Dynamic electron correlations in single capture from helium by fast protons

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(Received 27 January 1997; revised manuscript received 14 July 1997)

We employ the four-body continuum distorted-wave (CDW-4B) method to compute the *total* cross sections for the single electron-capture process $H^+ + He(1s^2) \rightarrow H(1s) + He^+(1s)$ at incident energies ranging from 20 to 20 000 keV. The purpose of the present work is twofold: (i) to verify whether the CDW-4B approximation for one-electron transfer is as successful as for double charge exchange in fast proton-helium collisions and (ii) to search for evidence of dynamic electron correlation effects as a function of increased projectile energy. The validity of our findings is critically assessed in comparisons with the available experimental data in the quoted impact energy range. [S1050-2947(97)01311-5]

PACS number(s): 34.70.+e, 82.30.Fi

I. INTRODUCTION

The simple four-body problem of the basic single charge exchange $p + He(1s^2) \rightarrow H(1s) + He^+(1s)$ offers an intriguing task of establishing the relative importance of the interelectron and electron-projectile potentials. In principle, both interactions can lead to one-electron capture, but the invoked mechanisms differ considerably from each other. The interaction V_{p1} of the ''active'' electron e_1 to be captured with the incident proton p leads to single charge exchange and forms the basis of the so-called ''velocity-matching'' mechanism [1]. This mechanism can be best conceived by resorting to the transition probability in terms of the initial $\widetilde{\varphi}_{n_i l_i m_i}$ and final $\widetilde{\varphi}_{n_f l_f m_f}$ bound-state wave functions in momentum space. When a fast impinging proton p of mass m_p passes by the helium target with a large momentum $m_p \vec{v}_p$ and velocity $\vec{v}_p$, the electron e_1 of mass $m_e \ll m_p$, which is orbiting about the α particle with the classical velocity $v_{e_1} \ll v_p$, could be captured via a single binary collision p-e_1 only if considerable momentum, of the order of $m_e \vec{v}_p$, is imparted onto e_1. Since this displacement $m_e \vec{v}_p$ in the momentum components of $\widetilde{\varphi}_{n_f l_f m_f}$ will increase with augmentation of v_p, it is clear that only the largest components of the momentum-space wave functions would be able to provide the ''velocity matching,'' which should yield a nonvanishing overlap of the initial and final orbitals. Nevertheless, the resulting probability is exceedingly small, giving a cross section with the typical behavior $v_p^{-12-2l_i-2l_f}$ for large v_p, since both orbitals $\widetilde{\varphi}_{n_i l_i m_i}$ and $\widetilde{\varphi}_{n_f l_f m_f}$ fall off too rapidly with increasing values of their momentum variables. A large momentum $m_e \vec{v}_p$ could be transferred to e_1 only if the impinging proton p comes close to electron e_1, which possesses a very small initial momentum in the target ($m_e v_{e_1} \ll m_e v_p$). Hence, the velocity-matching mechanism is expected to be operative mainly at small impact parameters ρ. This is a common feature of all first Born-type models [2].

One can alternatively choose the potential V_{p1} as a perturber of the asymptotic state Φ_i in the entrance channel, with Φ_i given by the product of the two-electron target wave function φ_i and the plane wave for the relative motion of the projectile. This is accomplished through the usual multiplication of the channel state Φ_i by the appropriate Coulomb wave and an automatic cancellation of V_{p1} from the entrance channel perturbation V_i in the transition T matrix. This procedure is reminiscent of the four-body continuum distorted-wave (CDW-4B) theory [3–6], which represents a rigorous first-order approximation of the Dodd and Greider [7,8] distorted-wave perturbation expansion without any divergencies, such as disconnected Feynman diagrams and the like. In the CDW-4B model, the projectile does not directly impart a large momentum of the order $\sim m_e \vec{v}_p$ onto the ''active'' electron e_1. Instead, this momentum is transferred indirectly via the long-range distortion effects and, hence, close encounters between p and e_1 are not mandatory any longer. This illustrates that the small size of the impact parameter ρ cannot be used as an unambiguous signature or a characterization of the velocity-matching mechanism. A much clearer situation emerges from the analysis of recoiled particle He^+ of the target remainder. Namely, in order to conserve the total momentum of the whole four-body collision system, the residual He^+ ion in the exit channel must recoil in the backward direction. This is readily observed by means of the well-established experimental technique known as the recoiled ion momentum spectroscopy (RIMS) [9,10].

Additionally, the interaction V_{p2} of the presumably ''passive'' electron e_2 with the projectile can also lead to capture of electron e_1. Here, electron e_2 receives a large momentum $m_e \vec{v}_p$, which is afterwards transferred onto e_1. This is possible only if the static correlation of the two electrons in the helium target plays a non-negligible role. The relative importance of V_{p2} as a perturbation in a T matrix has not been previously estimated and this will be thoroughly investigated in the present work by means of the CDW-4B method.

