

Symmetric double charge exchange in fast collisions of bare nuclei with heliumlike atomic systems

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Double charge exchange in fast collisions between completely stripped projectiles and heliumlike atomic systems is investigated by means of the correct first Born approximation. The theory is devised beyond the usual independent-particle model. For the reason of consistency, the usual proper boundary conditions must be reformulated when dealing with atoms or ions containing more than one electron. Consequently an appropriate correction ought to be introduced in the perturbation potential, which conveniently deals with the difficulty related to the unavailability of exact two-electron bound-state wave functions. For the purpose of illustration, numerical computations are performed for electron capture by α particles from helium. Total cross sections are found to be in satisfactory agreement with the available experimental data from 100 to 2000 keV.

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I. INTRODUCTION

Double electron capture from multielectron atoms or ions by completely stripped projectiles has received considerable attention over a long period of time from both experimental and theoretical points of view. Most of the measurements cover the low and intermediate incident-energy region [1–16] [50,500] keV/amu, whereas the experimental data at higher energies are sparse [17–20] and hence still awaiting completion. The measured total cross sections are far from forming a fully satisfactory data base and much further effort is required to fill in the existing gaps. This is particularly important in view of the relative significance of the electronic-correlation effects. These effects are manifested through the electronic repulsion $1/r_{12}$, which prevents the two electrons from coming too close to each other in space. The correlations of the electrons play a marginal role in the intermediate-energy range, but they become of considerable importance at low and, quite interestingly, also at high energies.

As to the theoretical studies, they were mostly concentrated upon the so-called independent-particle model (IPM) [21–35], in which the interelectron potential is substituted by an average field introduced within various perturbative or nonperturbative approximations. The IPM consists of treatment of the double charge exchange as two independent single-electron transfers. As a consequence, the overall transition probability \mathcal{P} for the total event is given as the product $\mathcal{P}_1\mathcal{P}_2$ of the two individual probabilities \mathcal{P}_1 and \mathcal{P}_2 for each of the participating electrons. Such an approach then completely ignores the *dynamic* correlations, as one of the causes of the transition from the initial to the final state of the whole *four-body* system. Consequently, e.g., capture of a given target electron resulting from its interaction with the other electron in the presence of the projectile field is entirely neglected. In other words, the inability of the IPM to account for

the dynamic correlations stems from the very definition of total probability \mathcal{P} , which is given only in terms of certain single-electron perturbation potentials.

In addition to the dynamic, there exist also the *static* correlations, which originate from the Coulomb interaction $1/r_{12}$ between the two electrons in the heliumlike atomic systems *before* the collision takes place. This kind of correlation is reminiscent of a given isolated two-electron atomic particle and, therefore, has nothing to do with the scattering event, since, e.g., a quantum-mechanical bound state of the target is by definition prepared in the absence of the incident beam. Strictly speaking, a fully adequate description of the static correlations for heliumlike atomic systems must explicitly include the *two* electronic coordinates $\mathbf{r}_{1,2}$ and directly or indirectly the interelectronic distance $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$. When this is accomplished, the resulting correlated theory departs in a clear manner from the standard Hartree-Fock method. As the best known representative of the single-particle model, the Hartree-Fock self-consistent-field procedure encompasses the so-called *single-electron approximation*, which provides a heliumlike orbital in terms of only *one* electronic coordinate. Recall that the correlation effects are by definition referred to as the phenomena which cannot be described by a single-particle model. A well-known example is the notion of the correlation energy, which is introduced as the difference between the “exact” and the corresponding Hartree-Fock energy [36]. From the physical point of view, the electron correlation is plausibly understood as the phenomenon by which the electrons try to *avoid* each other through the Coulomb repulsion $1/r_{12}$ in order to *lower* the binding energy of a given heliumlike atomic system. For an instructive analysis of the role of the correlation effects concerning the single and double charge exchange in α -He collisions at low and intermediate energies, see Schaudt, Kwong, and Garcia [37].

Here the natural question emerges as to whether there

is any reason to go beyond the above-mentioned standard IPM or eventually to abandon it altogether. This is a matter of principle, since it is necessary to inspect whether the IPM possibly violates certain *ab initio* conditions. Such a question is then put on a qualitatively different footing from previous judgments about the validity of the IPM based upon *empirical* evidence collected merely by checking the theory against the experimental data. The answer to the above question cannot *a priori* be negative, before we verify whether a purely *three*-body nature of the IPM is justified on a *theoretical* basis, when dealing with the true *four*-body problem under study. Of course, a proper four-body treatment is a more satisfactory starting point, because it offers various possibilities to incorporate adequately both dynamic and static correlations. The dynamic correlations would be included by selecting the appropriate forms of the four-body perturbation potentials, which could not be done at all in the IPM. The static correlations of a four-body scattering theory can also be treated in an adequate manner, because the heliunlike orbitals would automatically contain both electronic coordinates $\mathbf{r}_{1,2}$ together with an implicit (configuration interaction [38]) or explicit [39] inclusion of the interelectron distance r_{12} . Hence the justification for introduction of new theories, which would preserve the genuine four-body nature of double charge exchange in collisions between bare nuclei and two-electron atoms or ions.

Once the single-electron transition amplitudes are available in any of the existing approximations, the predictions on double charge exchange can easily be obtained within the IPM. In this way, Gayet, Rivarola, and Salin [28] and more recently Deco and Grün [30] have used the general algorithm of Belkić, Gayet, and Salin [40] for one-electron transfer in the framework of the continuum-distorted-wave (CDW) approximation of Cheshire [41] to readily deduce the cross sections for double charge exchange in α -He collisions at intermediate and high energies. The major reason for the fact that the previous studies of two-electron transfer processes have predominantly been concentrated upon the IPM was the computational complexity of the proper four-body treatment. Most researchers have limited themselves to analytically calculating the transition amplitude for double charge exchange [20,28–32], just as easily as in the case of single-electron transitions, so that resorting to the IPM became unavoidable.

However, it is quite clear *a priori* that *formal* theories for single-electron transfer, built for pure three-body problems, can be directly generalized, without any difficulty, to double charge exchange in four-body collisions. Nevertheless, it was only recently that, e.g., the CDW method was properly formulated and implemented by Belkić and Mančev [42,43] to double-electron transfer as a correct four-body theory. The CDW approximation of Refs. [42] and [43] was devised within the well-known distorted-wave formalism of Dodd and Greider [44] in such a manner that the four-body nature of the problem is fully preserved. Such a CDW method has emerged as a first-order approximation to Dodd and Greider's modified perturbation expansion [44] in which all the dia-

grams are kept connected by an adequate choice of the distorting potentials. At the same time, the new CDW method [42,43] belongs to a class of so-called second-order theories, which relate to the methods including the continuum intermediate states of the two electrons in one and/or both channels of the double-charge-exchange reaction. Such a strict four-body CDW method of Refs. [42] and [43] is not only theoretically more satisfactory than all the previous IPM versions [28–31] of Cheshire's [41] theory, but also provides excellent agreement with the existing experimental data on two-electron capture from He by fast protons [42,43]. Further work is required along these lines for other systems to assess the validity of the four-body CDW approximation in systematic comparisons with the measurements on other colliding particles. Also the actual validity of the IPM three-body variant [28–31] of the CDW approximation should now be established by comparisons with the four-body CDW theory [42,43] and that certainly represents a much more stringent test than the previous checking against the measurements.

Considering the single-electron transfer problems, the former detailed experience [45,46] confirmed that, for reliable predictions on total cross sections, it is not mandatory at all to use the second-order theories, at impact energies which are small in comparison with the range dominated by the Thomas double scattering. In particular, it has been convincingly demonstrated [45,46] that the first Born (CB1) approximation with the correct boundary conditions is systematically in excellent agreement with the experiment on one-electron capture from hydrogenic and multielectron targets. It would then appear desirable to see whether an analogous conclusion would also hold true for the two-electron capture process. Hence the need to devise a four-body CB1 approximation. This is the subject of the present work. We shall first formulate the CB1 theory for a general case (heteronuclear and/or homonuclear) of two-electron capture from heliumlike systems by completely stripped projectiles. The explicit calculation of the matrix elements will, however, presently be accomplished for the homonuclear collisions and applied to the symmetric resonant double charge exchange in α -He($1s^2$) scattering. Particular attention is focused upon a consistent introduction of the proper asymptotic channel states, despite the fact that the exact bound-state wave function of the two-electron systems is unknown.

II. THEORY

We study a collision in which the nucleus P of charge Z_P is impinging upon a heliumlike atomic system consisting of two electrons e_1 and e_2 bound to the nucleus T of charge Z_T , i.e.,

$$Z_P + (Z_T; e_1, e_2)_i \rightarrow (Z_P; e_1, e_2)_f + Z_T. \quad (2.1)$$

The parentheses in double-charge-exchange process (2.1) symbolize the bound states, whose quantum numbers are given by the collective label i or f . Let us denote by \mathbf{R} the position vector of P relative to T . Further, the position vectors of e_1 and e_2 relative to P and T will, respec-

tively, be represented by $\mathbf{s}_{1,2}$ and $\mathbf{x}_{1,2}$. Thus the interelectron distance $r_{12} \equiv |\mathbf{r}_{12}|$ can be defined by the vector $\mathbf{r}_{12} = \mathbf{x}_1 - \mathbf{x}_2 \equiv \mathbf{x}_{12} = \mathbf{s}_1 - \mathbf{s}_2 \equiv \mathbf{s}_{12}$. We also introduce \mathbf{r}_i and \mathbf{r}_f as the position vectors of P and T relative to the center of mass of $(T, 2e)$ and $(P, 2e)$, respectively.

