Total and single differential cross sections for simple resonant collisions using a fully orthonormal continuum-distorted-wave basis

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Simple electron capture processes are studied using an orthonormal two state continuum-distorted-wave (CDW) basis. The suitability of the basis set is tested by comparing predictions for total and differential cross sections with available experimental data. Overall good agreement is obtained and the authors conclude that a relatively small CDW basis set may be suitable to model a wide variety of low-energy collisions if the members of this extended set are astutely chosen.

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I. INTRODUCTION

Charge transfer processes are of fundamental interest, to physicists studying a wide range of phenomena in astrophysics, where the displacement of electrons affects the behavior of all interstellar gases [1], and to plasma physics where edge effects, in part due to electron transfer, have detrimental consequences on the process of thermonuclear fusion [2]. Concurrent improvement in the accuracy of detection methods, like photon emission spectroscopy (PES) and translational energy spectroscopy (TES), has allowed charge transfer to be studied at the lowest impact energies leading to a wealth of experimental data being available. Unfortunately the development of theoretical models has not advanced at the same pace and while models exist which can produce reliable cross sections for charge transfer at moderate and high energies there is little consensus at impact energies below 1 keV/a.m.u. [3].

The purpose of this discussion is to assess the suitability of a continuum-distorted-wave (CDW) based model to study charge transfer. The advantages of this treatment should be many-fold. First the inclusion of electron translation factors (ETF's) implies that the system will be Galilean invariant. Second the distorted waves used will automatically satisfy the relevant boundary conditions, an attribute which has been shown to be a necessity in any reliable theory [4]. Finally, a fully orthogonal and normalized CDW basis set has been used when deriving the appropriate coupled equations. This feature ensures that probability is conserved throughout the collision and that estimates for cross sections remain sensible regardless of the impact velocity.

The scope of this paper will be confined to resonant collisions where the entrance and exit channels of the active electron are both 1*s* states and the transfer of the electron leaves the binding energy of the electron unchanged. This transfer process should be dominant during the collision and the coupling between the entrance and exit channels will be much stronger than that in any other reaction path. Hence a two state approximation should be valid and any error in the results can be attributed to the use of a CDW basis set rather than to the truncation of the total wave function to two terms.

Throughout this paper the projectile will be assumed to follow a straight line trajectory and atomic units will be used unless otherwise stated.

II. THEORY

Working with the straight line impact parameter representation the initial-(i) and final-(f) state wave functions,

$$\psi_i(\mathbf{r},t) = N(\nu_P)\varphi_i(\mathbf{r_T})\exp\left(-i\varepsilon_i t - \frac{i\mathbf{v}\cdot\mathbf{r}}{2} - \frac{iv^2t}{8}\right) \times {}_1F_1(i\nu_P;1;i(vr_P+\mathbf{v}\cdot\mathbf{r_P}))(vR-v^2t)^{iZ_TZ_P/v}, \quad (1)$$

$$\psi_f(\mathbf{r},t) = N^*(\nu_T)\varphi_f(\mathbf{r_P})\exp\left(-i\varepsilon_f t + \frac{i\mathbf{v}\cdot\mathbf{r}}{2} - \frac{iv^2t}{8}\right) \times {}_1F_1(-i\nu_T;1;-i(vr_T+\mathbf{v}\cdot\mathbf{r_T}))(vR+v^2t)^{-iZ_TZ_P/v}, \quad (2)$$

are used to construct a fully orthogonal basis set to describe the collision:

$$P^{Z_P+} + T^{(Z_T-1)+}(1s) \rightarrow P^{(Z_P-1)+}(nl) + T^{Z_T+}, \quad (3)$$

where φ_i and φ_f are representations of the motion of the single electron present in the appropriate undisturbed state and the remaining variables are defined in Crothers [5]. In a two-state approximation the total wave function for this collision can be written as

$$\Psi(\mathbf{r},t) = c_i(\boldsymbol{\rho},t)\hat{\psi}_i + c_f(\boldsymbol{\rho},t)\hat{\psi}_f, \quad (4)$$

where

$$\hat{\psi}_i = \frac{\psi_i}{\sqrt{\langle\psi_i|\psi_i\rangle}}, \quad (5)$$

$$\hat{\psi}_f = a(\boldsymbol{\rho},t)\psi_i + b(\boldsymbol{\rho},t)\psi_f, \quad (6)$$

$$a(\boldsymbol{\rho},t) = \frac{-s_{if}}{\sqrt{s_{ii}}\sqrt{s_{ii}s_{ff}-s_{if}s_{fi}}}, \quad (7)$$