We shall mainly focus on the role of the interelectronic (e_1-e_2) potential V_{12} from the *dynamic* point of view. To achieve this goal within the CDW-4B method, one ought to employ the ''post'' formalism with the appropriate full per-

turbation V_f in the exit channel. A contribution from V_{12} to single capture in the p-He collisions has not been previously assessed and it is our main goal to bridge this gap with the help of the CDW-4B model. The mechanism of the dynamic electron correlation does not necessitate close encounters with a projectile. Moreover, when the dynamic correlations are operating, the target remainder He^+ is at rest as a mere spectator, in sharp contrast to the backward recoil in the velocity-matching mechanism [11].

The above-listed mechanisms should be completed by yet another pathway, commonly known as the Thomas [12] double scattering (p-e_1-α). In this two-step mechanism of the p-He single capture, the electron e_1 first collides with the incident proton p and then scatters elastically on the α particle of the target, acquiring finally the ejection momentum $m_e\vec{v}_p$, which is sufficient to form atomic hydrogen. Such a mechanism operates only at very high energies, yielding the v^{-11} Thomas-type behavior of the cross section. This is correctly predicted by the CDW-4B theory. The purely classical mechanism of the Thomas double encounter is comprised of two consecutive Rutherford scatterings each yielding the v_p^{-4} behavior of the cross section. When the ensuing result v_p^{-8} is further multiplied by the volume element v_p^{-3} of momentum space, the overall Thomas cross section v_p^{-11} is obtained. The second-Born approximation describes this classical effect by means of the transition operator $V_{\alpha 1}G_0^+V_{p1}$. Here, $V_{\alpha 1}$ is the Coulomb interaction between the α particle and e_1, whereas G_0^+ is the free-particle Green's operator. A slower decrease of the Thomas cross section with rising v_p in comparison with the velocity-matching mechanism can be mathematically interpreted as an enlarged overlap between the initial and final bound states. This is also expected from the physical viewpoint, since the stringent condition for velocity matching in the p-e_1 encounter is partially relaxed via the subsequent e_1-α collision, where the target nucleus could carry some excess of energy. Clearly, this surplus of energy and momentum taken by the α particle is severely limited by the heavy mass of the target nucleus. A much more pronounced reduction of the cross section, however, is expected if the energy excess is taken by, e.g., a photon, which indeed yields the v_p^{-5} behavior [13] of the cross sections for the ensuing radiative electron capture (REC). A similar argument could be evoked to anticipate a considerably weaker dependence than the v_p^{-11} asymptote of the second Born cross section [14] for transfer ionization (TI) in the p-He collision, where e_1 is captured by the proton and e_2 is simultaneously ionized. Here, the second electron e_2 could readily carry away the excess of energy and momentum and, therefore, maximally relax the strict velocity-matching requirement. Indeed, a very recent experiment by Mergel *et al.* [15] provides evidence that the total cross section for TI in the p-He collision behaves like $v_p^{-7.4\pm 1.0}$ with increasing v_p at impact energies ranging from 300 to 1400 keV.

Atomic units will be used throughout unless stated otherwise.

II. THEORY

It is important to investigate the influence of the dynamic electron correlation effects on *total* cross sections for single capture in the p-He collision, particularly with respect to the increasing values of the incident proton velocity v_p, but still below the region of the dominance of the Thomas double scattering p-e_1-α. In this way, one could monitor an interplay between the *single*-step velocity-matching mechanism and the dynamic electron correlations and, hence, determine their relative importance. Here, the electron dynamics enter the composite process under investigation via a *two-step* p-e_1-e_2 Thomas-type mechanism, which corresponds to the propagator $V_{12}G_0^+V_{p1}$ of the second Born approximation. The first p-e_1 step in the CDW-4B method is not accomplished directly via an explicit appearance of the the electrostatic interaction V_{p1} in the transition T operator, but rather indirectly through dressing of the unperturbed states Φ_i and Φ_f with the Coulomb waves centered on p and α, respectively. The transfer of large momentum $m_e\vec{v}_p$ from p to e_1, mediated by these long-range distortions of the asymptotic channel states, enables the two electrons to interact strongly in the second e_1-e_2 step of the above p-e_1-e_2 mechanism via the explicit V_{12} potential in the V_f perturbation of the exit channel. Although e_2 remains on the target rest He^+, as opposed to TI, the e_1-e_2 scattering should be able to considerably relax the velocity-matching condition of the preceding p-e_1 step. Our goal is to determine whether such an effect could be detected already on the level of the total cross sections, since these observables are easier to measure experimentally. There exist several measurements of differential cross sections for the Thomas double scattering p-e_1-Z_T in the p-He or p-H_2 single capture at high energies [16,17]. These data indicate that the width of the Thomas p-e_1-Z_T peak is larger for p-He or p-H_2 than in the case of the p-H collision. Such a phenomenon could be due a broader momentum distribution of the initial state of the ''active'' electron in p-He than in p-H case. In addition, the dynamic correlation effect might change the shape of the conventional Thomas peak in the p-e_1-Z_T encounter. This is supported by our preliminary computation for p-He single charge exchange within the the CDW-4B method, which shows that the Thomas peaks for the double p-e_1-e_2 and p-e_1-α collisions occur at the same critical angle.