When treating a general collision, one formally begins with the *exact* transition amplitude in either its standard *prior* \mathcal{T}_{if}^- or *post* \mathcal{T}_{if}^+ form. These two starting expressions are identical to each other on the energy shell, if the initial φ_i and final φ_f bound-state wave functions are exact. Whenever the latter conditions are not fulfilled, as in the case of reaction (2.1), we say that there is a so-called *post-prior* discrepancy. In such a circumstance, one cannot decide with certainty on a purely theoretical basis which of the two forms, *prior* or *post*, is more physically acceptable. It then appears reasonable to introduce a modified transition amplitude, which would be, e.g., an average value [45(d)] of the quantities \mathcal{T}_{if}^- and \mathcal{T}_{if}^+ , such as $\mathcal{T}_{if} = (\mathcal{T}_{if}^- + \mathcal{T}_{if}^+)/2$. Clearly, this new starting point of the full transition amplitude \mathcal{T}_{if} would yield the same result as its prior or post form on the energy shell and for the exact bound-state wave functions $\varphi_{i,f}$. The first-order T_{if} of such an average full transition amplitude \mathcal{T}_{if} in the distorted-wave formalism of Belkić, Gayet, and Salin [47] reads as follows:

$$2T_{if} = \langle \Phi_f^- | \Omega_f^{-\dagger} [(V_i - W_i) + (V_f - W_f^\dagger)] \Omega_i^+ | \Phi_i^+ \rangle, \quad (2.2)$$

where henceforth the atomic units are used. Here $\Phi_{i,f}^\pm$ are the entrance and exit channel states, $\Omega_{i,f}^\pm$ represent the Möller wave operators, $V_{i,f}$ denote the channel perturbation interactions, and $W_{i,f}$ are certain distorting potentials to be conveniently specified,

$$(E - H_{i,f} - W_{i,f}^d) \Phi_{i,f}^\pm = 0, \quad (2.3a)$$

$$\Omega_{i,f}^\pm = 1 + \frac{1}{E - H_{i,f} - W_{i,f}^\pm i\epsilon} U_{i,f}, \quad \epsilon \rightarrow 0^+, \quad (2.3b)$$

$$W_{i,f} = U_{i,f} + W_{i,f}^d, \quad (2.3c)$$

$$V_i = \frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}, \quad V_f = \frac{Z_P Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2}. \quad (2.3d)$$

The initial and final bound-state wave functions will be labeled by $\varphi_i \equiv \varphi_i(\mathbf{x}_1, \mathbf{x}_2)$ and $\varphi_f \equiv \varphi_f(\mathbf{s}_1, \mathbf{s}_2)$ and they correspond to the *exact* electronic binding energies E_i and E_f , respectively. Here the term “exact” refers to the most accurate variational calculations such as those of Pekeris [39], but if these are unavailable then the experimentally determined values of $E_{i,f}$ should be used. Quantity E is the total energy of the four-body system, whereas \mathbf{k}_i and \mathbf{k}_f are the initial and final wave vectors,

$$E = \frac{k_i^2}{2\mu_i} + E_i = \frac{k_f^2}{2\mu_f} + E_f. \quad (2.4a)$$

Further, H_i and H_f are the channel Hamiltonians,

$$H_{i,f} = K_{i,f} + H_{T,P}, \quad K_{i,f} = -\frac{1}{2\mu_{i,f}} \nabla_{\mathbf{r}_{i,f}}^2, \quad (2.4b)$$

$$H_T = K_T + V_T, \quad H_P = K_P + V_P, \quad (2.4c)$$

$$K_T = -\frac{1}{2b_1} \nabla_{x_1}^2 - \frac{1}{2b_2} \nabla_{x_2}^2, \quad V_T = -\frac{Z_T}{x_1} - \frac{Z_T}{x_2} + \frac{1}{x_{12}}, \quad (2.4d)$$

$$K_P = -\frac{1}{2a_1} \nabla_{s_1}^2 - \frac{1}{2a_2} \nabla_{s_2}^2, \quad V_P = -\frac{Z_P}{s_1} - \frac{Z_P}{s_2} + \frac{1}{s_{12}}, \quad (2.4e)$$

where $\mu_i = [m_P(m_T + 2)]/m$, $\mu_f = [m_T(m_P + 2)]/m$, $a_1 = m_P/(m_P + 1)$, $m = m_P + m_T + 2$, $a_2 = (m_P + 1)/(m_P + 2)$, $b_1 = m_T/(m_T + 1)$, $b_2 = (m_T + 1)/(m_T + 2)$, and m_P (m_T) is the mass of the projectile (target) nucleus.

Distorting potentials $W_{i,f}$ from (2.3c) are conveniently written in the additive form $W_{i,f} = U_{i,f} + W_{i,f}^d$, which is particularly advantageous for construction of the Möller wave operator from (2.3b), by *independent* choices of the constituent parts $U_{i,f}$ and $W_{i,f}^d$. Operators $U_{i,f} \equiv U_{i,f}(\mathbf{r}_{i,f})$ are short-range potentials, which are assumed, without loss of generality, to be dependent only on the coordinates $\mathbf{r}_{i,f}$. On the other hand, in addition to the eventual appearance of short-range interactions in $W_{i,f}^d$ these operators must contain the Coulomb distorting potentials $Z_P(Z_T - 2)/r_i$ and $Z_T(Z_P - 2)/r_f$ between the two aggregates $P - (T, 2e)$ and $T - (P, 2e)$ in the entrance and exit channels of the process (2.1). If the perturbations $V_{i,f}$ were some short-range interactions, as in nuclear physics, we would then put $W_{i,f}^d = 0$ from the onset. We shall presently make the simplest choice of the short-range distorting potentials, i.e., $U_{i,f} = 0$, which implies $\Omega_{i,f}^\pm = 1$, so that

$$2T_{if} = \langle \Phi_f^- | (V_i - W_i^d) + (V_f - W_f^{d\dagger}) | \Phi_i^+ \rangle. \quad (2.5a)$$

Distorting potentials $W_{i,f}^d$ must be chosen from Eq. (2.3a) by requiring that the asymptotic states $\Phi_{i,f}^\pm$ exhibit the prescribed correct boundary conditions. In other words, we shall determine $W_{i,f}^d$ by looking for the solutions of Eq. (2.3a) in the following proper forms;

$$\begin{aligned} \Phi_{i,f}^\pm &= \varphi_{i,f} \exp[\pm i \mathbf{k}_{i,f} \cdot \mathbf{r}_{i,f} \pm i \xi_{i,f} \ln(k_{i,f} r_{i,f} - \mathbf{k}_{i,f} \cdot \mathbf{r}_{i,f})] \\ &\equiv \varphi_{i,f} g_{i,f}^\pm, \end{aligned} \quad (2.5b)$$

where $\xi_i = Z_P(Z_T - 2)/u_i$, $\xi_f = Z_T(Z_P - 2)/u_f$, and $\mathbf{u}_{i,f} = \mathbf{k}_{i,f}/\mu_{i,f}$. Before we make a particular selection of the potentials $W_{i,f}^d$, we shall resort to the well-known eikonal approximation (small scattering angles and $\mu_{i,f} \gg 1$), which is appropriate for heavy particle collisions, such as reaction (2.1), for which the total cross sections are predominantly determined by a narrow cone near the forward direction. The error invoked by use of this additional approximation is of the order of $\max\{1/\mu_i, 1/\mu_f\}$, which is typically less than or equal to $\sim 10^{-4}$. We are then justified in employing the following

useful linearization of the kinetic-energy operators $K_{i,f}$, i.e.,

$$K_{i,f} \approx \frac{k_{i,f}^2}{2\mu_{i,f}} - \mathbf{u}_{i,f} \cdot (\mathbf{k}_{i,f} \pm i \nabla_{\mathbf{r}_{i,f}}), \quad \mu_{i,f} \gg 1. \quad (2.6a)$$

By means of this expression, it immediately follows that in the limit $\mu_{i,f} \gg 1$ the wave functions $\Phi_{i,f}^\pm$ satisfy the equations

$$\left[\frac{k_{i,f}^2}{2\mu_{i,f}} - K_{i,f} - V_{i,f} - V_{i,f}^a \right] \Phi_{i,f}^\pm \approx [\mathbf{u}_{i,f} \cdot (\mathbf{k}_{i,f} \pm i \nabla_{\mathbf{r}_{i,f}}) - V_{i,f}^a] \Phi_{i,f}^\pm = 0, \quad (2.6b)$$

where $V_{i,f}^a$ are the asymptotic forms of $V_{i,f}$ as $r_{i,f} \rightarrow \infty$,

$$V_i^a = \frac{Z_P(Z_T - 2)}{r_i}, \quad V_f^a = \frac{Z_T(Z_P - 2)}{r_f}. \quad (2.6c)$$

Utilizing energy conservation (2.4a) and applying the operator $E - H_{i,f} - W_{i,f}^d$ from Eq. (2.3a) to the required explicit expression (2.5b) of the wave functions $\Phi_{i,f}^\pm$, we find with the help of Eq. (2.6b),

$$0 = (E - H_{i,f} - W_{i,f}^d) \Phi_{i,f}^\pm = (V_{i,f}^a - W_{i,f}^d) \Phi_{i,f}^\pm + g_{i,f}^\pm (E_{i,f} - H_{T,P}) \varphi_{i,f}. \quad (2.6d)$$

