Theoretical fully differential cross sections for double-charge-transfer collisions

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(Received 21 January 2010; published 26 August 2010)

We present a four-body model for double charge transfer, called the four-body double-capture model. This model explicitly treats all four particles in the collision, and we apply it here to fully differential cross sections (FDCSs) for proton + helium collisions. The effects of initial- and final-state electron correlations are studied, as well as the role of the projectile-nucleus interaction. We also present results for proton + helium single capture, as well as single-capture:double-capture ratios of FDCSs.

DOI: 10.1103/PhysRevA.82.022714 PACS number(s): 34.50.−s, 34.70.+e

I. INTRODUCTION

Study of the few-body scattering problem has advanced significantly in the last decade, thanks to advances in experimental technology and computational resources. On the computational side, the three-body scattering problem of atomic ionization by electron impact has been solved for simple target atoms [1–4]. Experimental advances now make it possible to measure fully differential cross sections (FDCSs), and recently Schulz *et al.* [5] have published experimental four-body FDCS results for single and double charge transfer for the proton-helium collision system. We have previously proposed a four-body model for charge transfer and presented results for the four-body process of charge transfer with target excitation (TTE). Here, we use the same model to examine double and single charge transfer.

The three-body process of single charge transfer (or single capture; SC) has been studied intensively [6–63], and several reviews of this work have been published [64–72]. The first quantum mechanical calculation for single charge transfer was performed by Oppenheimer [7] in 1928, followed two years later by Brinkman and Kramers [12]. Their model would later become known as the OBK approximation. In the OBK approximation, the projectile is treated as a plane wave in both the initial and the final states, and only the interaction between the projectile and the atomic electron is included. The projectile-nucleus interaction is ignored based on the assumption that this term only contributes due to the nonorthogonality of the initial- and final-state wave functions [7]. The OBK calculation yielded results that were at least a factor of 4 too large, and nearly 15 years passed before Jackson and Schiff [13] (hereafter, JS) performed a calculation using the full interaction potential, including the projectile-nuclear term.

The JS results agreed with experiment much better than the OBK results and correctly predicted the magnitude of the cross sections [13,38]. Since the OBK and JS models were introduced, much discussion has centered around the inclusion of the projectile-nucleus term. It has been shown by Belkić and Salin [16] that including the projectile-nucleus term in the perturbation improves the agreement with experiment, particularly at large angles. When this interaction is ignored, the differential cross section drops off much more quickly than when it is included. This can be attributed to the idea that scattering of the projectile through a large angle is typically the result of scattering from the nucleus. Classically, this is analogous to small impact parameter scattering, where the projectile penetrates the electron cloud and scatters elastically from the nucleus. It is now accepted that the projectile-nucleus term in the perturbation needs to be included to accurately predict the magnitude of the charge-transfer cross section.

Most of the work done on charge transfer has involved total cross sections, but a more stringent test of theory is the study of cross sections that are differential in projectile scattering angle. In general, the differential cross sections for single charge transfer decrease rapidly as the scattering angle increases, and they typically exhibit a change in slope between a scattering angle of 0.3 mrad and one of 0.8 mrad. This change in slope represents the boundary between small- and large-angle scattering. At small angles, the projectile scattering is a result of scattering from the atomic electrons, whereas for large angles, it is a result of nuclear scattering, as already discussed [20].

A process similar to single charge transfer, but one that is a true four-body process, is that of double charge transfer (or double capture; DC). In DC, the incident proton captures both atomic electrons from the target helium atom and leaves the collision as an H^- ion. DC was first studied in the mid to late 1960s, but the vast majority of work on this problem has been completed in the last 30 years. This is due mostly to the difficulty of treating a full four-body problem and the fact that DC cross sections are typically two to three orders of magnitude smaller than SC cross sections, making measurements difficult. Recent reviews of the previous DC work and other four-body processes have been published by Belkić and co-workers [8,9,71,72].

Like SC, most work on DC has involved total cross sections, typically for the resonant process of α particles incident on helium atoms. DC via the ground-state to ground-state transition in α + He collisions is resonant, and therefore, excited states play a negligible role. However, for projectile nuclear charges > 3, any calculations performed would need to include capture into excited states to be accurately compared with experiment [37,73–75]. In the case of DC proton collisions, the electrons are guaranteed to be captured to the ground state because the H^- ion has no stable excited states. This greatly reduces the amount of computation required.