In a search for the signature of the p-e_1-e_2 mechanism in the p-He single-electron transfer, we will also be in a position to verify whether a four-body distorted-wave formalism, such as the presently used CDW-4B model for this process, would be of comparable adequacy in regard to the results of a previously reported study on double charge exchange for the same colliding system [3]. This is important in view of some evidence within another four-body formalism known as the forced impulse approximation (FIA), which is successful for double ionization, but has very recently been reported to break down for single ionization in p-He collisions [18].

In all the previous studies of a general one-electron capture from a heliumlike atomic systems of the nuclear charge Z_T by a completely stripped projectile of the charge Z_P:

$$Z_P+(Z_T;e_1,e_2)_i\rightarrow(Z_P,e_1)_{f1}+(Z_T,e_2)_{f2}, \qquad (1)$$

the electron e_2 has been considered as being ''passive'' in the sense of occupying the same orbital before and after collision. Moreover, all the residual interactions of e_2 with Z_P and e_1 in the form V_{p2} and V_{12} mentioned in the Introduction

have systematically been neglected from distorted-wave models in order to bypass several complicated bound-free multicenter atomic form factors with Coulomb functions. The net result of such a ''frozen-core'' approximation is an explicit reduction of the four-body formalism to essentially a three-body problem [19,20]. Here, the electron e_2 is *de facto* ''phased out'' from the otherwise onset four-body starting point. This is customarily accomplished by using, e.g., the Slater-screened hydrogenic wave function [21] for a helium-like target: $\varphi_i(\vec{x}_1,\vec{x}_2)=(\lambda^3/\pi)\exp[-\lambda(x_1+x_2)]$, where $\lambda=Z_T-\lambda_S$ and $\lambda_S=0.3125$. In such a way, all the interesting features of the pure dielectronic dynamics are washed out from the four-particle formalism, which, therefore, does not introduce anything new with respect to a pure three-body problem. If instead of the hydrogenic wave functions [21], some more elaborate orbitals are used via configuration interactions (CI) to describe $\varphi_i(\vec{x}_1,\vec{x}_2)$, one will end up with a reduction of a four-body T matrix to a linear combination of three-body T matrices and again no new insight would be gained on the electronic dynamics [22]. Moreover, such a four-body formalism that neglects V_{p2} and V_{12} would be, in a sense, equivalent to the independent particle model (IPM), which discards the dynamic electron correlations from the onset [23,24]. Nowadays, however, with the advent of fast computers, there is no need any longer to overlook the contributions from V_{p2} and V_{12}. Taking the Fourier transforms of these residual potentials, one finally arrives at convenient distorted-wave four-body T matrices for Eq. (1) in terms of some readily manageable triple numerical integrations. A similar technique has already been implemented in double charge exchange [3], resonant or nonresonant transfer excitation [4,5] and in transfer ionization [6] treated by means of the CDW-4B approximation. For this reason, there should be no need to give here any details of the derivation, but merely to quote the final expressions of the total cross sections for the process (1) in the prior (Q_{if}^-) and post (Q_{if}^+) forms:

$$Q_{if}^{\pm}(a_0^2)=\int d\vec{\eta}\left|\frac{R_{if}^{\pm}(\vec{\eta})}{2\pi v}\right|^2, \tag{2}$$

where $\vec{\eta}$ is the usual transverse momentum transfer and $\vec{v}=\vec{v}_p$ is the incident velocity ($\vec{\eta}\cdot\vec{v}=0$). The integrals $R_{if}^-(\vec{\eta})$ and $R_{if}^+(\vec{\eta})$ in Eq. (2) are given by the following matrix elements with the *complete* prior V_i and post V_f perturbations, respectively:

$$R_{if}^-(\vec{\eta})=N_{PT}\int\int\int d\vec{R}\; d\vec{x}_1\; d\vec{x}_2\; e^{i\vec{q}\cdot\vec{s}_1+i\vec{p}\cdot\vec{x}_1}\varphi_{f_1}^*(\vec{s}_1)\varphi_{f_2}^*(\vec{x}_2)\,{}_1F_1(i\nu_T;1;ivx_1+i\vec{v}\cdot\vec{x})[V_i\varphi_i(\vec{x}_1,\vec{x}_2)$$
$$\times\,{}_1F_1(i\nu_P;1;ivs_1+i\vec{v}\cdot\vec{s}_1)], \tag{3}$$

$$V_i=\Delta V_{P2}-\vec{\nabla}_{x_1}\ln\varphi_i(\vec{x}_1,\vec{x}_2)\cdot\vec{\nabla}_{s_1}, \tag{4}$$

$$\Delta V_{P2}=V_{P2}-V_{P2}^{\infty},\quad V_{P2}=-\frac{Z_P}{s_2},\quad V_{P2}^{\infty}=-\frac{Z_P}{R}, \tag{5}$$