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$$b(\boldsymbol{\rho},t) = \sqrt{\frac{s_{ii}}{s_{ii}s_{ff} - s_{if}s_{fi}}}, \tag{8}$$

$$s_{jk}(\boldsymbol{\rho},t) = \langle \psi_j | \psi_k \rangle, \tag{9}$$

$$s_{kj}(\boldsymbol{\rho},t) = s_{jk}(\boldsymbol{\rho},t)^*, \tag{10}$$

$$\langle \hat{\psi}_j | \hat{\psi}_k \rangle = \delta_{jk}. \tag{11}$$

Defining:

$$H = -\frac{1}{2}\nabla_{\mathbf{r}}^2 - \frac{Z_T}{r_T} - \frac{Z_P}{r_P} + \frac{Z_P Z_T}{R}, \tag{12}$$

and applying the variational principle of Sil [6]

$$\delta \int_{-\infty}^{+\infty} dt \langle \Psi(\mathbf{r},t) | \left(H - i\frac{d}{dt} \right) | \Psi(\mathbf{r},t) \rangle = 0, \tag{13}$$

to the coefficients $c_i(\boldsymbol{\rho},t)$ and $c_f(\boldsymbol{\rho},t)$, it can be deduced that the coupled equations governing the system are

$$i\frac{d}{dt}c_i(\boldsymbol{\rho},t) = c_i(\boldsymbol{\rho},t)\langle \hat{\psi}_i | \left(H - i\frac{d}{dt} \right) | \hat{\psi}_i \rangle + c_f(\boldsymbol{\rho},t)\langle \hat{\psi}_i | \left(H - i\frac{d}{dt} \right) | \hat{\psi}_f \rangle, \tag{14}$$

$$i\frac{d}{dt}c_f(\boldsymbol{\rho},t) = c_i(\boldsymbol{\rho},t)\langle \hat{\psi}_f | \left(H - i\frac{d}{dt} \right) | \hat{\psi}_i \rangle + c_f(\boldsymbol{\rho},t)\langle \hat{\psi}_f | \left(H - i\frac{d}{dt} \right) | \hat{\psi}_f \rangle, \tag{15}$$

which is a result identical to one obtained by a second-order Euler-Lagrange method.

A. Evaluation of matrix elements

In order to solve the coupled equations it is necessary to evaluate the matrix elements:

$$s_{jk}(\boldsymbol{\rho},t) = \langle \psi_j | \psi_k \rangle, \tag{16}$$

and

$$h_{jk}(\boldsymbol{\rho},t) = \langle \psi_j | \left(H - i\frac{d}{dt} \right) | \psi_k \rangle. \tag{17}$$

This is done by treating $\mathbf{r_P}$, $\mathbf{r_T}$, and t as generalized nonorthogonal coordinates in a manner similar to the method used in Crothers [5]. As the entrance and exit channels in this discussion are both 1*s* states, the matrix element $h_{fi}^{1s-1s}(\boldsymbol{\rho},t)$ is evaluated here explicitly with the evaluation of the elements $s_{if}^{1s-1s}(\boldsymbol{\rho},t)$ and $h_{if}^{1s-1s}(\boldsymbol{\rho},t)$ being achieved in an almost identical manner.