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Initially the independent electron model, which ignores electron-electron correlation, was used to simplify the calculation [76]. This model is typically valid for a high target nuclear charge [77] and high incident projectile velocity [78], where electron-electron correlation within the target atom is not important. Since DC is a true four-body problem, it would seem reasonable to expect that some correlation should be included. However, several full four-body models [39,79–82] have been developed, all of which found that correlation had little effect on the total or differential cross sections. The inclusion of correlation generally decreased the cross section by a factor of <3 but did not alter the shape.

The first differential DC cross section was presented in 1991 by Schuch *et al.* [79] for α + helium resonant capture. A few calculations of differential cross sections for DC have been performed, all for α + helium collisions. Schuch *et al.* [79] and Gravielle and Miraglia [83] showed that electron correlation is not very important; Belkić [84] showed that the boundary-corrected first Born approximation has a 0 in the differential cross section at 0.112 mrad due to the potential vanishing at this scattering angle; Schöffler *et al.* [85] found a minimum in the DC cross section similar to that in the SC cross section when using the Born distorted wave model; and Martínez *et al.* [75] showed that a double-peak structure due to a double-scattering mechanism is observed when the energy is high enough.

At this point, only three sets of experimental differential cross section results exist for nonresonant DC, and there is only one theoretical calculation that has been reported. Schulz *et al.* [5] reported experimental results for proton + helium, Afrosimov *et al.* [86] reported experimental results for proton + argon, and Martínez *et al.* [87] reported theoretical and experimental results for proton + argon. Here, we present theoretical differential cross sections for proton + helium DC.

The fundamental T matrix for a four-body process contains a nine-dimensional (9D) integral. For the DC work that has been done previously, a scattering model was developed such that at least part of the T matrix could be integrated analytically. This reduced the dimensionality of any required numerical integration, making the calculation more tractable. The required integrals for several different models of DC are presented by Belkić [8]. To avoid model-dependent integrals, we have developed a computer code to directly evaluate the four-body 9D integral numerically. The advantage of this approach is that we can calculate cross sections for any arbitrary model. The disadvantage is the enormous amount of computer time required. We have previously tested this approach by calculating very recently measured FDCSs for proton-helium collisions in which one electron is captured and the other electron is left in an excited state of helium [88]. Here we report a test of this approach for DC. Atomic units are used throughout, unless noted otherwise.

II. THEORY

The FDCS for SC, DC, and TTE is differential only in projectile scattering angle and can be written as

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \mu_{\text{pa}} \mu_f \frac{k_f}{k_i} |T_{fi}|^2, \tag{1}$$

where μ_{pa} is the reduced mass of the projectile and target atom, μ_f is the reduced mass of the outgoing particle and the residual ion, and $\vec{k}_i$ ($\vec{k}_f$) is the wave vector of the incident (scattered) projectile.

A. The four-body transfer with target excitation (4BTTE) theory

The 4BTTE model [88] is used to calculate the SC cross sections. In [88] we called this model 4BTE. However, Belkić [89] pointed out that this terminology could lead to some confusion since TE has previously been used to mean transfer into an excited state of the projectile. To avoid confusion, we use TTE to indicate that the excited state is associated with the target and not the projectile. The details of this calculation are presented in [88], and thus we only summarize the main features here.

The exact transition matrix in the two-potential formulation is given by

$$T_{fi} = \langle \chi_f^{(-)} | V_i | \beta_i \rangle + \langle \chi_f^{(-)} | W_f^{\dagger} | (\Psi_i^{(+)} - \beta_i) \rangle, \tag{2}$$

where $\chi_f^{(-)}$ is an approximate final-state wave function, $\Psi_i^{(+)}$ is the exact initial-state wave function, and β_i is the asymptotic initial-state wave function. The final-state perturbation is W_f, and the initial-state projectile-atom interaction is V_i.

Past work on total cross sections has shown that it is important for the initial- and final-state wave functions to satisfy the asymptotic boundary conditions [8]. For the TTE calculations reported in [88], we examined initial-state plane waves and eikonal waves, both of which satisfy the asymptotic boundary conditions. The eikonal initial state (EIS) has been extremely successful in treating the three-body problem. However, Belkić [8] has shown that the EIS may not be appropriate for the four-body problem. Consequently, in our initial attempt to calculate the differential cross section for DC, we use a plane wave for the projectile wave function.

