Single-electron capture from hydrogenlike atomic systems

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The total cross sections for single-charge transfer in H + H, He^+ + H, He^+ + He^+, and Li^{2+} + H collisions have been calculated in the framework of four-body (4B) formalism of boundary corrected continuum intermediate state (BCCIS) approximation in the energy range 20–5000 keV/amu. The dynamic electron correlation is explicitly taken into account through the complete perturbation potentials. In the initial channel, the passive electron plays the role of screening of the projectile ion. However, continuum states of the target ion and the electron in the field of the residual projectile ion are included. In all cases, total single-electron capture cross sections have been calculated by summing over all contributions up to $n = 2$ shells and subshells, respectively, except the H-H collision. The present computed results, both in prior and post forms of BCCIS-4B method for symmetric and asymmetric cases have been compared with the available theoretical and experimental results. We found that our computed results, particularly in the prior form, are in better agreement with the experimental observations in comparison to other theoretical findings. Post-prior discrepancy has been found to be within 20% above 70 keV/amu for all interactions.

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I. INTRODUCTION

In recent years much work has been devoted to the study of single-electron capture by multicharged ions interacting with few-electron atoms. When many active electrons are involved in high energy ion-atom collisions, one has to face the question of the influence of electronic correlations on the magnitude of cross section for the process. The study of interelectronic correlation has played a central role in atomic collision physics for a long time [1]. Not only is this research motivated by the quest for a better understanding of the fundamental few-body dynamics, but it has also practical implications for applied field, such as plasma physics and fusion research. For a long time, theoretical and experimental efforts concentrated on the energy dependence of total cross sections (TCSs) for a single-electron transfer from single-electron target atoms or ions colliding with hydrogenlike projectiles. In this respect, previous theoretical work consists of calculations in the framework of three-body (3B) formalism such as the continuum distorted wave (CDW-3B) approximation of Belkic [2], coupled-channel calculations of Ford *et al.* [3], Oppenheimer-Brinkman-Kramers (OBK) approximation [4,5], classical trajectory Monte Carlo (CTMC) method [6,7], CDW-3B and continuum intermediate state (CIS) approximations [8] and the two-center atomic-orbital close-coupling method of Liu *et al.* [9]. Some of these three-body models show a satisfactory agreement with experimental data, but these models completely neglect electronic correlations. In the present paper we shall be particularly interested in processes of the single-electron capture, in which the two electrons take part. Such processes involve scattering between the two hydrogenlike atoms. However, different quantum-mechanical four-body formalisms for such reactions have been proposed. Different four-body theories such as the boundary corrected first Born approximation (CB1-4B) of Mancev [10,11], the CIS approximation of Banyard and Shirtcliffe [12], the CTMC method of Becker and MacKellar [13], the atomic-orbital expansion method of Fritsch and Lin [14], the time-dependent Hartree-Fock approximation (TDHF) of Henne *et al.* [15], the CDW-4B method [16,17], and the CDW-4B and CB1-4B methods of Mancev [18,19]. In the present theoretical investigation, we have focused our attention on charge transfer of hydrogenlike ions or atoms by the impact of H, He^+, and Li^{2+} ions in the incident energy range between 20 and 5000 keV/amu.

The total and partial single-electron capture cross sections in the He^+-He^+ collision has been studied within the two-electron form of the atomic-orbital expansion method [14]. The calculated results are in very close agreement with experimental data at lower energies. Cross sections for single-electron capture in the collision of partially and completely stripped projectile ions with hydrogenlike atoms were calculated by Belkic [2] in the framework of three-body CDW approximation at incident energies ranging from 25 keV to 10 MeV. In this method, the dynamic correlations have been neglected. The calculation shows that in the low-energy range, the computed results are not in satisfactory agreement. The problem of single-charge exchange in collision of hydrogenlike atoms with ground-state hydrogenlike atoms or ions was investigated by Mancev [10] in the framework of CB1-4B theory within the distorted wave four-body formalism. In such investigation, they have studied the sensitivity of the total cross sections to the choice of ground-state wave function for heliumlike atoms and the influence of noncaptured electrons on the final results. However, the agreements of the obtained results with the experimental findings are not satisfactory in the low-energy range. Mancev [11] also investigated the cross sections for single-electron transfer from helium atoms by the impact of hydrogen atoms and helium ions using the same method. They have used an independent particle model with a one-electron Roothan-Hartree-Fock (RHF) orbital for the target atom. Agreement of the obtained results with the experimental data for the He^+ + He collision is not