If the bound-state wave functions for two-electron systems were known exactly, the terms $g_{i,f}^\pm (E_{i,f} - H_{T,P}) \varphi_{i,f}$ on the right-hand side of Eq. (2.6b) would vanish identically. Since such wave functions are unavailable, the contributions $g_{i,f}^\pm (E_{i,f} - H_{T,P}) \varphi_{i,f}$ to the solutions $\Phi_{i,f}^\pm$ are generally nonzero and, as such, should be kept in the analysis. The distorted-wave formalism provides a convenient framework to deal with this term through the appropriate selection of the potentials $W_{i,f}^d$. A choice of these distorting potentials implied by (2.6b) is given by

$$W_{i,f}^d = V_{i,f}^a + (E_{i,f} - H_{T,P}) \varphi_{i,f} \circ \frac{1}{\varphi_{i,f}} \equiv V_{i,f}^a + W_{i,f}^{\text{op}}. \quad (2.7a)$$

Here, it is understood that the symbol (\circ) requires that any function $\Theta_{i,f}^\pm$ from the domain of the definition of operators $W_{i,f}^{\text{op}}$ must be given in the form $\Theta_{i,f}^\pm = \varphi_{i,f} \theta_{i,f}^\pm(\mathbf{r}_{i,f})$, so that $W_{i,f}^d \Theta_{i,f}^\pm = V_{i,f}^a \Theta_{i,f}^\pm - \theta_{i,f}^\pm(\mathbf{r}_{i,f})(H_{T,P} - E_{i,f}) \varphi_{i,f}$. In particular, we have

$$\begin{aligned} W_{i,f}^d \Phi_{i,f}^\pm &= V_{i,f}^a \Phi_{i,f}^\pm - g_{i,f}^\pm(\mathbf{r}_{i,f})(H_{T,P} - E_{i,f}) \varphi_{i,f} \\ &\equiv V_{i,f}^a \Phi_{i,f}^\pm - g_{i,f}^\pm(\mathbf{r}_{i,f}) \varphi'_{i,f}. \end{aligned} \quad (2.7b)$$

The overall factorizing functions $\varphi_{i,f}$ in $\Theta_{i,f}^\pm$ preserve the regular behavior of the operator $W_{i,f}^{\text{op}}$ at the eventual nodes of the bound-state wave functions $\varphi_{i,f}$. For *nonexact* state vectors $\varphi_{i,f}$, the functions $\varphi'_{i,f} \equiv (H_{T,P} - E_{i,f}) \varphi_{i,f}$ are not equal to zero. Instead of the exact Schrödinger equations, such quantities $\varphi_{i,f}$ satisfy a *model* eigenvalue problem of the sort,

$$(E'_{i,f} - H'_{T,P}) \varphi_{i,f} \equiv (E'_{i,f} - K_{T,P} - V'_{T,P}) \varphi_{i,f} = 0. \quad (2.8a)$$

Here $V'_{T,P}$ represent, respectively, the selected model potentials of the isolated bound systems $(Z_T; e_1, e_2)_i$ and $(Z_P; e_1, e_2)_f$, whereas $E'_{i,f}$ are the corresponding *approximate* electronic binding energies. Employing the identity $(E_{i,f} - H_{T,P}) \varphi_{i,f} \equiv [(E_{i,f} - H_{T,P}) - (E'_{i,f} - H'_{T,P})] \varphi_{i,f} + (E'_{i,f} - H'_{T,P}) \varphi_{i,f} \equiv [(E_{i,f} - H_{T,P}) - (E'_{i,f} - H'_{T,P})] \varphi_{i,f}$, we shall have from (2.8a),

$$W_{i,f}^d = V_{i,f}^a + (V''_{T,P} - V_{T,P}) \varphi_{i,f} \circ \frac{1}{\varphi_{i,f}}, \quad (2.8b)$$

where $V''_{T,P}$ are the model interactions $V'_{T,P}$ shifted through the constant potentials $V_{T,P}^{(0)}$ appearing as the energy discrepancy terms $\Delta_{i,f}$,

$$V''_{T,P} = V'_{T,P} + \Delta_{i,f}, \quad \Delta_{i,f} = E_{i,f} - E'_{i,f}. \quad (2.8c)$$

Interestingly, the shifting constant potentials $V_{P,T}^{(0)} \equiv \Delta_{i,f}$ are such that they render the expectation values of the exact Hamiltonians $H_{T,P} = K_{T,P} + V_{T,P}$ and the operators $K_{T,P} + V''_{T,P}$ identical to each other. Namely, by defining the exact eigenenergies $E_{i,f}$ as the average values of the true Hamiltonians $H_{T,P}$ over the best known variational bound-state wave functions $\varphi_{i,f}^V$,

$$\langle \varphi_{i,f}^V | H_{T,P} | \varphi_{i,f}^V \rangle = E_{i,f}, \quad (2.9a)$$

we shall have for the normalized approximate orbitals $\varphi_{i,f}$,

$$\begin{aligned} \langle \varphi_{i,f} | K_{T,P} + V''_{T,P} | \varphi_{i,f} \rangle &= \langle \varphi_{i,f} | K_{T,P} + V'_{T,P} + \Delta_{i,f} | \varphi_{i,f} \rangle \\ &= \langle \varphi_{i,f} | E'_{i,f} + \Delta_{i,f} | \varphi_{i,f} \rangle \\ &= \langle \varphi_{i,f} | E'_{i,f} + E_{i,f} - E'_{i,f} | \varphi_{i,f} \rangle \\ &= E_{i,f}, \end{aligned} \quad (2.9b)$$

where the model eigenvalue equations from (2.8a) are utilized.

Next, by consistently proceeding with the eikonal approximation, i.e., by ignoring every term smaller than or equal to $1/\mu_{i,f}$ and dropping out the unimportant phase factors, the expressions for the distorted waves $\Phi_{i,f}^\pm$ can further be simplified as follows:

$$\begin{aligned} \Phi_{i,f}^\pm &= \varphi_{i,f} \exp[\pm i \mathbf{k}_{i,f} \cdot \mathbf{r}_{i,f} \pm i v_{i,f} \ln(vR \mp \mathbf{v} \cdot \mathbf{R})] \\ &\equiv \varphi_{i,f} \mathcal{F}_{i,f}^\pm, \end{aligned} \quad (2.10a)$$

where

$$v_i = \frac{Z_P(Z_T - 2)}{v}, \quad v_f = \frac{Z_T(Z_P - 2)}{v}, \quad (2.10b)$$

with \mathbf{v} being the vector of the incident velocity. In the same mass approximations $\mu_{i,f} \gg 1$, we shall have $V_i^a = Z_P(Z_T - 2)/R$ and $V_f^a = Z_T(Z_P - 2)/R$. The transition amplitude (2.2a) then becomes

$$2T_{if} = \langle \varphi_f | \mathcal{F}(V_i^d + V_f^d) | \varphi_i \rangle - (\mathcal{A}_{if}^- + \mathcal{A}_{if}^+), \quad (2.11a)$$

where

$$\mathcal{A}_{if}^- = \langle \varphi_f \mathcal{F}^* | \varphi_i' \rangle, \quad \mathcal{A}_{if}^+ = \langle \varphi_f' | \mathcal{F} \varphi_i \rangle, \quad (2.11b)$$

$$\varphi_{i,f}' = (H_{T,P} - E_{i,f}) \varphi_{i,f} = (V_{T,P} - V_{T,P}'') \varphi_{i,f}, \quad (2.11c)$$

$$\begin{aligned} \mathcal{F} &\equiv \mathcal{F}_f^* \mathcal{F}_i^+ = \exp\{i[Z_P(Z_T - 2)/v] \ln(vR - \mathbf{v} \cdot \mathbf{R})\} \exp\{i[Z_T(Z_P - 2)/v] \ln(vR + \mathbf{v} \cdot \mathbf{R})\} \exp(i\mathbf{k}_i \cdot \mathbf{r}_i + i\mathbf{k}_f \cdot \mathbf{r}_f) \\ &= (\rho v)^{2iZ_P Z_T / v} \exp\{-2i[Z_P/v] \ln(vR - \mathbf{v} \cdot \mathbf{R})\} \exp\{-2i[Z_T/v] \ln(vR + \mathbf{v} \cdot \mathbf{R})\} \exp(i\mathbf{k}_i \cdot \mathbf{r}_i + i\mathbf{k}_f \cdot \mathbf{r}_f) \\ &= (\rho v)^{2iZ_T(Z_P - 2)/v} \exp\{2i[(Z_T - Z_P)/v] \ln(vR - \mathbf{v} \cdot \mathbf{R})\} \exp(i\mathbf{k}_i \cdot \mathbf{r}_i + i\mathbf{k}_f \cdot \mathbf{r}_f) \\ &= (\rho v)^{2iZ_P(Z_T - 2)/v} \exp\{2i[(Z_P - Z_T)/v] \ln(vR + \mathbf{v} \cdot \mathbf{R})\} \exp(i\mathbf{k}_i \cdot \mathbf{r}_i + i\mathbf{k}_f \cdot \mathbf{r}_f), \end{aligned} \quad (2.11d)$$