If the exact initial-state wave function is approximated as a plane wave times an atomic wave function, Eq. (2) reduces to

$$T_{fi} = \langle \chi_f^{(-)} | V_i | \beta_i \rangle. \tag{3}$$

The initial-state projectile-atom interaction is given by

$$V_i = \frac{Z_p Z_{\text{nuc}}}{r_1} + \frac{Z_p Z_e}{r_{12}} + \frac{Z_p Z_e}{r_{13}}, \tag{4}$$

where r_1, r_{12}, and r_{13} are the distances from the projectile to the nucleus and two atomic electrons respectively. The quantities Z_p, Z_e, and Z_{nuc} are the electric charges of the projectile, electron, and target nucleus. This perturbation potential corresponds to that of JS.

The calculations are performed in the center-of-mass frame, using the Jacobi coordinates [90] shown in Figs. 1 and 2.

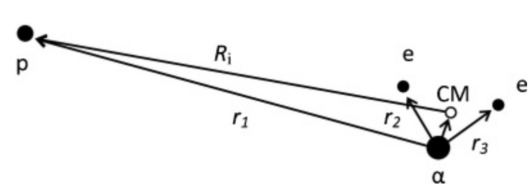

FIG. 1. Jacobi coordinate system for the projectile–helium-atom system.

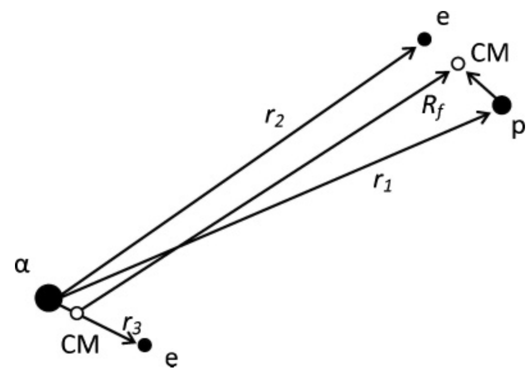

FIG. 2. Jacobi coordinate system for the hydrogen–helium-ion system.

In this coordinate system, $\vec{R}_i$ is the relative vector between the projectile and the center of mass of the helium atom, and $\vec{R}_f$ is the relative vector between the center of mass of the hydrogen atom and the center of mass of the He^+ ion. They are given by

$$\vec{R}_i = \vec{r}_1 - \frac{m_e}{m_\alpha + 2m_e}(\vec{r}_2 + \vec{r}_3) \tag{5}$$

and

$$\vec{R}_f = \frac{m_e\vec{r}_2 + m_p\vec{r}_1}{m_p + m_e} - \frac{m_e}{m_e + m_\alpha}\vec{r}_3, \tag{6}$$

where m_e, m_α, and m_p are the masses of the electron, α particle, and projectile, respectively.

We approximate the exact initial-state wave function as

$$\Psi_i^{(+)} \approx \beta_i = \chi_p^i(\vec{R}_i)\,\xi_{\mathrm{He}}(\vec{r}_2,\vec{r}_3), \tag{7}$$

where $\chi_p^i(\vec{R}_i)$ is a plane wave for the incident projectile, and $\xi_{\mathrm{He}}(\vec{r}_2,\vec{r}_3)$ is a fully correlated Hylleraas wave function for the ground-state helium atom [91]. The incident projectile plane wave is given by

$$\chi_p^i(\vec{R}_i) = \frac{e^{i\vec{k}_i\cdot\vec{R}_i}}{(2\pi)^{3/2}}. \tag{8}$$

The approximation we use for the final-state wave function is

$$\chi_f^{(-)} = \chi_p^f(\vec{R}_f)\phi_{\mathrm{H}}(\vec{r}_{12})\psi_{\mathrm{He}^+}(\vec{r}_3), \tag{9}$$

where $\chi_p^f(\vec{R}_f)$ is a Coulomb wave for the scattered hydrogen wave function. It is given by

$$\chi_p^f(\vec{R}_f) = \frac{e^{i\vec{k}_f\cdot\vec{R}_f}}{(2\pi)^{3/2}}e^{-\pi\gamma/2}\Gamma(1+i\gamma) \times {}_1F_1\big(-i\gamma,1,i(k_fR_f + \vec{k}_f\cdot\vec{R}_f)\big), \tag{10}$$

where $\gamma = \frac{Z_pZ_{\mathrm{He}^+}}{v_{\mathrm{H}}}$. The quantity Z_{He}^+ is the electric charge of the He^+ ion, and v_{H} is the speed of the outgoing hydrogen atom.