Consider

$$\frac{h_{fi}^{1s-1s}(\boldsymbol{\rho},t)}{\beta_{1s1s}} = \frac{\langle \psi_f | \left(H - i\frac{\partial}{\partial t} \right) | \psi_i \rangle}{\beta_{1s1s}} = \int d\mathbf{r} e^{-i\boldsymbol{v}\cdot\mathbf{r}} {}_1F_1(i\nu_T;1;i(vr_T + \boldsymbol{v}\cdot\mathbf{r_T}))\boldsymbol{\nabla}_{r_T}[e^{-Z_T r_T}] \cdot e^{-Z_P r_P}\boldsymbol{\nabla}_{\mathbf{r_P}}\left[{}_1F_1(i\nu_P;1;i(vr_P + \boldsymbol{v}\cdot\mathbf{r_P})) \right]$$
$$= \int d\mathbf{r} e^{-i\boldsymbol{v}\cdot\mathbf{r}} \overline{g}(\mathbf{r_T})\overline{f}(\mathbf{r_P}) = \int \frac{d\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{R} + (1/2)i\boldsymbol{v}\cdot\mathbf{R}}}{(2\pi)^3} \overline{F}_{1s-1s}^{hfi}(\mathbf{q}) \cdot \overline{G}_{1s-1s}^{hfi}(-\mathbf{v}-\mathbf{q}), \tag{18}$$

where

$$\alpha_{1s1s} = \frac{(Z_P Z_T)^{3/2}}{\pi} N(\nu_P) N(\nu_T), \tag{19}$$

$$\Delta\epsilon = \varepsilon_i - \varepsilon_f, \tag{20}$$

$$\beta_{1s1s} = -\alpha_{1s1s} e^{-i\Delta\epsilon t} (\rho v)^{2iZ_P Z_T/v}, \tag{21}$$

$$\overline{G}_{1s-1s}^{hfi}(\mathbf{q}) = \int d\mathbf{r_T} e^{i\mathbf{q}\cdot\mathbf{r_T}} \overline{g}(\mathbf{r_T}) = \int d\mathbf{r_T} e^{i\mathbf{q}\cdot\mathbf{r_T}} {}_1F_1(i\nu_T;1;i(vr_T + \boldsymbol{v}\cdot\mathbf{r_T}))\boldsymbol{\nabla}_{\mathbf{r_T}} e^{-Z_T r_T}$$
$$= \boldsymbol{\nabla}_{\mathbf{q}} \int \frac{iZ_T d\mathbf{r_T}}{r_T} e^{i\mathbf{q}\cdot\mathbf{r_T} - Z_T r_T} {}_1F_1(i\nu_T;1;i(vr_T + \boldsymbol{v}\cdot\mathbf{r_T})) = iZ_T \boldsymbol{\nabla}_{\mathbf{q}} \Lambda(\mathbf{q}, Z_T, 0, \nu_T, 0, \boldsymbol{v}), \tag{22}$$

$$\overline{F}_{1s-1s}^{hfi}(\mathbf{q}) = \int d\mathbf{r_T} e^{i\mathbf{q}\cdot\mathbf{r_T}} \overline{f}(\mathbf{r_T}) = \int \frac{d\mathbf{r_P}}{r_P} e^{i\mathbf{q}\cdot\mathbf{r_P} - Z_P r_P} \boldsymbol{\nabla}_{\mathbf{r_P}} \left[{}_1F_1(i\nu_P;1;i(vr_P + \boldsymbol{v}\cdot\mathbf{r_P})) \right]$$
$$= \mathcal{L}\left[\int \frac{d\mathbf{r_P}}{r_P} e^{i\mathbf{q}\cdot\mathbf{r_P} - Z_P r_P} {}_1F_1(i\nu_P;1;i(vr_P + \boldsymbol{v}\cdot\mathbf{r_P})) \right] = \mathcal{L}[\Lambda(\mathbf{q}, Z_P, 0, \nu_P, 0, \boldsymbol{v})]. \tag{23}$$

The operator $\mathcal{L}$ is defined as

$$\mathcal{L} = \left[iZ_P \boldsymbol{\nabla}_{\boldsymbol{q}} - i\boldsymbol{q}\frac{d}{dZ_P} \right], \tag{24}$$

and $\Lambda(\boldsymbol{q}, Z, a_1, a_2, \boldsymbol{p}_2, \boldsymbol{p}_2)$ is obtained from the standard Nordsieck integral [7]). If $\boldsymbol{q}$ is expressed in terms of cylindrical polar coordinates the angular dependence is contained entirely in the exponential term of Eq. (18) and thus one integration can be performed analytically and the resulting function is *independent* of the orientation of the vector $\boldsymbol{\rho}$. Unfortunately the matrix elements $s_{jj}^{1s-1s}(\rho,t)$ and $h_{kk}^{1s-1s}(\rho,t)$ do not lend themselves to calculation via a Fourier transform and are most efficiently evaluated as they stand, using a parabolic coordinate system with the origin chosen so that the number of evaluations of the Kummer function is minimized. These integrals could be reduced to a lower dimension but the method is tedious and does not give any significant advantage numerically. The remaining quantities required can be deduced since