$$V_i^d = \frac{2Z_P}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_1}, \quad V_f^d = \frac{2Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_1}, \quad (2.11e)$$

and $\rho = \mathbf{R} - (\hat{\mathbf{v}} \cdot \mathbf{R})\mathbf{v}$, $\rho \cdot \mathbf{v} = 0$, and $\hat{\mathbf{v}} = \mathbf{v}/v$. Since the interelectron potential $1/r_{12}$ is contained in both Hamiltonians H_P and H_T , it follows that the transition amplitude (2.8a) approximately includes, to a certain extent, the correlation effects in $(Z_T; e_1, e_2)_i$ and $(Z_P; e_1, e_2)_f$. This is so even if the bound-state wave functions $\varphi_{i,f}$ are chosen to be completely uncorrelated, such as the well-known one-parameter Hylleraas [48] orbital $(\gamma^3/\pi)e^{-\gamma(r_1+r_2)}$. We emphasize, however, that *consistency* is the sole cause of the appearance of the corrections $\varphi_{i,f}'$, which must also be taken into account for highly correlated bound-state functions $\varphi_{i,f}$. Namely, by using any of the existing approximate orbitals $\varphi_{i,f}$ in place of the exact ones, we immediately have that $\varphi_{i,f}' \equiv (H_{T,P} - E_{i,f})\varphi_{i,f} \neq 0$, so that the correct boundary conditions are consistently formulated for a *model* problem only if the nonzero terms $\varphi_{i,f}'$ are taken into account. In fact, the inequality $\varphi_{i,f}' \neq 0$ signifies that we are treating a model problem instead of the one from which we have started and where $\varphi_{i,f}' \equiv 0$ by definition.

Calculation of the term $\mathbf{k}_i \cdot \mathbf{r}_i + \mathbf{k}_f \cdot \mathbf{r}_f$ is very simple in the eikonal approximation, since

$$\mathbf{k}_i \cdot \mathbf{r}_i + \mathbf{k}_f \cdot \mathbf{r}_f = \mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2) + \mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2), \quad (2.12a)$$

with

$$\begin{aligned} 2\mathbf{q}_P &= +\boldsymbol{\eta} - q^+ \hat{\mathbf{v}}, \quad 2\mathbf{q}_T = -\boldsymbol{\eta} - q^- \hat{\mathbf{v}}, \\ q^\pm &= v \pm \frac{E_f - E_i}{v}, \end{aligned} \quad (2.12b)$$

where vector $\boldsymbol{\eta} = (\eta \cos \phi, \eta \sin \phi, 0)$ stands for the usual transverse momentum transfer. Notice that the momentum transfers $\mathbf{q}_{P,T}$ from (2.12b) contain the “exact,” i.e., the most accurate variational values or the best experimental findings for the binding energies $E_{i,f}$ and *not* the

observables $E_{i,f}'$ from a given model. Thus the total cross section for the two-electron transfer reaction (2.1) is introduced by

$$Q_{if}(a_0^2) = \int d\boldsymbol{\eta} \left| \frac{R_{if}(\boldsymbol{\eta})}{2\pi v} \right|^2, \quad (2.13)$$

where

$$\begin{aligned} 2R_{if}(\boldsymbol{\eta}) &= \langle \varphi_f | \mathcal{G}(V_i^d + V_f^d) | \varphi_i \rangle \\ &\quad + [\mathcal{B}_{if}^-(\boldsymbol{\eta}) + \mathcal{B}_{if}^+(\boldsymbol{\eta})], \end{aligned} \quad (2.14a)$$

$$\mathcal{B}_{if}^+(\boldsymbol{\eta}) = \langle \varphi_f \mathcal{G}^* | \varphi_i' \rangle, \quad \mathcal{B}_{if}^-(\boldsymbol{\eta}) = \langle \varphi_f' | \mathcal{G} \varphi_i \rangle, \quad (2.14b)$$

$$\begin{aligned} \mathcal{G} &= \exp[i\mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2) + i\mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2) \\ &\quad - i\xi \ln(vR + \mathbf{v} \cdot \mathbf{R})], \\ \xi &= \frac{2(Z_T - Z_P)}{v}. \end{aligned} \quad (2.14c)$$

We see that the internuclear potential $Z_P Z_T / R$ does not contribute to the total cross sections, whenever the eikonal mass limit holds true, in precise agreement with the well-known conclusion reached previously for single charge exchange [47].

III. CALCULATION OF THE MATRIX ELEMENTS WITH THE HYLLEAAS WAVE FUNCTIONS

We shall henceforth concentrate on the symmetric version of reaction (2.1) obtained for $Z_P = Z_T$ in which case $\xi = 0$. Nevertheless, since cross section Q_{if} depends only parametrically on ξ , it is convenient to put $\xi \equiv 0$ and continue considering the two labels Z_P and Z_T as if they were generally unequal. In such a case, we need to calculate the following matrix element for the determination of the cross section (2.10):

$$\begin{aligned} 2R_{if}(Z_P, Z_T; \boldsymbol{\eta}) &= \int \int \int d\mathbf{R} d\mathbf{x}_1 d\mathbf{x}_2 \exp[i\mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2) + i\mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2)] \\ &\quad \times \left\{ \varphi_f^*(\mathbf{s}_1, \mathbf{s}_2) \left[\left[Z_P \left(\frac{2}{R} - \frac{1}{s_1} - \frac{1}{s_2} \right) + (H_T - E_i) \right] \varphi_i(\mathbf{x}_1, \mathbf{x}_2) \right] \right. \\ &\quad \left. + \varphi_i(\mathbf{x}_1, \mathbf{x}_2) \left[\left[Z_T \left(\frac{2}{R} - \frac{1}{x_1} - \frac{1}{x_2} \right) + (H_P - E_f) \right] \varphi_f(\mathbf{s}_1, \mathbf{s}_2) \right]^* \right\}, \end{aligned} \quad (3.1a)$$

or equivalently

$$2R_{if}(Z_P, Z_T; \eta) = \int \int \int d\mathbf{R} d\mathbf{x}_1 d\mathbf{x}_2 \exp[i\mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2) + i\mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2)] \\ \times \left\{ \varphi_f^*(\mathbf{s}_1, \mathbf{s}_2) \left[Z_P \left[\frac{2}{R} - \frac{1}{s_1} - \frac{1}{s_2} \right] + (V_T - V_T'') \right] \varphi_i(\mathbf{x}_1, \mathbf{x}_2) \right\} \\ + \varphi_i(\mathbf{x}_1, \mathbf{x}_2) \left\{ \left[Z_T \left[\frac{2}{R} - \frac{1}{x_1} - \frac{1}{x_2} \right] + (V_P - V_P'') \right] \varphi_f(\mathbf{s}_1, \mathbf{s}_2) \right\}^* \right\} . \quad (3.1b)$$

The CB1 approximation for homonuclear double charge exchange is obtained by specification $Z_P = Z_T \equiv Z$ in the final result,

$$R_{if}(\eta) \equiv R_{if}^{\text{CB1}}(\eta) = R_{if}(Z, Z; \eta) . \quad (3.1c)$$

In order to perform the explicit calculations of the matrix elements in (3.1a), and (3.1b), we shall presently choose the bound-state wave functions $\varphi_{i,f}$ in the form of the one-parameter Hylleraas orbitals [48],

$$\varphi_i(\mathbf{x}_1, \mathbf{x}_2) = \phi_\alpha(\mathbf{x}_1) \phi_\alpha(\mathbf{x}_2) , \quad (3.2a)$$

$$\varphi_f(\mathbf{s}_1, \mathbf{s}_2) = \phi_\beta(\mathbf{s}_1) \phi_\beta(\mathbf{s}_2) ,$$

with the corresponding approximate binding energies $E_i' = -\alpha^2$, $E_f' = -\beta^2$, and

$$\phi_\gamma(\mathbf{r}) = \left[\frac{\gamma^3}{\pi} \right]^{1/2} e^{-\gamma r} \quad (\gamma = \alpha, \beta) , \quad (3.2b)$$

$$\alpha = Z_T - a, \quad \beta = Z_P - b, \quad a = b = \frac{5}{16} = 0.3125 . \quad (3.2c)$$

The two-electron Hylleraas orbitals $\varphi_{i,f}$ from (3.2a) satisfy the eigenvalue problem (2.8a), where the potentials $V'_{T,P}$ are given by

$$V'_T = -\frac{\alpha}{x_1} - \frac{\alpha}{x_2}, \quad V'_P = -\frac{\beta}{s_1} - \frac{\beta}{s_2} . \quad (3.2d)$$