The final-state He^+ wave function $\psi_{\mathrm{He}^+}(\vec{r}_3)$ and the outgoing hydrogen wave function $\phi_{\mathrm{H}}(\vec{r}_{12})$ are both hydrogenic wave functions and, thus, known exactly. The final-state wave function has been properly symmetrized in the calculations, but the electrons have been labeled here for clarity.

B. The four-body double-capture (4BDC) theory

We present here the 4BDC model. The theory for DC is quite similar to that for SC, and because the fully differential cross section for DC is again differential only in projectile scattering angle, it is given by Eq. (1). The corresponding T matrix is given by Eq. (3). The initial-state wave function is the same as that for SC and Eq. (7). However, the final-state wave function is now given by

$$\chi_f^{(-)} = \chi_p^f(\vec{R}_f)\psi_{\mathrm{H}^-}(\vec{r}_{12},\vec{r}_{13}), \tag{11}$$

where $\psi_{\mathrm{H}^-}(\vec{r}_{12},\vec{r}_{13})$ is the wave function for the outgoing H^- ion, and $\chi_p^f(\vec{R}_f)$ is the scattered projectile wave function. The calculation is again performed in the center-of-mass frame, and the Jacobi coordinate $\vec{R}_f$ is now the relative vector between the α particle and the center of mass of the H^- ion.

Unlike for SC, it is now possible to examine the effects of correlation in both the initial and the final bound-state wave functions. Thus, in the calculations presented here, either an analytic Hartree-Fock wave function [92] or a 20-parameter Hylleraas [91] wave function is used for the helium atom, and either a two-parameter variational wave function [93] or a 20-parameter Hylleraas [91] wave function is used for the H^- ion. The initial projectile is again treated as a plane wave, and the final projectile is treated as a Coulomb wave, where $\gamma = \frac{Z_{\mathrm{H}^-}Z_{\mathrm{He}^{2+}}}{v_{\mathrm{H}^-}}$. The quantities Z_{H^-} and $Z_{\mathrm{He}^{2+}}$ are the charges of the H^- and He^{2+} ions, and v_{H^-} is the speed of the H^- ion. Unlike the JS model, this wave function satisfies the final-state asymptotic boundary conditions, which is now known to be important [8].

III. RESULTS

A. Single charge transfer

There is a large amount of experimental data available for three-body single charge transfer, and the model used in these calculations is not new. However, the calculations were necessary to compare single and double charge transfer using equivalent models, and so our results are presented in Fig. 3 for the specific energies needed. Results are presented

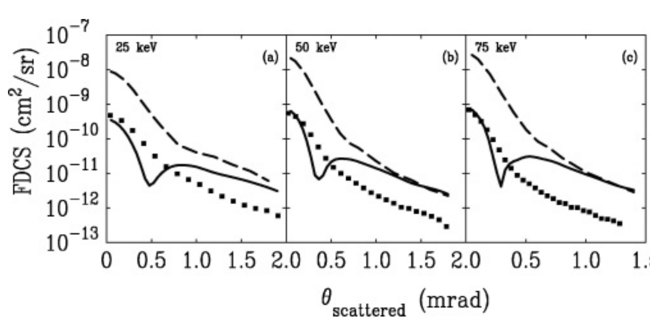

FIG. 3. FDCS as a function of projectile scattering angle for $p + \mathrm{He}$ SC. Experiment: Solid squares show results of Schulz *et al.* [5] for the incident projectile energies shown. Both theoretical curves are from the 4BTTE model with a plane wave for the incident projectile, Hylleraas wave function for the helium atom, and Coulomb wave for the scattered projectile. Theory: Solid curve shows results with all three terms in the perturbation; dashed curve, with no projectile-nucleus term in the perturbation.

both including and excluding the projectile-nucleus term in the perturbation.