$$h_{jk}(\rho,t) - h_{kj}^{*}(\rho,t) = -i\langle\overline{\psi_j}|\frac{d}{dt}|\psi_k\rangle - i\langle\psi_k|\frac{d}{dt}|\psi_j\rangle^{*}$$

$$= -i\frac{d}{dt}\langle\psi_j|\psi_k\rangle. \tag{25}$$

Thus

$$h_{if}(\rho,t) - h_{fi}^{*}(\rho,t) = -i\frac{d}{dt}s_{if}(\rho,t), \tag{26}$$

and

$$\Im(h_{jj}(\rho,t)) = -\frac{1}{2}\frac{d}{dt}s_{jj}(\rho,t). \tag{27}$$

B. Total and differential cross sections

The probability amplitude associated with electron capture to the state ψ_f at impact parameter $\boldsymbol{\rho}$ is defined as $c_f(\boldsymbol{\rho}, t=+\infty)$. The capture probability $|c_f(\boldsymbol{\rho}, t=+\infty)|^2$ will be independent of the orientation of the collision plane with respect to any fixed plane including the incident polar axis, and the cross section σ, for capture to this state is simply defined as

$$\sigma = 2\pi\int_0^{\infty} \rho|c_f(\rho, t=+\infty)|^2 d\rho. \tag{28}$$

It should be noted that the total cross section for capture is independent of the term $Z_P Z_T/R$, which could have been removed from Eq. (12) by means of a simple transformation. Consequently the phase factors $(vR - v^2t)^{iZ_TZ_P/v}$ and $(vR + v^2t)^{-iZ_TZ_P/v}$ could have been omitted from $\psi_i(\mathbf{r},t)$ and $\psi_f(\mathbf{r},t)$.

In ion-atom collisions many important quantities need to be measured in order to accurately compare experimental data and theoretical predictions. The more quantities that can be measured the more stringent a test may be placed upon the theoretical predictions and thus assess their suitability at describing a particular physical situation. Otherwise the unmeasured quantities must be integrated over all possible values and possibly mask important insights and hinder understanding of the associated problem. For this reason predictions of differential cross sections are much more useful than that of total cross sections. The differential cross section $d\sigma/d\Omega$ in the straight line impact parameter formulation is calculated from McCarroll and Salin [8] and is defined as

$$\frac{d\sigma}{d\Omega} = \mu^2 v^2 \left| \int_0^{\infty} \rho J_0(\eta\rho) c_f(\rho, t=+\infty) d\rho \right|^2, \tag{29}$$

where

$$\eta = 2\mu v \sin\frac{\theta}{2}, \tag{30}$$

μ is the heavy particle reduced mass, θ is the scattering angle in the center of mass system, and $c_f(\rho, t=+\infty)$ is the charge exchange amplitude at impact parameter ρ. This expression is calculated by starting from the fully quantal expression for the differential cross section, and retaining only the first term in an expansion in m/M (m and M are the electron and proton masses, respectively). In contrast to the total cross section the differential cross section is *not* independent of the phase introduced by the internuclear potential $Z_T Z_P/R$ and so this term may not be omitted from Eq. (12) during calculations for differential cross sections.

III. RESULTS

The preceding theory, now called CDW2S is applied to two of the most basic resonant charge-transfer processes; First to electron capture between atomic hydrogen and a proton and second to a collision between a singly charged He ion and a He atom. In the first collision the total cross section, σ_T has been estimated using the n^{-3} scaling law [9]:

$$\sigma_T \approx 1.202\sigma_{1s\to 1s}. \tag{31}$$

The second collision, involving the He nuclei, presents the dilemma of how to model the motion of the electrons present. As CDW2S is not versatile enough to account for the motion of two electrons simultaneously, the He atom (ion) is approximated using a H-like atom (ion) with an appropriately chosen charge. This charge is chosen using a variational principle, and also so that the energy levels of the electron in the replacement system and that in the H atom coincide. In both cases a multiplying factor is used in order to account for the fact that two electrons are available for capture.

