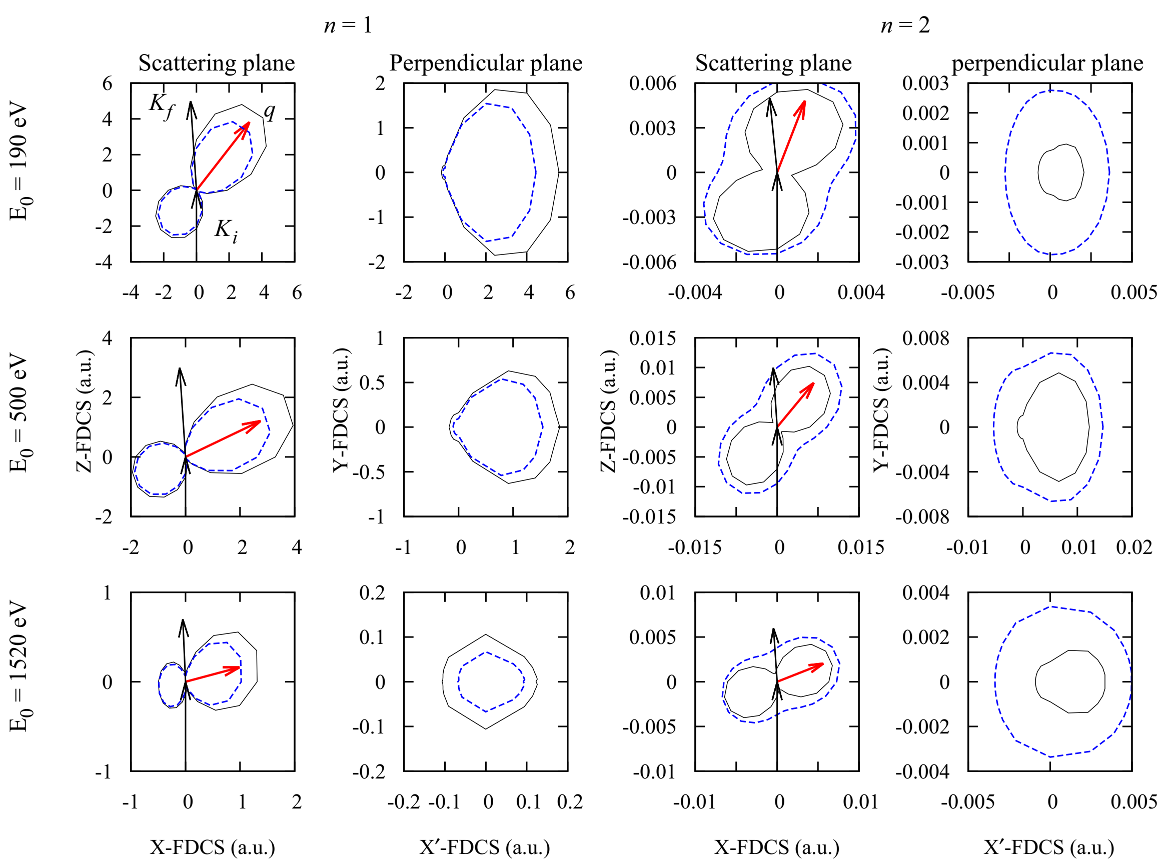

FIG. 4. (Color online) Two-dimensional FDCS slices for electron-impact excitation-ionization of helium using the FBA-HY (solid line) and FBA-VAR (dashed line) models in the scattering plane and plane perpendicular to the momentum transfer. Results are shown for an ionized electron energy of 3 eV and a projectile scattering angle of 4.1°. The incident projectile energy and final state of the He^+ ion are labeled in the figure as are the incident projectile (k_i), scattered projectile (k_f), and momentum-transfer (q) vectors.