These results exhibit some well-known features and trends. The unphysical minimum seen in the calculation with the full perturbation is typically attributed to a cancellation of the terms in the perturbation [46]. Note that this minimum becomes deeper and shifts to smaller angles as the projectile energy increases, as previously observed by Band [94] and Sil *et al.* [95]. The removal of the projectile-nucleus term in the perturbation results in the elimination of this minimum and an increase in the overall magnitude of the cross section, something seen by Belkić and Salin [16]. When the projectile-nucleus term is included in the perturbation, we get good agreement with the magnitude of the absolute experimental cross sections for small scattering angles. Since the total cross sections represent an integral over angles, it is clear that our results would be in reasonable agreement with the magnitude of the absolute total cross sections since the integral would be dominated by small angles.

B. Double electron capture

It has been shown that electron correlation is not important for total DC cross sections at high incident projectile energies [96–98]. However, the effect of correlation for differential cross sections at intermediate energies has not been studied. One would be inclined to think that correlation would play an important role in a first-order model of the DC process since the only interactions included in the perturbation are between the projectile and each individual electron, as well as the projectile-nucleus interaction. Thus, for both electrons to be captured, it seems reasonable to expect correlation to play a role. The effect of angular correlation in both the initial and the final states is shown in Fig. 4. Four calculations are shown, using either a 20-term Hylleraas wave function or an analytic Hartree-Fock wave function for the initial-state helium atom. For the final-state H^- ion, either a 20-term Hylleraas wave function or a two-parameter variational wave function is used. All four of the calculations shown are similar in both shape and magnitude, indicating that angular correlation is not important in differential cross sections for the DC process at intermediate energies. In the initial-state helium atom, the inclusion of correlation lowered the magnitude of the FDCS slightly, while in the final-state H^- ion, the inclusion of correlation increased the magnitude of the FDCS slightly. This is consistent with the previous work on total cross sections.

The effect of the projectile-nucleus term in the perturbation of Eq. (4) is shown in Fig. 5 for DC. Comparing SC and DC results, we see that the experimental results for DC are about three orders of magnitude smaller than those for SC. There is also a strong similarity between the theoretical DC differential cross sections and the SC differential cross sections. Like SC, a minimum is again observed in the DC cross section, and excluding the projectile-nucleus term from the perturbation results in the removal of this minimum. Also, the location of this minimum moves to smaller angles as the energy increases. As expected, theory requires inclusion of the projectile-nucleus term to more accurately predict the magnitude of experimental results. However, the DC model still overestimates experiment by a factor of 100.

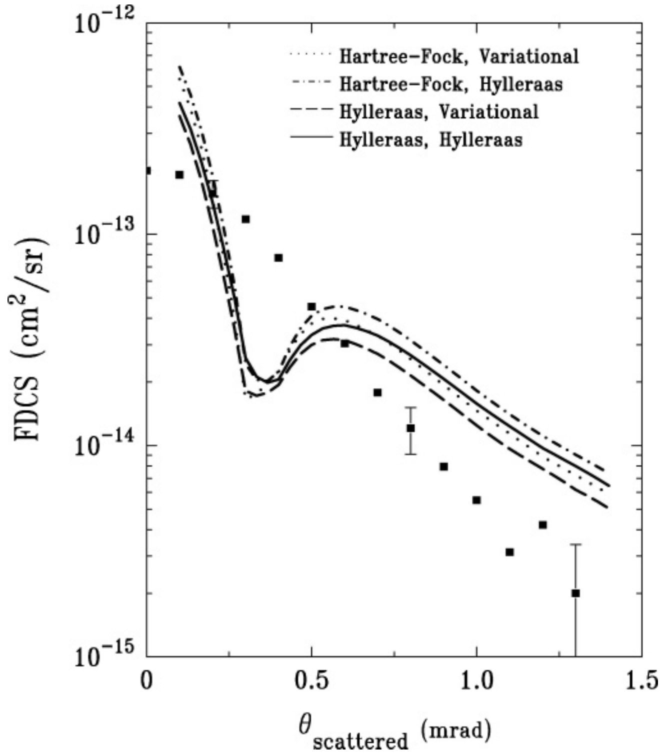

FIG. 4. FDCS for 75-keV p + He DC showing the effect of electron correlation in the target atom and the scattered ion. Experiment: Solid squares show results of Schulz *et al.* [5]. All calculations are for the 4BDC model with a plane wave for the incident projectile and Coulomb wave for the scattered projectile. Labels indicate the helium atom and H^- wave functions, respectively. All calculations have been divided by 100.