$$R_{if}^+(\vec{\eta})=N_{PT}\int\int\int d\vec{R}\; d\vec{s}_1\; d\vec{s}_2 e^{i\vec{q}\cdot\vec{s}_1+i\vec{p}\cdot\vec{x}_1}\varphi_i(\vec{x}_1,\vec{x}_2)\varphi_{f_2}^*(\vec{x}_2)\,{}_1F_1(i\nu_P;1;ivs_1+i\vec{v}\cdot\vec{s}_1)[V_f\varphi_{f_1}^*(\vec{s})\,{}_1F_1(i\nu_T;1;ivx_1+i\vec{v}\cdot\vec{x}_1)], \tag{6}$$

$$V_f=\Delta V_{P2}+\Delta V_{12}-\vec{\nabla}_{s_1}\ln\varphi_f^*(\vec{s}_1)\cdot\vec{\nabla}_{x_1}. \tag{7}$$

$$\Delta V_{12}=V_{12}-V_{12}^{\infty},\quad V_{12}=\frac{1}{x_{12}}=\frac{1}{|\vec{x}_1-\vec{x}_2|},\quad V_{12}^{\infty}=\frac{1}{x_1}, \tag{8}$$

The symbol ${}_1F_1$ in Eqs. (3) and (6) denotes the confluent hypergeometric Kummer function, whereas φ_i and φ_{f_j} ($j=1,2$) are the initial and final bound-state orbitals. The quantity N_{PT} in $R_{if}^{\pm}(\vec{\eta})$ is given by $N_{PT}=N^+(\nu_P)N^{-*}(\nu_T)$ and $N^{\pm}(\nu_K)=\Gamma(1\mp i\nu_K)\exp(\pi\nu_K/2)$ $(K=P,T)$, where $N^+(\nu_P)$ and $N^-(\nu_T)$ are the standard normalization Coulomb constants with the Sommerfeld parameters $\nu_P=Z_P/v$ and $\nu_T=(Z_T-1)/v$. The two momentum transfers $\vec{p}$ and $\vec{q}$ in Eqs. (3) and (6) are defined as follows:

$$\vec{q}=\vec{\eta}-\left(\frac{v}{2}-\frac{\Delta E}{v}\right)\hat{v},\quad \vec{p}=-\vec{\eta}-\left(\frac{v}{2}+\frac{\Delta E}{v}\right)\hat{v},$$
$$\Delta E=E_i-(E_{f_1}+E_{f_2}), \tag{9}$$

where E_i and $E_{f_{1,2}}$ are the initial (helium) and final (hydrogenic) binding energies, respectively. In the course of deriving Eq. (2) from the corresponding T matrices $T_{if}^{\pm}(\vec{\eta})$, the term $\rho^{2iZ_P(Z_T-1)/v}$ disappears from the total cross sections $Q_{if}^{\pm}$. This phase, however, is present in the corresponding differential cross sections $dQ_{if}^{\pm}/d\Omega$, describing the Z_P-Z_T Rutherford internuclear scattering [1]. Notice that the Z_P-e_2 Coulomb interaction of the ''passive'' electron e_2 at finite and infinite distances is present in the same fashion in both V_i and V_f from Eqs. (4) and (7) through ΔV_{P2}. This is because the potential V_{P2} is chosen as inactive in the course of dynamic distortion of total scattering states in the entrance and exit channels. However, the e_1-e_2 potential appears only in V_f, since V_{12} emerges in the definition of the exit channel

perturbation through the difference between the total interaction $V=Z_PZ_T/R-Z_P/s_1-Z_P/s_2-Z_T/x_1-Z_T/x_2+1/x_{12}$ and the binding potentials in the noninteracting hydrogenic atomic systems $(Z_P,e_1)_{f_1}$ and $(Z_T,e_2)_{f_2}$. Additionally, a residual potential $V_{12}^{\infty}=1/x_1$, as the limiting value of V_{12} at infinitely large x_1 and finite x_2, consistently appears in V_f. This is because at infinitely large x_1, the ''active'' electron e_1 from $(Z_P,e_1)_{f_1}$ cannot discern the individual constituents in $(Z_T,e_2)_{f_2}$, which is, therefore, conceived as the net charge Z_T-1. In order to account for this correct screened nuclear charge, the genuine potential $V_{T1}=-Z_T/x_1$ is written as $-(Z_T-1)/x_1+1/x_1\equiv-(Z_T-1)/x_1+V_{12}^{\infty}$. Here, the term $-(Z_T-1)/x_1$ is used to produce the distortion $\Gamma(1+i\nu_T)e^{\pi\nu_T/2}{}_1F_1(i\nu_T;1;ivx_1+i\vec{v}\cdot\vec{x}_1)$ with $\nu_T=(Z_T-1)/v$, whereas the potential V_{12}^{∞} is joined together with V_{12} to yield ΔV_{12}. On the other hand, the term V_{12} does not appear in V_i, since the e_1-e_2 interaction is, in principle, *exactly* included in the initial eigenvalue problem: $(-\nabla_{x_1}^2/2-\nabla_{x_2}^2/2-Z_T/x_1-Z_T/x_2+1/x_{12}-E_i^{\rm ex})\varphi_i^{\rm ex}(\vec{x}_1,\vec{x}_2)=0$. In practice, however, the exact wave function $\varphi_i^{\rm ex}(\vec{x}_1,\vec{x}_2)$ is unavailable and the nonzero term $O_i\equiv(-\nabla_{x_1}^2/2-\nabla_{x_2}^2/2-Z_T/x_1-Z_T/x_2+1/x_{12}-E_i^{\rm ex})\varphi_i(\vec{x}_1,\vec{x}_2)\neq0$ should be incorporated in V_i as an additional perturbation for any particular approximation φ_i of $\varphi_i^{\rm ex}$ [25]. For example, using the Slater-screened hydrogenic wave function [21], we shall have $O_i=(1/x_{12}-\lambda_S/x_1-\lambda_S/x_2+E_i-E_i^{\rm ex})\exp[-\lambda(x_1+x_2)]$, where $E_i=-\lambda^2$ and $E_i^{\rm ex}$ is the ''exact'' initial binding energy, the best estimate of which is given by the CI ansatz of Drake [26]. In this way, V_{12} would also appear in V_i, but only in the role of static electron correlations. The initial eigenvalue correction O_i was recently found to be negligible at high energies for α-He transfer ionization treated by means of the CDW-4B method [6]. Assuming that this will also be the case with single-electron capture (1), we shall not consider the correction O_i in the present work.