This implies

$$(H_T - E_i) \varphi_i(\mathbf{x}_1, \mathbf{x}_2) \\ = (V_T - V_T'') \varphi_i(\mathbf{x}_1, \mathbf{x}_2) \\ = \left[\frac{1}{x_{12}} - \frac{a}{x_1} - \frac{a}{x_2} + \Delta_i \right] \varphi_i(\mathbf{x}_1, \mathbf{x}_2) , \quad (3.3a)$$

$$(H_P - E_f) \varphi_f(\mathbf{s}_1, \mathbf{s}_2) \\ = (V_P - V_P'') \varphi_f(\mathbf{s}_1, \mathbf{s}_2) \\ = \left[\frac{1}{s_{12}} - \frac{b}{s_1} - \frac{b}{s_2} + \Delta_f \right] \varphi_f(\mathbf{s}_1, \mathbf{s}_2) , \quad (3.3b)$$

where the shifting constant potentials $\Delta_{i,f}$ are defined in Eq. (2.8c). This derivation allows us to write Eq. (3.1a) in the following concise form:

$$R_{if}(\eta) = (Z_P + Z_T)J + I_{12} - (a + Z_T) \frac{I_1 + I_2}{2} \\ - (b + Z_P) \frac{K_1 + K_2}{2} + \frac{\Delta_i + \Delta_f}{2} L , \quad (3.4)$$

where

$$I_k = \int \int \int d\mathbf{R} d\mathbf{x}_1 d\mathbf{x}_2 \varphi_f^*(\mathbf{s}_1, \mathbf{s}_2) \\ \times \frac{\exp[i\mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2) + i\mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2)]}{x_k} \\ \times \varphi_i(\mathbf{x}_1, \mathbf{x}_2) , \quad (3.5a)$$

$$I_{12} = \int \int \int d\mathbf{R} d\mathbf{x}_1 d\mathbf{x}_2 \varphi_f^*(\mathbf{s}_1, \mathbf{s}_2) \\ \times \frac{\exp[i\mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2) + i\mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2)]}{x_{12}} \\ \times \varphi_i(\mathbf{x}_1, \mathbf{x}_2) , \quad (3.5b)$$

$$K_k = \int \int \int d\mathbf{R} d\mathbf{x}_1 d\mathbf{x}_2 \varphi_f^*(\mathbf{s}_1, \mathbf{s}_2) \\ \times \frac{\exp[i\mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2) + i\mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2)]}{s_k} \\ \times \varphi_i(\mathbf{x}_1, \mathbf{x}_2) , \quad (3.5c)$$

$$J = \int \int \int d\mathbf{R} d\mathbf{x}_1 d\mathbf{x}_2 \varphi_f^*(\mathbf{s}_1, \mathbf{s}_2) \\ \times \frac{\exp[i\mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2) + i\mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2)]}{R} \\ \times \varphi_i(\mathbf{x}_1, \mathbf{x}_2) , \quad (3.5d)$$

$$L = \int \int \int d\mathbf{R} d\mathbf{x}_1 d\mathbf{x}_2 \varphi_f^*(\mathbf{s}_1, \mathbf{s}_2) \\ \times \exp[i\mathbf{q}_T \cdot (\mathbf{x}_1 + \mathbf{x}_2) + i\mathbf{q}_P \cdot (\mathbf{s}_1 + \mathbf{s}_2)] \\ \times \varphi_i(\mathbf{x}_1, \mathbf{x}_2) . \quad (3.5e)$$

By making the transformation $\mathbf{x}_1 \leftrightarrow \mathbf{x}_2$ and $\mathbf{s}_1 \leftrightarrow \mathbf{s}_2$ in the integrals (3.5a), (3.5c), and (3.5e) and using the symmetry property $\varphi_i(\mathbf{x}_1, \mathbf{x}_2) = \varphi_i(\mathbf{x}_2, \mathbf{x}_1)$ and $\varphi_f(\mathbf{s}_1, \mathbf{s}_2) = \varphi_f(\mathbf{s}_2, \mathbf{s}_1)$ of the Hylleraas orbitals from (3.2a), it is at once seen that

$$I_1 = I_2 \equiv I, \quad J_1 = J_2 \equiv J , \quad (3.6)$$

which yields

$$R_{if}(\eta) = (Z_P + Z_T)J + I_{12} - (a + Z_T)I \\ - (b + Z_P)K + \frac{\Delta_i + \Delta_f}{2} L . \quad (3.7)$$

In order to carry out the integrations in (3.5a)–(3.5d), we now employ the usual asymmetric Fourier transform $\tilde{f}(\mathbf{p})$ and its inverse $f(\mathbf{r})$ by

$$\begin{aligned}\tilde{f}(\mathbf{p}) &= \int d\mathbf{r} e^{i\mathbf{p}\cdot\mathbf{r}} f(\mathbf{r}), \\ f(\mathbf{r}) &= (2\pi)^{-3} \int d\mathbf{p} e^{-i\mathbf{p}\cdot\mathbf{r}} \tilde{f}(\mathbf{p}).\end{aligned}\quad (3.8)$$

Furthermore, it will prove convenient to introduce the following auxiliary functions:

$$\begin{aligned}\chi_\alpha^{(l)}(\mathbf{x}_k) &= \frac{e^{i\mathbf{q}_T \cdot \mathbf{x}_k}}{x_k^l} \phi_\alpha(\mathbf{x}_k), \\ \psi_\beta^{(l)}(\mathbf{s}_k) &= \frac{e^{i\mathbf{q}_P \cdot \mathbf{s}_k}}{s_k^l} \phi_\beta^*(\mathbf{s}_k) \quad (l=0,1).\end{aligned}\quad (3.9)$$

By first taking the inverse Fourier transform of the functions $\psi_\beta^{(l)}(\mathbf{s}_2)$ in the integrands of Eqs. (3.5a)–(3.5d), we arrive at the result

$$I = (2\pi)^{-3} \int d\mathbf{p} \tilde{\psi}_\beta^{(0)}(\mathbf{p}) \tilde{\psi}_\beta^{(0)}(-\mathbf{p}) \tilde{\chi}_\alpha^{(1)}(\mathbf{p}) \tilde{\chi}_\alpha^{(0)}(-\mathbf{p}), \quad (3.10a)$$

$$K = (2\pi)^{-3} \int d\mathbf{p} \tilde{\psi}_\beta^{(0)}(\mathbf{p}) \tilde{\psi}_\beta^{(1)}(-\mathbf{p}) \tilde{\chi}_\alpha^{(0)}(\mathbf{p}) \tilde{\chi}_\alpha^{(0)}(-\mathbf{p}), \quad (3.10b)$$

$$L = (2\pi)^{-3} \int d\mathbf{p} \tilde{\psi}_\beta^{(0)}(\mathbf{p}) \tilde{\psi}_\beta^{(0)}(-\mathbf{p}) \tilde{\chi}_\alpha^{(0)}(\mathbf{p}) \tilde{\chi}_\alpha^{(0)}(-\mathbf{p}). \quad (3.10c)$$

As to the integrals (3.5b) and (3.5d), in addition to the variable \mathbf{s}_2 , we further need to introduce the Fourier transforms of the terms $1/R$ and $1/x_{12}$,

$$\begin{aligned}\frac{1}{R} &= \frac{1}{2\pi^2} \int \frac{d\mathbf{q}}{q^2} \exp[-i\mathbf{q} \cdot (\mathbf{x}_1 - \mathbf{s}_1)], \\ \frac{1}{x_{12}} &= \frac{1}{2\pi^2} \int \frac{d\mathbf{q}}{q^2} \exp[-i\mathbf{q} \cdot (\mathbf{x}_1 - \mathbf{x}_2)],\end{aligned}\quad (3.11)$$

which give

$$J = (2\pi)^{-3} \int d\mathbf{p} \tilde{\psi}_\beta^{(0)}(\mathbf{p}) \tilde{\chi}_\alpha^{(0)}(-\mathbf{p}) \mathcal{N}(\mathbf{p}), \quad (3.12a)$$

$$I_{12} = (2\pi)^{-3} \int d\mathbf{p} \tilde{\psi}_\beta^{(0)}(\mathbf{p}) \tilde{\psi}_\alpha^{(0)}(-\mathbf{p}) \mathcal{M}(\mathbf{p}), \quad (3.12b)$$

where

$$\mathcal{N}(\mathbf{p}) = \frac{1}{2\pi^2} \int \frac{d\mathbf{q}}{q^2} \tilde{\psi}_\beta^{(0)}(\mathbf{q} - \mathbf{p}) \tilde{\chi}_\alpha^{(0)}(\mathbf{p} - \mathbf{q}), \quad (3.12c)$$

$$\mathcal{M}(\mathbf{p}) = \frac{1}{2\pi^2} \int \frac{d\mathbf{q}}{q^2} \tilde{\chi}_\alpha^{(0)}(\mathbf{p} - \mathbf{q}) \tilde{\chi}_\alpha^{(0)}(\mathbf{q} - \mathbf{p}). \quad (3.12d)$$

The Fourier transforms of the auxiliary functions $\chi_\alpha^{(l)}$ and $\psi_\beta^{(l)}$ from Eq. (3.9) are readily obtained as

$$\tilde{\chi}_\alpha^{(1)}(\mathbf{p}) = 4\pi N_\alpha |\mathbf{q}_T + \mathbf{p}|^2 + \alpha^2, \quad (3.13a)$$

$$\tilde{\chi}_\alpha^{(0)}(\mathbf{p}) = \frac{8\pi\alpha N_\alpha}{(|\mathbf{q}_T + \mathbf{p}|^2 + \alpha^2)^2},$$

$$\tilde{\psi}_\beta^{(1)}(\mathbf{p}) = \frac{4\pi N_\beta^*}{|\mathbf{q}_P + \mathbf{p}|^2 + \beta^2}, \quad (3.13b)$$

$$\tilde{\psi}_\beta^{(0)}(\mathbf{p}) = \frac{8\pi\beta N_\beta^*}{(|\mathbf{q}_P + \mathbf{p}|^2 + \beta^2)^2}.$$