Of the two collisions the first has been most extensively studied with experimental data being available for total cross sections over a wide energy range and differential cross sections at a selection of impact energies. For this reason the discussion commences with this system. The total cross sections as a function of impact energy are presented in Fig. 1, along with the experimental results of Janev and Smith [10] and the theoretical predictions of Copeland and Crothers [11]. The differential cross sections as a function of labora-

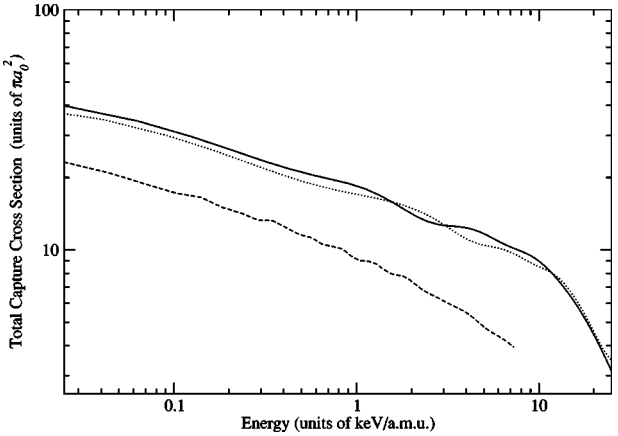

FIG. 1. Total capture cross sections σ_T for symmetric electron capture between H^+ and H(1*s*). Theory: solid line, CDW2S (this work); dashed line: Firsov approximation [11]) Experiment: dotted line, Janev and Smith [10].

tory scattering angle are shown in Figs. 2 and 3 at impact energies of 25 and 60 keV, respectively, along with the appropriate estimates of Martin *et al.* [12].

Generally, accord with experimental values for σ_T is good with the CDW2S theory differing by no more than 10% over the energy range considered and it is noted that the use of an orthonormal basis set has resulted in the estimates remaining realistic regardless of impact energy in contrast to previous CDW based models where lack of unitarity results in severely excessive cross sections as the impact velocity decreases.

A more rigorous test of the theory is provided by comparing estimates for differential cross sections with experimental values. In this respect agreement is excellent at energies of 25 and 60 keV, especially at the smaller scattering angles and though the level of accuracy does decrease as θ increases the CDW2S estimates do fall off at a rate comparable to experiment. Thus in relation to this collision it is concluded

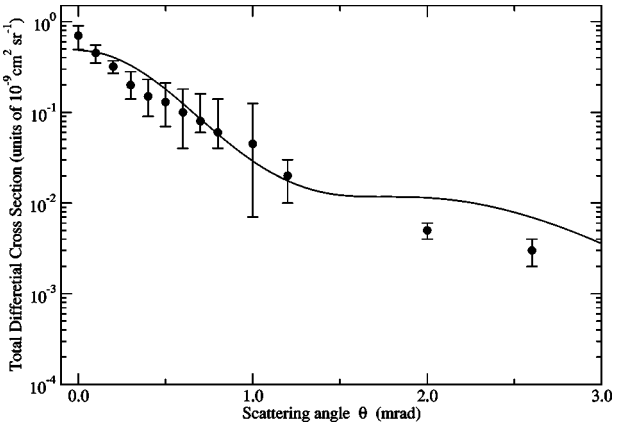

FIG. 2. Differential cross sections $d\sigma_T/d\Omega$ measured in the center-of-mass frame, at an impact energy of 25 keV for electron capture by H^+ from H(1*s*). Theory: solid line, CDW2S (this work). Experiment: circles, Martin *et al.* [12].

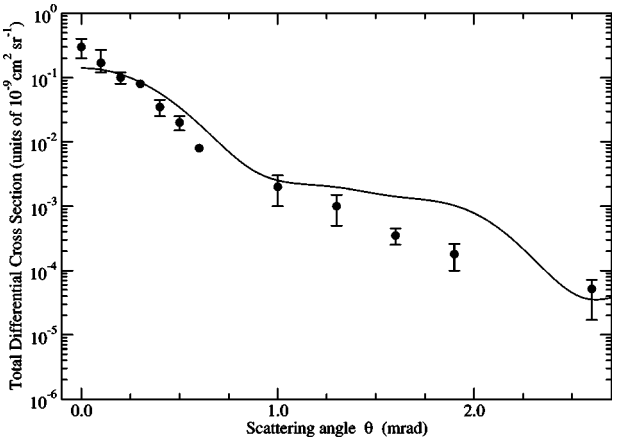

FIG. 3. Total differential cross sections $d\sigma_T/d\Omega$ measured in the center-of-mass frame, at an impact energy of 60 keV for electron capture by H^+ from H(1*s*). Theory: solid line, CDW2S (this work). Experiment: circles, Martin *et al.* [12].

that most of the physics of the problem has been included in the theory.