It is clear now from Eqs. (3) and (6) that the use of the uncorrelated closed-shell $(1s)^2$ Slater-screened hydrogenic wave function [21], accompanied with the neglect of ΔV_{P2} and ΔV_{12}, will effectively reduce the matrix elements of the CDW-4B method to those of its three-body counterpart, i.e., the CDW-3B model. In the present computations, however, we shall employ the radially correlated CI wave function $(1s1s')$ of Silverman *et al.* [27] for φ_i defined as $\varphi_i(\vec{x}_1,\vec{x}_2)=(\mathcal{N}/\pi)[\exp(-ax_1-bx_2)+\exp(-bx_1-ax_2)]$, where $\mathcal{N}^{-2}=2[(ab)^{-3}+(a/2+b/2)^{-6}]$. Despite this very simple form of the open shell of the helium ground-state wave function [27], the radial correlations are taken into account to a very high degree of the order of nearly 95%.

III. THE RESULTS

With the purpose of illustrating the CDW-4B method, we shall consider single-electron capture from helium by fast protons:

$$\mathrm{H}^+ + \mathrm{He}(1s^2) \rightarrow \mathrm{H}(1s) + \mathrm{He}^+(1s). \tag{10}$$

The results of the computations of prior and post total cross sections for the process (10) are summarized on Figs. 1–5. In our discussions, emphasis will be placed upon the relative role of various terms in the full prior V_i and post V_f perturbations from Eqs. (4) and (7), along the lines traced in the Introduction. The simplest forms of the perturbations V_i and V_f, used in all the previous computations of the CDW method for Eq. (10), as well as for other processes of the general type (1), are given by

$$V_i \approx -\vec{\nabla}_{x_1}\varphi_i(\vec{x}_1,\vec{x}_2)\cdot\vec{\nabla}_{s_1}, \quad V_f \approx -\vec{\nabla}_{s_1}\varphi_f^*(\vec{s}_1)\cdot\vec{\nabla}_{x_1}. \tag{11}$$

In comparison with the full prior perturbation V_i from Eq. (4), the choice (11) corresponds to neglect of $\Delta V_{p2}=V_{p2}-V_{p2}^{\infty}=-1/s_2+1/R$, where $P=p$ for $Z_P=1$. However, keeping only the scalar product of the gradient operators in the interaction V_f via the selection (11), will result in a more