Hence we shall have

$$I = \frac{1}{2} \beta^2 N_{\alpha\beta} \int d\mathbf{p} \mathcal{H}_{Te}^-(\mathbf{p}), \quad (3.14a)$$

$$\begin{aligned}I_{12} &= \frac{1}{2} \alpha \beta^2 N_{\alpha\beta} \int d\mathbf{p} \mathcal{H}_{ee}^-(\mathbf{p}), \\ J &= \frac{1}{2} \alpha \beta^2 N_{\alpha\beta} \int d\mathbf{p} \mathcal{H}_{PT}^-(\mathbf{p}),\end{aligned}\quad (3.14b)$$

$$\begin{aligned}K &= \frac{1}{2} \alpha \beta N_{\alpha\beta} \int d\mathbf{p} \mathcal{H}_{Pe}^-(\mathbf{p}), \\ L &= \alpha \beta^2 N_{\alpha\beta} \int d\mathbf{p} \mathcal{L}(\mathbf{p}),\end{aligned}\quad (3.14c)$$

where

$$N_{\alpha\beta} = \frac{512}{\pi} \alpha^4 \beta^3, \quad (3.15a)$$

$$\mathcal{H}_{Te}^-(\mathbf{p}) = F'(\mathbf{p}) G'(\mathbf{p}), \quad \mathcal{H}_{ee}^-(\mathbf{p}) = F'(\mathbf{p}) B''(\mathbf{p}), \quad (3.15b)$$

$$\mathcal{H}_{Pe}^-(\mathbf{p}) = F'''(\mathbf{p}) G''(\mathbf{p}), \quad \mathcal{H}_{PT}^-(\mathbf{p}) = A'(\mathbf{p}) B'(\mathbf{p}), \quad (3.15c)$$

$$F'(\mathbf{p}) = \frac{1}{q_{P\beta}^2}, \quad G'(\mathbf{p}) = \frac{1}{q_{T\alpha} q_{T\alpha}^2}, \quad (3.16a)$$

$$F'''(\mathbf{p}) = \frac{1}{q_{P\beta} q_{P\beta}^+}, \quad G''(\mathbf{p}) = \frac{1}{q_{T\alpha}^2}, \quad (3.16b)$$

$$A'(\mathbf{p}) = \frac{1}{(q_{T\alpha}^+ q_{P\beta}^+)^2}, \quad \mathcal{L}(\mathbf{p}) = F'(\mathbf{p}) G''(\mathbf{p}), \quad (3.16c)$$

$$\begin{aligned}B'(\mathbf{p}) &= \mathcal{D}_{22}(\mathbf{q}'_1, \alpha; -\mathbf{q}'_2, \beta), \\ B''(\mathbf{p}) &= \mathcal{D}_{22}(\mathbf{q}''_1, \alpha; -\mathbf{q}''_2, \alpha),\end{aligned}\quad (3.17a)$$

$$\begin{aligned}\mathcal{D}_{n_1 n_2}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) \\ = \frac{1}{\pi^2} \int d\mathbf{q} \frac{1}{q^2 (|\mathbf{q} - \mathbf{q}_1|^2 + \mu_1^2)^{n_1} (|\mathbf{q} - \mathbf{q}_2|^2 + \mu_2^2)^{n_2}},\end{aligned}\quad (3.17b)$$

$$q_{T\alpha} = q_{T\alpha}^+ q_{T\alpha}^-, \quad q_{T\alpha}^\pm = |\mathbf{q}_T \pm \mathbf{p}|^2 + \alpha^2, \quad (3.18a)$$

$$q_{P\beta} = q_{P\beta}^+ q_{P\beta}^-, \quad q_{P\beta}^\pm = |\mathbf{q}_P \pm \mathbf{p}|^2 + \beta^2, \quad (3.18b)$$

$$\mathbf{q}'_1 = \mathbf{q}_T + \mathbf{p}, \quad \mathbf{q}'_2 = \mathbf{q}_P - \mathbf{p}, \quad \mathbf{q}''_1 = \mathbf{q}'_1, \quad \mathbf{q}''_2 = \mathbf{q}_T - \mathbf{p}. \quad (3.18c)$$

Quantity $\mathcal{D}_{n_1 n_2}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2)$ defined by Eq. (3.17b) belongs to the class of the Dalitz three-denominator integrals [49]. The basic variant $\mathcal{D}_{11}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2)$ was also considered by Lewis [50] in the most general case of arbitrary (real or complex) parameters μ_1 and μ_2 with the final result,

$$\mathcal{D}_{11}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) = \frac{1}{D^{1/2}} \ln \left[\frac{B + D^{1/2}}{B - D^{1/2}} \right], \quad (3.19)$$

where the values of the function $\ln[(B + D^{1/2})/(B - D^{1/2})]$ are computed from the difference $\ln(B + D^{1/2}) - \ln(B - D^{1/2})$, with each logarithm being taken at its principal branch,

$$B = \mu_1 T_2 + \mu_2 T_1, \quad D = B^2 - C = -T_1 T_2 \tau^2 - \lambda \Delta, \quad (3.20a)$$

$$C = T_1 T_2 T,$$

$$T = \tau^2 + \mu^2, \quad T_i = q_i^2 + \mu_i^2 \quad (i=1,2), \quad (3.20b)$$

$$\tau = \mathbf{q}_1 - \mathbf{q}_2, \quad \mu = \mu_1 + \mu_2, \quad (3.20c)$$

$$\Delta = T_1 - T_2, \quad \lambda = \mu_1^2 T_2 - \mu_2^2 T_1.$$

For a detailed study of a larger class of the three-denominator Dalitz integrals including the general momentum space hydrogenic orbitals, see the work of Belkić [51]. The result for $\mathcal{D}_{22}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2)$ is obtained from $-[1/(2\mu_1)](\partial/\partial\mu_1)\mathcal{D}_{12}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2)$, where

$$\mathcal{D}_{12}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) = -[1/(2\mu_2)](\partial/\partial\mu_2)\mathcal{D}_{11}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2).$$

As an intermediate expression, we also need the values of

$$\mathcal{D}_{21}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) = -[1/(2\mu_1)](\partial/\partial\mu_1)\mathcal{D}_{11}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2).$$

By carrying out these partial differentiations with respect to parameters μ_1 and μ_2 , we arrive at

$$\mathcal{D}_{12}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) = [\xi_1^- \mathcal{D}_{11}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2)/2 - \omega_{12}^+/C]/D,$$

$$\mathcal{D}_{21}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) = [-\xi_2^+ \mathcal{D}_{11}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2)/2 - \omega_{21}^+/C]/D,$$

and finally,

$$\mathcal{D}_{22}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) = \frac{1}{2D} \left[\frac{D'}{2D} \mathcal{D}_{11}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) + \frac{\xi_1^-}{CD} \omega_{21}^- - \frac{2g\omega_{12}^+ - h}{\mu_1 C} \right], \quad (3.21)$$

where

$$D' = 2D(\tau^2 - \kappa^2) - 3\xi_1^- \xi_2^+, \quad (3.22a)$$

$$\kappa^2 = q_1^2 + q_2^2, \quad \xi_i^\pm = \lambda_i \pm \tau^2 T_i, \quad \lambda_i = \lambda + q_i^2 \Delta, \quad (3.22b)$$

$$\omega_{ij}^\pm = \frac{\mu_j(\nu\tau^2 T_i + \lambda_i B) \pm \sigma\tau_i^\pm \pm \tau^2 T_i^2 T_j}{\mu_j}, \quad (3.22c)$$

$$\nu = \mu_1 T_2 - \mu_2 T_1, \quad \sigma = \lambda \Delta, \quad \tau_i^\pm = 2\mu_1 \mu_2 \pm T_i, \quad (3.23a)$$

$$g = \frac{T_2(\mu_1 T + \mu T_1)}{C} - \frac{\mu_1 \xi_2^+}{D}, \quad (3.23b)$$

$$h = \tau^2(2\nu\mu_1 - T_1\tau_2^-) + \lambda_1\tau_2^+ + \frac{2\mu_1(\mu_2\kappa^2 B + \lambda_2\tau_1^+ + 2\tau^2 T_1 T_2) + 2\mu\sigma}{\mu_2}. \quad (3.23c)$$

Further, it can easily be shown that quantity D from (3.20a) takes the equivalent values,

$$D = -Q^2, \quad Q = T_2 \mathbf{q}_1 - T_1 \mathbf{q}_2. \quad (3.24)$$

Using this result, the following convenient expression can be given for the basic Dalitz-Lewis integral (3.19) in the case of the real parameters μ_1 and μ_2 , such as in Eq. (3.17a):

$$\mathcal{D}_{11}(\mathbf{q}_1, \mu_1; \mathbf{q}_2, \mu_2) = \frac{2}{Q} \tan^{-1} \left[\frac{Q}{B} \right] = \frac{1}{Q} \cos^{-1} \left[\frac{2B^2 - C}{C} \right], \quad (3.25)$$

where formulas 1.622/3 and 1.628/2 of Gradshteyn and Ryzhik [52] are employed. This completes the calculation of the matrix elements R_{if} from Eq. (3.1a), so that

$$R_{if}(\boldsymbol{\eta}) = \frac{1}{2} \beta N_{\alpha\beta} \int d\mathbf{p} [(Z_p + Z_T) \alpha \beta \mathcal{H}_{pT}(\mathbf{p}) + \alpha \beta \mathcal{H}_{ee}(\mathbf{p}) - (b + Z_p) \alpha \mathcal{H}_{pe}(\mathbf{p}) - (a + Z_T) \beta \mathcal{H}_{Te}(\mathbf{p}) + \frac{1}{2} (\Delta_i + \Delta_f) \alpha \beta \mathcal{L}(\mathbf{p})]. \quad (3.26)$$

Let us notice that setting $a = b \equiv 0$, $\mathcal{H}_{ee} \equiv 0$, and $\Delta_{i,f} \equiv 0$ in Eq. (3.26) we could obtain a version of the CB1 approximation, which would be a direct generalization to double charge exchange (2.1) of the same kind of theory introduced in the one-electron capture problems [45–47]. The rationale for introduction of the additional terms in (3.26) with $a = b \neq 0$, $\mathcal{H}_{ee} \neq 0$, and $\Delta_{i,f} \neq 0$ is to correct such a CB1 theory for the fact that the functions $\varphi'_{i,f}$ ($\equiv [H_{T,p} - E_{i,f}] \varphi_{i,f}$) are never strictly equal to the zero state vector for any of the existing approximate two-electron orbitals $\varphi_{i,f}$.