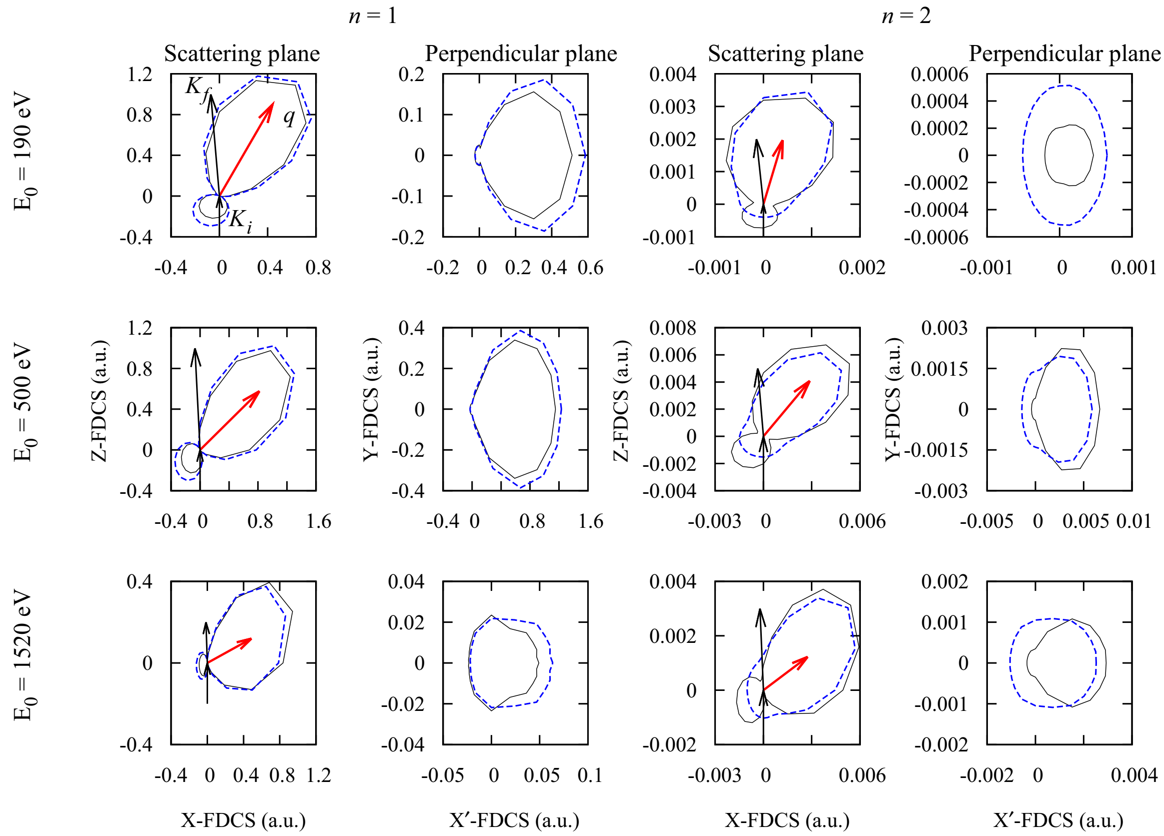

FIG. 5. (Color online) The same as Fig. 4 but for an ionized electron energy of 20 eV.

energy of 3 than 20 eV. The recoil lobe is a result of the ionized electron being given an initial "kick" in the direction of the nucleus. The interaction between the nucleus and the ionized electron then results in a backscattering of the ionized electron in the direction opposite the momentum transfer. For a smaller ejected electron energy, the nucleus has a greater influence, and therefore a larger recoil peak is seen for the $n = 1$ results at $E_2 = 3$ eV compared to those at $E_2 = 20$ eV. For the $n = 1$ results, very little difference is observed between the calculation with correlation and the calculation without correlation. This is entirely reasonable given that the ionization without excitation process is often considered a quasi-three-body process where the nonionized electron is simply a bystander and the three-body "frozen core" approximation has long been known to be valid [1–8].

Although the $n = 1$ results are exactly as anticipated, the same is not true for the $n = 2$ FDCS. Binary and recoil lobes are still observed, but now significant differences are observed between the correlated and the uncorrelated wave-function calculations, particularly at the lowest and highest incident projectile energies. The FBA-HY calculations show virtually zero cross section in a plane perpendicular to the momentum transfer, and the binary and recoil lobes are very distinct. However, the FBA-VAR calculations do show structure in this perpendicular plane, and the two lobes are smeared out near the collision region. This is contrary to what one would expect from an independent electron model where very little out-of-plane structure is expected.

To take a more quantitative look at the differences between the FBA-VAR and the FBA-HY results, we focus on two slices (or planes) through the three-dimensional FDCS. These two planes are the scattering plane (x-z plane) and the plane perpendicular to the momentum-transfer vector (x'-y' plane). A diagram of the geometry is shown in Fig. 3.