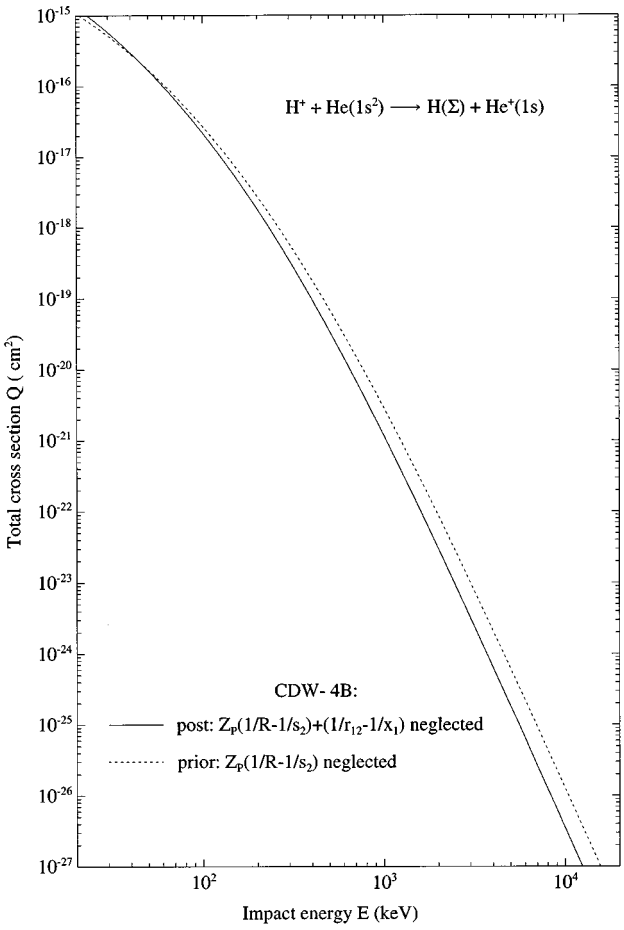

FIG. 1. Total cross sections for single capture from helium by protons as a function of the laboratory impact energy E computed in the four-body continuum distorted wave (CDW-4B) approximation. The symbol Σ represents the summation over all the bound states of atomic hydrogen (H). The explicit computations of $Q_{1s}^{\pm}\equiv Q_{if}^{\pm}$ are carried out only for the ground state of H($1s$) and the n^{-3} Oppenheimer scaling law is used for H(n) to estimate the contribution from the whole spectrum of the excited states H(Σ) via $Q^{\pm}=1.202Q_{1s}^{\pm}$. The initial wave functions (φ_i) of Silverman *et al.* [27] is used. The full and the dashed lines correspond to the case where the potentials $\Delta V_{p2}+\Delta V_{12}$ and ΔV_{p2} are neglected in the *abbreviated* V_i and V_f according to Eq. (11), in a test of the post-prior discrepancy.

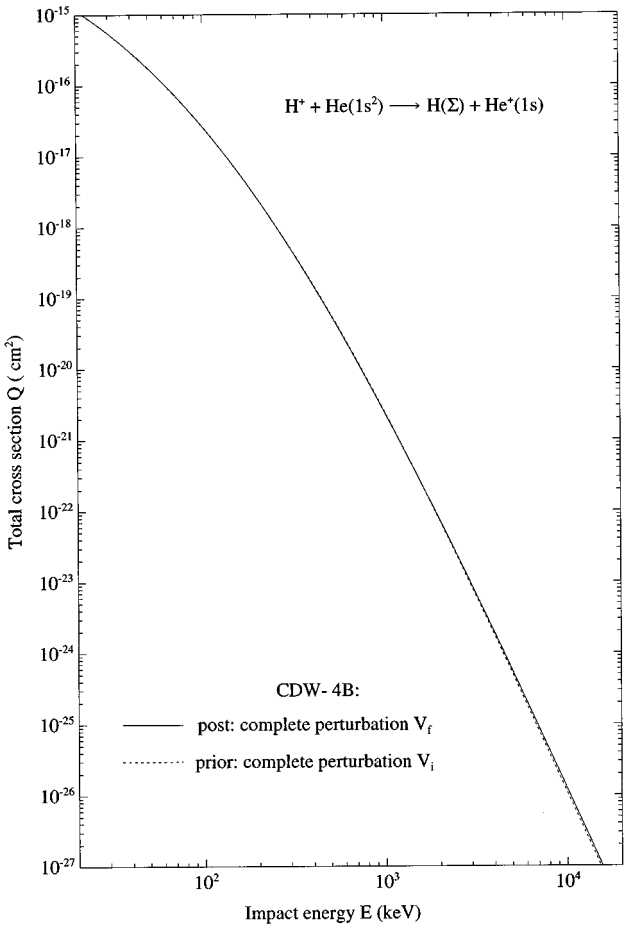

FIG. 2. The same as in Fig. 1, except for the *complete* perturbations V_i and V_f, according to Eqs. (4) and (7), respectively.

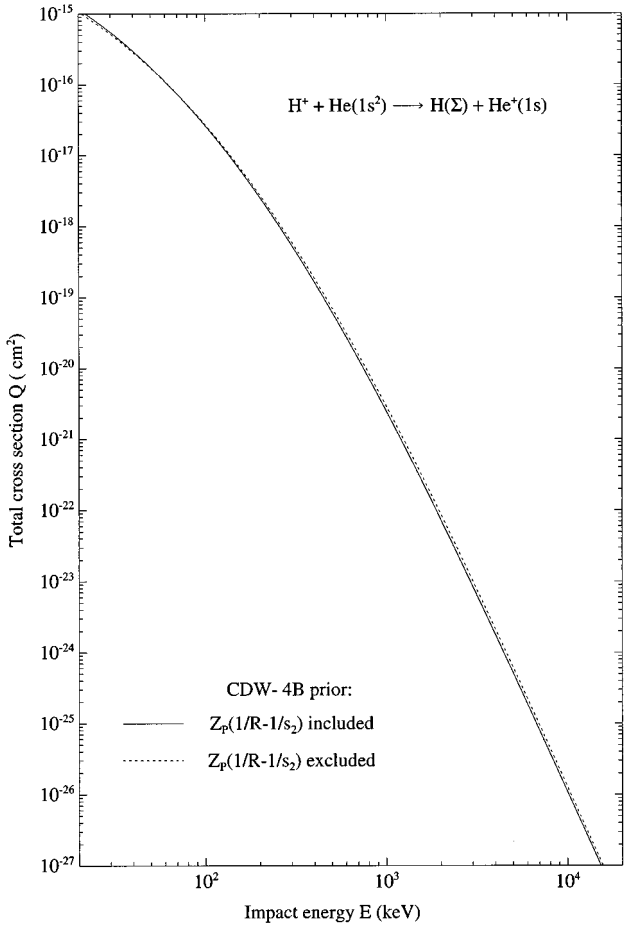

FIG. 3. The same as in Fig. 1, except for the limitation to the prior results only. The full and the dashed lines correspond to the case where the potential ΔV_{p2} is included or excluded from V_i, respectively.