IV. THE RESULTS OF THE NUMERICAL COMPUTATIONS

As an illustration of the present theory, we shall perform the numerical computations of the total cross sections (2.13) for two-electron capture from He by α particles,

$$\text{He}^{2+} + \text{He}(1s^2) \rightarrow \text{He}(1s^2) + \text{He}^{2+}. \quad (4.1)$$

In this case, the Hylleraas parameters are

$$\alpha = \beta = 1.6875, \quad E'_{i,f} = -2.847\,656\,3, \quad (4.2a)$$

$$E_{i,f} = -2.903\,724\,4, \quad \Delta_{i,f} = -0.056\,068\,1. \quad (4.2b)$$

It will prove convenient to carry out the integrations over the variables \mathbf{p} and $\boldsymbol{\eta}$ in the spherical $\mathbf{p} = (p, \theta, \phi)$ and polar $\boldsymbol{\eta} = (\eta \cos \phi_\eta, \eta \sin \phi_\eta, 0)$ coordinates, respectively. In such a case, we can choose the X and Z axis of the \mathbf{p} integral to be along the vectors $\boldsymbol{\eta}$ and \mathbf{v} . This implies that the integration over ϕ_η is done analytically with the result equal to 2π . Thus the final working formula for the observable Q_{if} will contain a *quadruple* integration over variables $\eta \in [0, \infty]$, $p \in [0, \infty]$, $\theta \in [0, \pi]$, and $\phi \in [0, 2\pi]$. For the innermost ϕ integral we directly employ the extremely efficient n -order Gauss-Mehler quadrature routine. On the other hand, the integration over θ is best suited for the application of the universal Gauss-Legendre method, after passing from the variable θ to u by the substitution $u = \cos \theta$, where $u \in [-1, +1]$. As to the remaining two semidefinite quadratures over η and p , it would naturally be most advantageous to introduce certain convenient changes of variables, so as to obtain

the integrals with finite lower *and* upper limits. In the case of the outermost η integral, we already have a guide for such a variable change, which stems from the fact that the total cross sections are dominated by the forward scattering. An inspection of the transverse momentum transfer η would show that the required substitution is supplied by the relation [45(d)]

$$\eta = \left(\frac{2+2\eta'}{1-\eta'} \right)^{1/2}, \quad (4.3)$$

where the variable η' belongs to the interval $[-1, +1]$. For simplicity, we shall adopt the same kind of change for the variable p by writing

$$p = \left(\frac{2+2p'}{1-p'} \right)^{1/2}, \quad (4.4)$$

with $p' \in [-1, +1]$. Consequently, we can also employ the variable-order Gauss-Legendre quadrature for integrations over η' and p' . The integrand in (2.13) is smooth in the new variables, so that a moderate size of the quadrature points over all the four axes suffices to provide excellent convergence of the results to within at least two accurate decimal places. Notice that the new variables η' and p' from Eqs. (4.3) and (4.4) are obviously of such a nature that it is necessary to investigate the regularity of the integrand in (2.13) at $\eta'=1$ and $p'=1$. However, there is no problem in this regard, since it can be shown that the function $|R_{if}(\eta)|^2$ scales according to

$$\begin{aligned} d\eta \eta |R_{if}(\eta)|^2 &= \int_{-1}^{+1} d\eta' (1-\eta')^{10} \\ &\times \left[\int_{-1}^{+1} dp' \int_{-1}^{+1} du \int_0^{2\pi} d\phi (1-p')^{7/2} R'_{if} \right]^2, \end{aligned} \quad (4.5)$$

where R'_{if} is a regular function everywhere along the four integration axes including the points $\eta'=1$ and $p'=1$. The explicit form of *real* function R'_{if} will not be given here, since it can readily be identified from Sec. II by using the result (3.25) for the Dalitz integral \mathcal{D}_{11} . Of course, in the actual computations, we use the expression of the type (4.5). It should be noticed that there is no post-prior discrepancy in the CB1 approximation for reaction (4.1), so that

$$T_{if} = T_{if}^- = T_{if}^+. \quad (4.6)$$

The present algorithm performs the computation of the total cross sections with and without the corrective terms $\varphi'_{i,f} \equiv (H_{T,P} - E_{i,f})\varphi_{i,f}$. Hence any numerical difference found between the results for $\varphi'_{if} \equiv 0$ and $\varphi'_{if} \neq 0$ would be a direct measure of the significance of the correlation effects which are present in the former and absent in the latter case. The terms in question would provide an assessment of the relative importance of the correlation effects for the process under investigation since the Hamiltonians $H_{T,P}$ contain the interelectron potential $1/r_{12}$, independent of any particular form of the initial and final bound-state orbitals $\varphi_{i,f}$. The results of the

computations of the total cross sections obtained with $\varphi'_{i,f} \equiv 0$ and $\varphi'_{i,f} \neq 0$ in the CB1 approximations for double charge exchange (4.1) are displayed in Fig. 1 at impact energies ranging from 100 to 2000 keV. The present theory is found to be in satisfactory agreement with the available measurements. At lower incident energies, the results relating to the case $\varphi'_{if} \neq 0$ are smaller than the corresponding data computed with $\varphi'_{i,f} = 0$ and the pattern is precisely reverse at higher energies. This trend indicates the relative importance of the correlation effects in the symmetric double charge exchange (4.1). Notice that a similar pattern at lower and high energies has previously been found [20,30,53] in the case of single and double charge exchange in collisions between bare nuclei and multielectron target atoms, by using the correlated configuration-interaction orbitals, but without the corrections $\varphi'_{i,f}$.

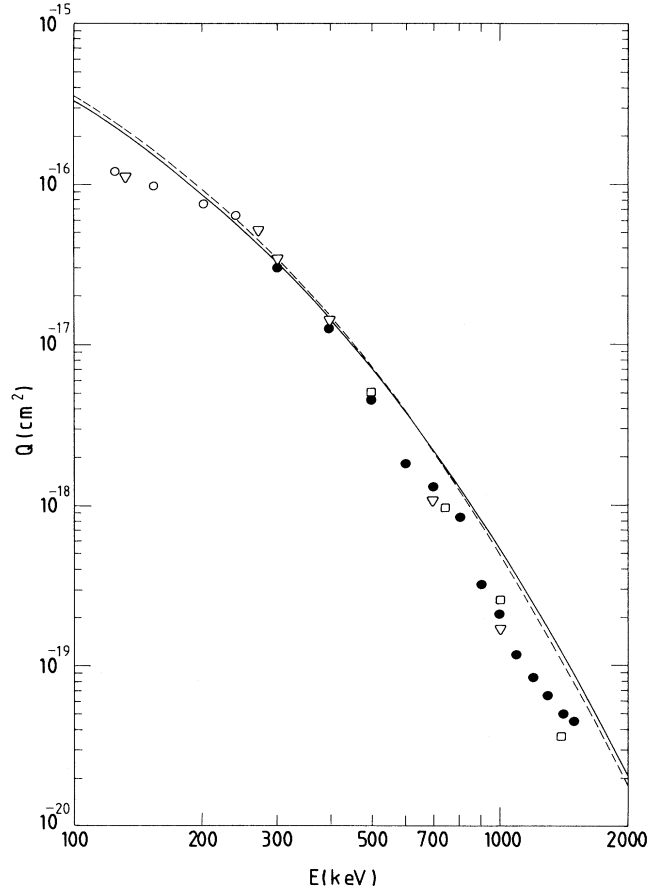


FIG. 1. Total cross section for the double-charge-exchange reaction ${}^4\text{He}^{2+} + {}^4\text{He} \rightarrow {}^4\text{He} + {}^4\text{He}^{2+}$. The displayed theoretical results relate only to the symmetric resonant case $1s^2 \rightarrow 1s^2$ and originate from the present correct first Born (CB1) approximation employing the completely uncorrelated Hylleraas orbitals. The *dashed* curve corresponds to the case *without* the dynamic correlations (perturbation operator potentials W_{if}^{op} neglected), whereas the *full* curve represents the results obtained *with* inclusion of the dynamic correlations (W_{if}^{op} retained; see text). Experimental data: \circ , Berkner *et al.* (Ref. [1]); \square , McDaniel *et al.* (Ref. [17]); \bullet , Pivovarov, Novikov, and Tubaev (Ref. [12]); and ∇ , DuBois (Ref. [8]).