It has been shown that for total DC cross sections, it is important to include the initial-state Coulomb interactions between the projectile and the target electrons as well as final-state Coulomb interactions between the target nucleus and the captured electrons. Belkić [8] has shown that the full Coulomb wave function, and not the eikonal asymptotic form that has been successful for three-body scattering, needs to be

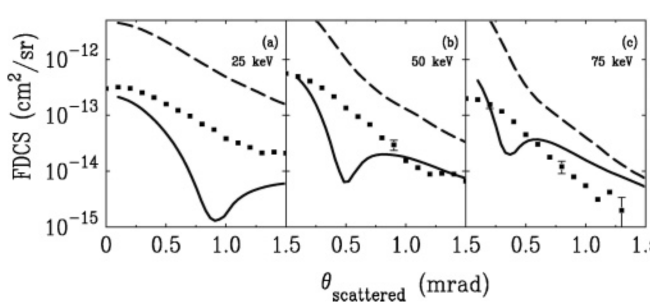

FIG. 5. FDCS as a function of projectile scattering angle for p + He DC. Experiment: Solid squares show results of Schulz *et al.* [5] for the incident projectile energies shown. Both theoretical curves are from the 4BDC model with a plane wave for the incident projectile, Hylleraas wave functions for the helium atom and H^- ion, and a Coulomb wave for the scattered projectile. Theory: The continuous curve shows all three terms in the perturbation; the dotted curve shows results without the projectile-nucleus term in the perturbation. Both calculations have been divided by 100.

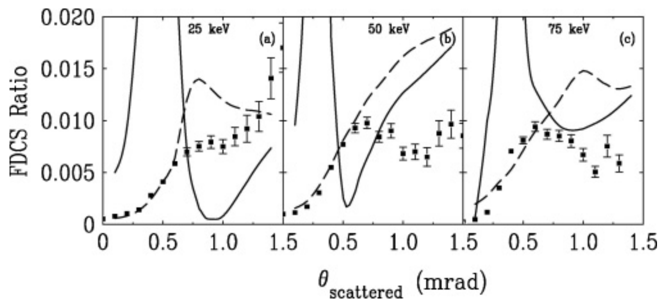

FIG. 6. FDCS ratios for $p+\mathrm{He}$ DC divided by $p+\mathrm{He}$ SC. Experiment: Solid squares show results of Schulz *et al.* [5] for the incident projectile energies shown. Theoretical curves are from the 4BTE and 4BDC models with a plane wave for the incident projectile, Hylleraas wave functions for the helium atom and H^- ion, and a Coulomb wave for the scattered projectile. Theory: The continuous curve shows all three terms in the perturbation, divided by (a) 100, (b) 35, and (c) 25; the dotted curve shows results without the projectile-nucleus term in the perturbation divided by 10 in (a)–(c).

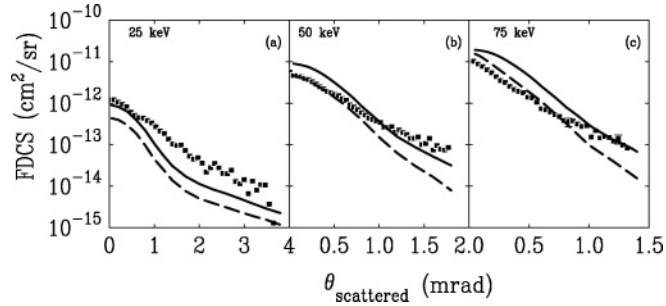

FIG. 7. FDCS as a function of scattering angle for $p+\mathrm{He}$ TTE showing the effect of the projectile-nucleus interaction. Experiment: Solid squares show results of Hasan *et al.* [99] for the incident projectile energies shown. Both theoretical curves are from the 4BTTE model with a plane wave for the incident projectile, Hylleraas wave function for the helium atom, and Coulomb wave for the scattered projectile. Theory: The continuous curve shows all three terms in the perturbation; the dotted curve shows results without the projectile-nucleus term in the perturbation.

used for these interactions. Including the initial-state Coulomb interactions between the projectile and the bound electrons is referred to as including the continuum intermediate states of the electrons in the field of the projectile [8]. We plan to investigate the importance of these interactions for differential cross sections in future work.