severe post approximation through omission of $\Delta V_{p2} + \Delta V_{12}$. The extent to which the dynamic electron correlation term $\Delta V_{12} = V_{12} - V_{12}^{\infty} = 1/x_{12} - 1/x_1$ is ignored can be at once seen on Fig. 1. It follows that above 100 keV, where the CDW-4B model is expected to be valid, the so-called ''post-prior'' discrepancy between V_i and V_f from Eq. (11) is seen as huge. In this region, the post cross sections are always smaller than those of the prior form. The discrepancy increases with augmentation of the incident energy. This indicates that the role of the dynamic electron correlation effect ΔV_{12} becomes more prominent at higher incident energies. Such an indication will be checked subsequently when we limit ourselves exclusively to the post approximation, considering the cases *with* and *without* ΔV_{12}. Once the complete perturbations V_i and V_f are retained in the computations, according to Eqs. (4) and (7), the full CDW-4B model emerges with the feature of a dramatically reduced post-prior discrepancy (see Fig. 2). This is an excellent property of the method, since the same physical assumptions are involved in both prior and post forms. Although the difference between the post and prior results with the complete V_i and V_f is small, it should be noticed that the two curves in Fig. 2 are *not parallel* to each other. This difference becomes more significant at higher energies, where the post results are larger than the prior ones, as opposed to the preceding situation in Fig. 1. Despite the fact that the post-prior discrepancy with the complete V_i and V_f from Eqs. (4) and (7) does not exceed 15%, the trend of this discrepancy is significant, indicating again an increasing role of the dynamic electron correlations at higher energies. Next we examine the role of the ''passive'' electron by displaying the results with and without ΔV_{p2} in Figs. 3 and 4. Above 100 keV, the cross sections accounting for ΔV_{p2} in V_i and V_f are smaller by some 10% than those neglecting this term. However, their difference remains constant with increasing impact energy. In order to critically assess the usefulness of the present model, a comparison with measurements is required, and this is carried out on Fig. 5. One can see from Fig. 5 that the CDW-4B approximation is in excellent agreement with the available experimental data, provided that the full perturbation V_f is included in the post formulation. This comparison, which extends over three orders of magnitude of the impact energy $E(20-20000\,\text{keV})$, where the cross sections vary within 12 orders of magnitude (10^{-15}–10^{-27} cm^2), establishes validity of the CDW-4B method at $E \geqslant 70$ keV. Moreover, it can be observed from Fig. 5 that the dynamic electron correlations are essential, since exclusion of the relevant term ΔV_{12} from V_f yields results that grossly underestimate the experiments at all energies above 100 keV.

IV. CONCLUSION

We have studied single charge exchange in proton-helium collisions at intermediate and high impact energies. This is

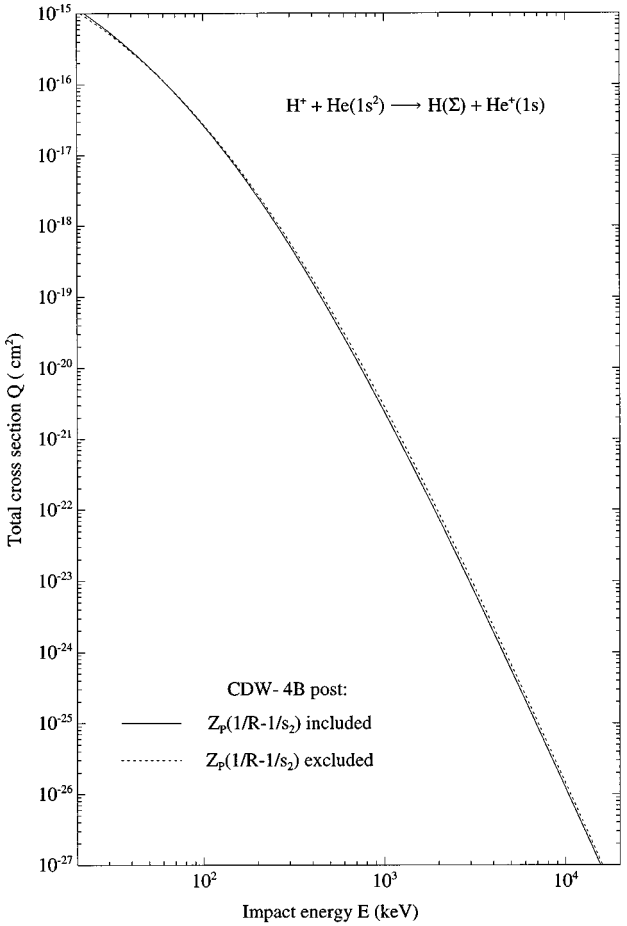

FIG. 4. The same as in Fig. 1, except for the limitation to the post results only. The full and the dashed lines correspond to the case where the potential ΔV_{p2} is included or excluded from V_f, respectively.