V. DISCUSSION

We have studied double charge exchange in fast collisions of bare nuclei of charge Z_P with the heliumlike atomic systems of the target nuclear charge Z_T , such as $Z_P + (Z_T; e_1, e_2)_i \rightarrow (Z_P; e_1, e_2)_f + Z_T$. The first Born approximation with the correct boundary conditions is formulated *beyond* the customary procedure. Namely, while solving the boundary-condition problem $(H_{i,f} - W_{i,f}^d - E)\Phi_{i,f}^\pm = 0$, for the asymptotic states $\Phi_{i,f}^\pm$ with given channel Hamiltonians $H_{i,f}$, it is always assumed that the corresponding eigenvalue equations $\Phi_{i,f}' \equiv (H_{T,P} - E_{i,f})\Phi_{i,f} = 0$ for the bound-state wave functions $\Phi_{i,f}$ are automatically satisfied. In other words, the functions $\Phi_{i,f}'$ coincide with the zero state vector by definition. One subsequently concentrates on the possible choices of the distorting potentials $W_{i,f}^d$ which must yield the state vectors $\Phi_{i,f}^\pm$ with the prescribed proper asymptotic behaviors at infinitely large interaggregate separations in the entrance and exit channels. At present, however, the exact bound-state wave functions $\Phi_{i,f}$ are unknown for the two-electron atomic systems, which implies that $\Phi_{i,f}' \neq 0$ for any of the existing heliumlike orbitals $\Phi_{i,f}$ utilized in the computations. Hence a *consistent* attainment of the asymptotically correct scattering wave functions for two-electron atomic systems requires that the following two conditions are satisfied.

(i) The unperturbed channel state $\Phi_{i,f}$ must be distorted whenever there are certain remaining Coulomb interactions of the type $V_i^a(R) = Z_P(Z_T - 2)/R$ and $V_f^a(R) = Z_T(Z_P - 2)/R$ between the two scattering particles at their infinite mutual separation R . This is accomplished by requiring that the distorting potential $W_{i,f}^d$ contain the long-range interactions $V_{i,f}^a$, which introduce the appropriate logarithmic Coulomb phase factors $\gamma_i = [Z_P(Z_T - 2)/v] \ln(vR - \mathbf{v} \cdot \mathbf{R})$ and $\gamma_f = [Z_T(Z_P - 2)/v] \ln(vR + \mathbf{v} \cdot \mathbf{R})$ into the wave functions $\Phi_{i,f}$, thus yielding $\Phi_{i,f}^\pm = \Phi_{i,f} e^{\pm i\gamma_{i,f}}$.

(ii) The unperturbed asymptotic states $\Phi_{i,f}$ ought to be given by the products $\Phi_{i,f} \exp(\pm i\mathbf{k}_{i,f} \cdot \mathbf{r}_{i,f})$ of the two-electron bound-state wave functions $\Phi_{i,f}$ and the plane waves $\exp(\pm i\mathbf{k}_{i,f} \cdot \mathbf{r}_{i,f})$ describing the relative motion of the scattering particles. In the *eikonal* approximation, various choices for the distorting potentials $W_{i,f}^d$ from the above defining equation $(H_{i,f} - W_{i,f}^d - E)\Phi_{i,f}^\pm = 0$ can be made, which could all lead to the asymptotically correct channel states $\Phi_{i,f}^\pm = \Phi_{i,f} \exp(\pm i\mathbf{k}_{i,f} \cdot \mathbf{r}_{i,f} \pm i\gamma_{i,f}) \equiv \Phi_{i,f} g_{i,f}^\pm$. However, each of the particular selection of the quantity $W_{i,f}^d \Phi_{i,f}^\pm$ must contain the terms $g_{i,f}^\pm \Phi_{i,f}' \equiv g_{i,f}^\pm (H_{T,P} - E_{i,f})\Phi_{i,f}$ as an unavoidable part of the application of the operator $H_{i,f} - W_{i,f}^d - E$ to the asymptotic wave function $\Phi_{i,f}^\pm$.

The present additional terms $g_{i,f}^\pm \Phi_{i,f}'$ in the resulting transition amplitudes T_{if} do not alter the explicit forms of the asymptotic configurations $\Phi_{i,f}^\pm$, but through the distorting potentials $W_{i,f}^d$ merely compensate for the lack of knowledge of the exact bound-state wave functions $\Phi_{i,f}$. With this important information included, the correct boundary conditions can be consistently formulated for a

model problem, despite the unavailability of the exact wave functions $\Phi_{i,f}$. Moreover, even if the bound-state wave functions $\Phi_{i,f}$ are completely uncorrelated such as the Hylleraas orbitals [48] of the type $(\gamma^3/\pi) e^{-\gamma(r_1+r_2)}$, the transition amplitudes will still approximately incorporate the electron-correlation effects through the terms $W_{i,f}^{\text{op}} \Phi_{i,f}^\pm = g_{i,f}^\pm \Phi_{i,f}'$. For the purpose of illustration, the present computation was limited to the uncorrelated Hylleraas [48] bound-state wave functions, but we could also employ highly correlated configuration-interactions orbitals [38]. In these latter orbitals, a high degree of angular and radial correlation effects is achieved by using a linear combination of a large number (~ 100) of the products the Slater-type orbitals (STO's) for each of the electrons. The price of avoiding the explicit appearance of the interelectron coordinate r_{12} in these wave functions is paid by the need to include many STO's. It should, however, be remarked that these wave functions originate from the studies of *bound-state* problems in which the main goal consists in obtaining the precise binding energies $E_{i,f}$, through the diagonalization of the exact two-electron Hamiltonians of the type $H_{T,P}$ in the basis span by the STO's. However, there is no *a priori* physical argument which would guarantee that these many-parameter wave functions are also best suited for the purpose of *scattering* problems. Furthermore, use of these orbitals in, e.g., the four-body CDW method [42,43] would be considerably computer-time consuming, since too many matrix elements ($\sim 4 \times 10^4$) need to be evaluated for a tremendous number of times for each point of the four *nested* integrations. We presently propose an opposite procedure by employing the simplest Hylleraas decoupled wave functions $\Phi_{i,f}$ and additionally including the correlation effects through the potential $1/r_{12}$, which is present in the transition amplitudes T_{if} as a part of the perturbation potentials, namely the correction terms $\Phi_{i,f}'$. The results obtained exhibit a familiar trend in which the correlation effects respectively decrease or increase the total cross sections depending on whether we are dealing with the lower or higher incident energies. The same pattern is observed through the use of the wave functions with a high degree of the static but without dynamic correlations, while studying single [53] as well as double charge exchange [20,30]. Of course, one could improve the proposed version of the CB1 theory by using the simple but correlated orbitals $(1s, 1s')$ or $(1s, 2p)$ of Eckart-Silverman [54] with two or three parameters, as a better input for the bound-state wave functions $\Phi_{i,f}$. In any case, the presently implemented variant employing the Hylleraas orbitals *together* with the corrections $\Phi_{i,f}'$ appears to be very useful, at least as a first guess in obtaining an estimate about the relative importance of electronic correlations. After having this quick estimate, one can then decide whether it is worthwhile to perform exhaustive computations with highly correlated wave functions $\Phi_{i,f}$, but still keeping the eigenproblem-type corrections $\Phi_{i,f}'$. The usefulness of this procedure could also be checked in other approximations for single and double charge exchange from heliumlike atomic systems. Thus we have verified that in the continuum-distorted-wave approximation of Cheshire [41] for single-electron capture

from H^- and He by fast protons, the present input with the Hylleraas orbitals and the corrective terms $\varphi'_{i,f}$ provide quantitatively very similar results to those obtained by Banyard and Szuster [53] with the highly correlated multiparameter two-electron wave functions in the configuration-interaction representation.

VI. CONCLUSION

We investigate the problem of double charge exchange in fast collisions of completely stripped projectiles and heliumlike atomic systems. An alternative version of the first Born approximation with the correct boundary conditions is formulated by an *ab initio* introduction of the perturbation operator potentials $W_{i,f}^{op} \equiv (H_{T,P} - E_{i,f})\varphi_{i,f} \circ [1/\varphi_{i,f}]$, which take proper care of the fact that the exact bound-state two-electron wave functions $\varphi_{i,f}$ are unknown. Here the symbol \circ indicates that all the functions from the domain of the definition of operators $W_{i,f}^{op}$ must contain the *factored* orbitals $\varphi_{i,f}$. As an important consequence of the introduction of this novel correction $W_{i,f}^{op}$, the interelectron repulsion $1/r_{12}$ *always* appears in the transition amplitude as a part of the whole perturbation potential for any of the available approximate two-electron orbitals. An illustrative computation *with* and *without* the correction term $W_{i,f}^{op}$ for the two-electron

bound-state eigenvalue problems is carried out on the symmetric resonant two-electron transfer in collisions between fast α particles and $He(1s^2)$. This is a prototype of a larger class of processes which directly participate in determining the transport characteristics of double charged particles and represent one of the primordial factors of the energy balance in the high-temperature thermonuclear fusion plasmas. The proposed CB1 method, exemplified with the uncoupled Hylleraas one-parameter bound-state orbitals, predicts the total cross sections which agree favorably with the experimental data at impact energies ranging from 100 keV to 2 MeV. We have found that cross sections with the correction $W_{i,f}^{op}$ are, respectively, decreased or increased in comparison to the theoretical results without the contribution $W_{i,f}^{op}$, depending upon whether we are considering the lower or higher impact energies.

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