With the success at modeling symmetric electron capture between protons attention now turns to the corresponding collision involving capture to and from the 1*s* states of H atoms and singly charged ions. For this system the dual-electron H atom has been replaced with a single electron hydrogenic ion with effective charges chosen as previously discussed. To account for the presence of the second electron, which will obviously contribute significantly to the capture process, factors of 2 and 1.95 are used in conjunction with effective charges of 2 and 1.6875 a.u., respectively, to calculate the capture cross section $\sigma_{1s\leftrightarrow 1s}$ (the second factor accounting for the overlap in the relevant electronic wave functions). The cross section for capture to the 1*s* state of the projectile, $\sigma_{1s\leftrightarrow 1s}$, as a function of the laboratory impact energy per atomic mass unit is shown in Fig. 4 with the differential cross section, $d\sigma_{1s\leftrightarrow 1s}/d\Omega$ as a function of the center-of-mass scattering angle and excluding the effect of the second electron, at an impact energy of 60 keV, given in Fig. 5.

Regardless of which of the two charges is used, CDW2S returns satisfactory estimates for capture cross sections in this relatively low collision energy range. However, the results generally overestimate the empirical data at almost all energies and hence it is deduced that the presence of the second electron does not increase the capture cross section by as much as a factor of 2. This observation is reinforced by the fact that the accuracy of the predictions of Copeland and Crothers [11] in this energy range relative to experiment has dramatically improved. In the *p*-H collision the Firsov approximation significantly underestimated the total capture cross section σ_T, and it would have been expected that this feature would have carried through to the He^+-He collision. This is not the case and is explained by the fact that Copeland and Crothers used a method similar to the one suggested here to account for the second electron. This has resulted in the capture probabilities, which were originally too small, being artificially inflated, inadvertently improving agreement with the experimental results. In any case the results show

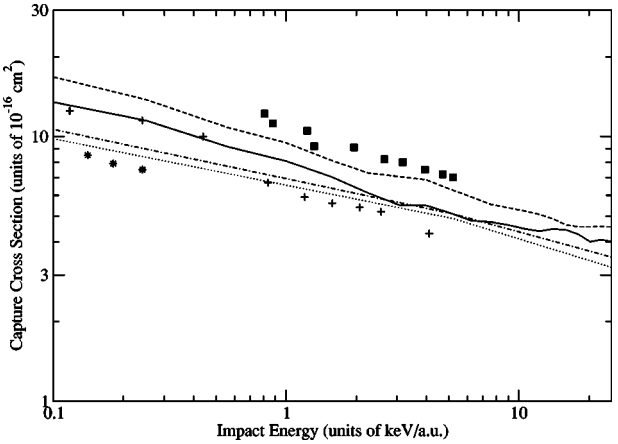

FIG. 4. Capture cross sections, $\sigma_{1s\leftrightarrow 1s}$, for symmetric electron capture between $He^+(1s)$ and $He(1s^2)$. Theory: solid line, CDW2S where $Z_{P,T}=1.34$ (this work); dashed line, CDW2S where $Z_{P,T}=1.6875$ (this work); dotted line, Firsov approximation (Copeland and Crothers [11]); dot-dashed line, Atomic orbital approximation (Sakabe and Izawa [13]). Experiment: Crosses, Gilbody and Hasted [14]; squares, Keene [15]; asterisks, Cramer and Simons [16].

that the multielectronic target or projectile may be adequately represented with a simpler single electronic system without having a detrimental effect on the accuracy of the total cross-section predictions.