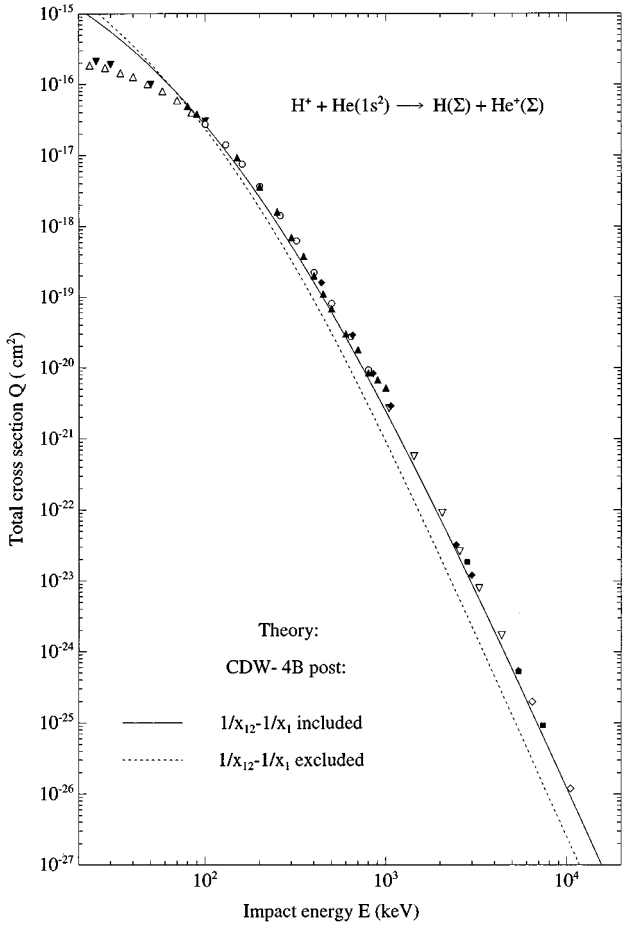

FIG. 5. Total cross sections for single capture from helium by protons as a function of the laboratory impact energy E. The symbol Σ represents the summation over all the bound states of atomic hydrogen (H) and helium ion (He^+) as measured experimentally. In the computations of the displayed post cross sections Q^+ only the ground states of $H(1s)$ and $He^+(1s)$ are accounted for. However, all the excited states $H(\Sigma)$ of atomic hydrogen are approximately included via $1.202Q_{1s}$ in terms of the n^{-3} Oppenheimer scaling law for $H(n)$. The initial wave function φ_i of Silverman *et al.* [27] is used. The full and the dashed lines obtained by means of the four-body continuum distorted-wave (CDW-4B) method correspond to the case where the potential ΔV_{12} is included or excluded from the complete perturbation V_f, respectively. Experimental data: ▽: Schryber [28]; △: Shah *et al.* [29]; ○: Shah and Gilbody [30]; ◇: Berkner *et al.* [31]; ▲: Williams [32]; ●: Horsdal-Pedersen *et al.* [33]; ▼: Martin *et al.* [34]; ◆: Welsh *et al.* [35].

accomplished by using the four-body continuum distorted wave (CDW-4B) theory, which was originally formulated for two-electron transitions, such as double charge exchange, transfer excitation, and transfer ionization. The obtained total cross sections for investigated p-He one-electron capture are presently found to be in excellent agreement with the available experimental data. Such a finding could also be used as an *a posteriori* justification of the physical assumptions of the original formulation of the CDW-4B model for more complex problems involving two active electrons. This is not surprising, since the four-body version of the CDW approximation is obtained as a direct extension of its well established three-body counterpart. Both three- and four-body formalisms of the same CDW theory are consistently derived as a first-order approximation of their respective Dodd-Greider perturbation developments. Such power series expansions are free from singular terms and this guarantees a meaningful interpretation of their first-order estimates. However, the employed CDW-4B method for the p-He single electron transfer is not unique, due to a multitude of choices for distorting potentials, and hence the need for a judicious choice of the prior and post perturbations V_i and V_f. The present selection of these perturbations, which are responsible for the transition under study, is guided by the correct boundary conditions as well as by the relative role of the competitive mechanisms of ''velocity matching'' (electron-projectile) and dynamic correlation effect (electron-electron interaction). The reported theoretical data provide evidence of the prevailing importance of the interelectron potential over the electron-nucleus interaction *at high* impact energies. This invalidates the widely accepted concept of considering the noncaptured electron as being ''passive'' in proton-helium single charge exchange. We emphasize that the present conclusion is reached on the level of the *total* cross sections. Since these observables are easier to measure, it is hoped that our findings would motivate further experimental studies on similar collisional systems at high energies, especially by means of storage rings equipped with the recoiled ion momentum spectroscopy.

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