The two-dimensional FDCS slices of the scattering plane and perpendicular plane are shown in Figs. 4 and 5. From these slices, it can be seen that only minor differences are observed for the He^+ ion being left in the $n = 1$ state, both in the scattering plane and in the perpendicular plane. This is further confirmation that correlation is not important in the single-ionization process. However, more obvious differences are seen for the He^+ ion being left in the $n = 2$ state. In particular, it is now clear that the inclusion of correlation in the $n = 2$ FBA-HY calculation leads to two very distinct binary and recoil lobes in the scattering plane, whereas this structure becomes washed out in the FBA-VAR calculation, and a more uniform distribution is seen. Despite the shape differences in the scattering plane, the magnitude of both calculations is similar. In the perpendicular plane, both calculations have a fairly uniform distribution with no distinct lobes observed. But, the inclusion of correlation reduces the magnitude of the perpendicular plane $n = 2$ FDCS and leads to the two distinct lobes observed in the three-dimensional plots. The inclusion of correlation also shifts the perpendicular plane distribution away from the scattered projectile direction (distribution shifted in $+x'$ direction). These perpendicular plane structures are similar to those seen in the heavy particle impact single ionization of helium [23–28], although the exact cause of those structures is still not well understood.

Dürr and co-workers have published some out-of-plane experimental data and theoretical calculations for the single ionization of helium without excitation [32,33] at 1-keV incident projectile energy. They also examine FDCS in the scattering plane and the plane perpendicular to the momentum-transfer direction. In general, the shape and magnitude of the theory and experiment presented in Refs. [32,33] is similar to that of our $n = 1$ FBA calculations, indicating that our calculations fit well with the already published data. In Ref. [32], the authors attribute the perpendicular plane structure to higher-order effects of the projectile-target interaction. Our results cannot confirm or reject this hypothesis for $n = 1$ FDCS since the projectile is treated as a plane wave in the FBA models. However, we do observe some perpendicular plane structure for excitation-ionization within the FBA models, indicating that higher-order projectile-target interactions cannot be wholly responsible for this structure. In fact, our results demonstrate that some of this structure is due to not including correlation in the target atom wave function. In the theoretical models of Dürr and co-workers, electron correlation was included, although as already mentioned, it is well known that correlation is not important in the single ionization without excitation process.

We note that the perpendicular plane structure exists for a range of incident projectile energies, which implies that it cannot be an effect of different energy projectiles probing different parts of the target atom wave function. Because of this, we find it unlikely that higher-order projectile-target effects are responsible for the structure. We hope to test this in the future by using our four-body distorted wave (4DW) model [29] to calculate three-dimensional FDCSs for the excitation-ionization process. The 4DW model treats the incident and scattered projectiles as a distorted wave and would therefore include some higher-order projectile-target interactions. The perpendicular plane structure also exists for two different ionized electron energies and therefore cannot be due to the distorted wave treatment of the ionized electron, which is known to be less accurate at lower ionized electron energies.

An *a priori* analysis of the two FBA models would lead one to hypothesize that the FBA-HY calculation with correlation would be the more physically correct model and should therefore produce the more accurate FDCSs. Thus, we predict that experiment will show almost no cross section in a plane perpendicular to the momentum-transfer direction. Unfortunately, there is currently no experimental data outside of the scattering plane that can be used to test this hypothesis. We hope that our colleagues will soon be able to provide some experimental data so that this question can be answered.

One effect that has been neglected in the FBA models is the postcollision interaction (PCI) between the scattered projectile and the ionized electron. This effect is known to be substantial in the excitation-ionization process [29], although for the asymmetric energy sharing here, the effect of the PCI is likely limited. Our 4DW model has the capability to include PCI, and this is another effect that we would like to examine in the future.

IV. CONCLUSION

To summarize, we have presented theoretical three-dimensional fully differential cross sections for electron-impact excitation-ionization of helium over a wide range of incident projectile energies designed to probe different parts of the target atom wave function. We studied the effects of electron correlation in the target helium atom and found that for ionization without excitation, correlation played very little role in predicting the shape or magnitude of the FDCS. This was consistent with the large body of already published papers on single ionization. However, we found surprising results for excitation-ionization to the $n = 2$ state. In this case, very little structure outside of the scattering plane was expected in the model without correlation, but structure was observed. The results were most striking in a plane perpendicular to the momentum-transfer direction. Here, both magnitude and shape differences were observed between the models with and without correlation. These results are reminiscent of recent heavy particle impact single-ionization FDCSs where structure was observed in experiment outside of the scattering plane. We hope that this paper prompts further theoretical and experimental studies of the excitation-ionization process outside of the scattering plane so that the role of electron correlation and the particle dynamics may be better understood.

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