Unfortunately, in Fig. 5 no experimental data are available for comparison with CDW2S predictions of $d\sigma_{1s\leftrightarrow 1s}/d\Omega$. The results correctly suggest that the projectile is much less likely to be scattered but it is expected that the magnitude of $d\sigma_{1s\leftrightarrow 1s}/d\Omega$ will only be reliable at very small scattering angles, corresponding to medium and large impact parameters, due to the manner in which the H atom (ion) has been described.

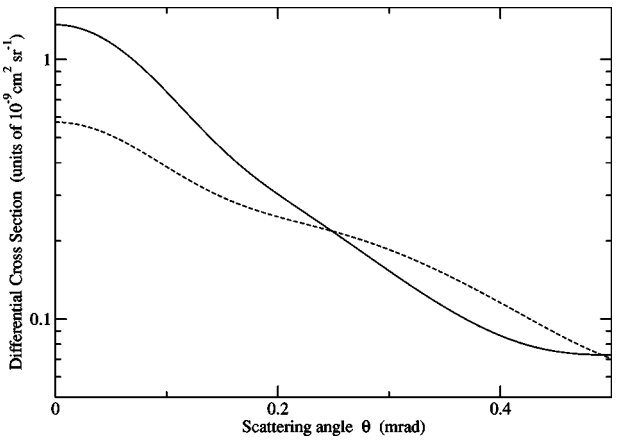

FIG. 5. Differential cross sections $d\sigma_{1s\leftrightarrow 1s}/d\Omega$ measured in the center-of-mass frame, at impact energy 60 keV for electron capture by $He(1s)^+$ from $He(1s^2)$. Theory: solid line, CDW2S where $Z_{P,T}=1.34$ (this work); dashed line, CDW2S where $Z_{P,T}=1.6875$ (this work).

IV. CONCLUSION

The CDW2S method described here is a definite improvement over many of the other existing models for studying charge transfer [17] at lower collision energies where results are in excellent agreement with experiment. The implementation of the model is relatively easy, providing reliable cross sections in relation to experiment over a wide range of collision energies. As the original CDW states become orthonormal as $v\rightarrow\infty$ the quantity $\dot{s}_{if}$ becomes negligible at high impact energies. Unsurprisingly then the CDW2S approximation concurs with the unnormalized CDW theory of Cheshire [20] and the previously proven symmetrized variational CDW theory of Brown and Crothers [18] at collision energies above 70 keV. At very low energies there is good accord with the Firsov approximation [19,11].

Unfortunately, the model has only been applied to a very restricted class of collision where two-states are very strongly coupled together so that a two state approximation is expected to be valid. In these instances CDW2S has performed admirably though its application to monoelectronic systems was more successful than to systems where more than one electron was present. The collision between the two H nuclei has demonstrated one of the model's inadequacies as the motion of only one electron is accounted for. Furthermore, the movement of this electron must be represented with a simple hydrogeniclike orbital. Fortunately this method of modeling the electronic motion is not severely restrictive as many of the most interesting collisions are between ions where the behavior of the active electron is essentially hydrogenic in character. Currently there is a wealth of experimental data relating to the collision of atomic hydrogen with multiply charged H-like ions [21].

Overall, the following inferences are drawn from the study. First a CDW based model will provide accurate cross sections only if all the dominant exit channels are explicitly included in the calculation. Thus to successfully model electron transfer between multiply charged ions it may be necessary to extend the basis set to include all the states whose energy levels lie in close proximity to that of the entrance channel. Without this refinement the model will fail regardless of the type of basis set used. The most notable feature of the model presented is that it adheres to the law of probability conservation at all times. Previous CDW based models have ignored the fact that in general the appropriate CDW functions are neither orthogonal nor normalized. While it may be valid to disregard this fact at moderate to high impact energies, the effect of this assumption becomes more pronounced as the energy decreases. This may lead to excessively large cross sections, like those in Crothers and Dunseath [22], and to unexpected features in the differential cross sections [23]. Thus the use of a fully orthonormal basis set is an essential component in any low-energy CDW approximation.

In conclusion CDW2S represents a sound platform on which to base future research. CDW (2S) is a dynamic molecular theory [24,25] in which the equivalent of perturbed

stationary states radial and rotational coupling is the proverbial dipole-dipole coupling. Further study should concentrate on extending the size of the basis set so that a wider range of collisions can be studied.

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