Schulz *et al.* [5] presented experimental results for the ratio of DC to SC. This ratio showed some structure, which they interpreted as potentially important physical effects that could be observed only in the ratio, and not in the absolute differential cross sections. Figure 6 shows this ratio of DC to SC for the differential cross sections. Clearly, since the absolute magnitude of the SC and DC theory is not in good agreement with experiment, the ratio results are not expected to have proper magnitude agreement either.

Structure in the DC-to-SC ratio is predicted by theory as well, and it can be traced to either the individual DC or the individual SC results. When the projectile-nucleus term is included in the perturbation, there is little similarity between experiment and theory due to the minima in the theoretical SC and DC cross sections, which are not seen in the experiment. When the projectile-nucleus term is excluded, there is some structure at 25 and 75 keV that is similar to that in the experiment. This structure results from the changes in slope in the individual SC and DC cross sections. Since slope changes have been attributed to a transition from electronic scattering to nuclear scattering, it is quite likely that the structure observed in the experimental data indicates this transition.

C. Transfer with target excitation

We have previously performed a detailed study of TTE for the three energies of interest here [88] using the 4BTTE model. Figure 7 presents TTE results for both including and excluding the projectile-nucleus interaction in the perturbation of Eq. (4). Experimentally, it is known that the outgoing hydrogen atom is in the ground state, and the residual helium ion is in an excited state. However, it is not known in which excited state the helium ion is left. Therefore, the cross sections must be summed over all possible excited states. The calculations shown here include s and p excited states for $2 \leqslant n \leqslant 4$. However, as we have shown in [88], the contributions of excited states above $n=4$ are negligible.

As shown in Fig. 7, the projectile-nucleus interaction has much less effect on the FDCSs for TTE than for SC or DC. Exclusion of this term from the perturbation lowers the magnitude but does not dramatically change the shape. This is in stark contrast to both SC and DC, where exclusion of the projectile-nucleus term removes the minimum in the FDCSs and increases the magnitude.

As already mentioned, the unphysical minimum seen in the SC and DC cross sections is typically attributed to a cancellation of amplitudes in the T matrix. However, if this was the only cause for the minimum, one would expect to see a minimum in TTE, where the only thing that has changed from SC is the state of the residual ion. Since we must sum over all possible excited states of the helium ion for the TTE calculations, we considered the possibility of a minimum if the helium ion is left in a particular state. However, we examined the individual angular momentum states for the dominant $n=2$ level and found no such minimum. This implies that since no minimum is observed for TTE, a cancellation of terms alone cannot account for the minimum.

IV. CONCLUSION

We have presented the 4BDC model here and applied it to proton + helium FDCSs. The effects of electron correlation in the initial and final state have been studied, and it is shown that correlation has little effect on the FDCSs. This is consistent with previous findings that correlation has little effect on total cross sections at a high incident projectile energy.

We have also compared the present SC and DC results with previously published results of the 4BTTE model for TTE. Within the 4BTTE and 4BDC models, the effect of the projectile-nucleus term has been studied. For SC and DC, inclusion of the projectile-nucleus term in the perturbation resulted in a minimum in the FDCS. When the projectile-nucleus term was excluded from the perturbation, this minimum was removed, and the magnitude of the FDCSs increased. However, for TTE, the effect of the projectile-nucleus term had much less effect on the FDCS, and no minima were observed in the calculations.

We have also examined ratios of DC-to-SC cross sections. When the projectile-nucleus term was included, there was no similarity between theory and experiment due to the theoretical minima that occur in the individual cross sections. When the projectile-nucleus term was excluded, some structure similar to the experimental data was observed for the lowest and highest energies. This structure was attributed to a transition from electronic scattering to nuclear scattering.

The 4BTTE model correctly predicts the magnitude of the SC and TTE results, but the 4BDC model overestimates the absolute experimental DC data by two orders of magnitude. Belkić [8] has shown that this magnitude discrepancy is likely due to the exclusion of the electron continuum intermediate states, and we plan to investigate this possibility in future work.

ACKNOWLEDGMENTS

This research was supported by the National Science Foundation (Grant No. PHY-0757749) and TeraGrid resources provided by the Texas Advanced Computing Center (Grant No. TG-MCA07S029). We would also like to thank Dž. Belkić for helpful discussions.

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