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satisfactory in the whole energy range. Becker and Mackellar [13] have developed a general four-body version of CTMC and calculated the electron transfer and ionization for He^+ + H and H + H collisions in the energy range 35–1000 keV, but there are substantial differences compared with the experimental results. The CDW-4B model [18] has been used to investigate the charge exchange between hydrogenlike projectiles and atoms. In this calculation, the effects of electron correlation have been explicitly taken into account in the complete perturbation potential. The calculation shows that below 200 keV/amu for the He^+ + He collision and 150 keV for the He^+ + H collision, respectively, the computed results are not in satisfactory agreement. Later, Mancev [19] investigated the total cross sections for change transfer in Li^{2+}-H and He^+-He^+ collisions using the CB1-4B and CDW-4B methods in the energy range 10–5000 keV/amu. In this calculation, the dynamic correlation has been taken into account through the perturbation potential. The computed results are not in agreement with the experimental results in the energy range 10–300 keV/amu. Recently, electron capture by fast Be^{q+} ($q = 2,3$) and B^{q+} (q = 3,4) ions in collisions with atomic hydrogen have been also studied by Liu *et al.* [9] in the framework of the the two-center atomic-orbital close coupling method (TC-AOCC) in the energy region from 0.1 to 100 keV/amu. Total and subshell state-selective cross sections are compared with available experimental and other theoretical data. These results are quite satisfactory. In this context, Belkic *et al.* [20] have extensively discussed different quantum mechanical four-body (4B) methods for various inelastic ion-atom collisions. Based on the success of four-body boundary corrected continuum intermediate state (BCCIS-4B) approximation [21], we are motivated to study the above-mentioned processes in the framework of the BCCIS-4B theory at impact energies of 20–5000 keV/amu.

The plan of this paper is as follows. We present the details of our calculations in Sec. II and discuss our computed results in Sec. III. Finally, we make our concluding remarks in Sec. IV. Atomic units will be used throughout unless otherwise stated.

II. THEORY

Single-electron capture in the process of the scattering between two hydrogenlike atomic systems may be written as

$$(Z_P;\ e_1)_{i_1} + (Z_T,\ e_2)_{i_2} \rightarrow (Z_P;\ e_1,e_2)_f + Z_T, \tag{1}$$

where Z_p and Z_T are, respectively, the nuclear charges of the projectile and the target. Here e, T, and P represent active electron, target ion, and projectile ion, respectively. e_1 and e_2 are the two electrons initially bound to the projectile and target nucleus, respectively. Finally the electron e_2 is captured by the projectile but e_1 occupies the same orbital before and after collision. Let $\vec{s}_1$ and $\vec{s}_2$ ($\vec{x}_1$ and $\vec{x}_2$) be position vectors of the first and second electrons (e_1 and e_2) relative to the nuclear charge of the projectile Z_p (target Z_T). The interelectronic coordinate is denoted by $\vec{r}_{12} = \vec{s}_1 - \vec{s}_2 = \vec{x}_1 - \vec{x}_2$. $\vec{R}$ denotes the position vector of the projectile (P) relative to the target (T) nucleus. In the entrance channel, it is convenient to introduce $\vec{R}_T$ as the position vector between the center of mass of (Z_P; e_1) and (Z_T; e_2) system, and $\vec{R}_P$ is the position vector of the center of mass of (Z_P; e_1,e_2) system relative to Z_T. The total Hamiltonian of the system may be written as

$$H = H_i + V_i = H_f + V_f, \tag{2}$$

where $H_{i,f}$ represents the Hamiltonian in the entrance and exit channels, respectively, and $V_{i,f}$ are the corresponding perturbation potentials, respectively. Let M_T (M_p) be the mass of the target (projectile) nucleus. In the initial channel, one may write

$$\begin{aligned} H_i &= -\frac{1}{2\mu_i}\nabla^2_{R_T} + \frac{(Z_P-1)(Z_T-1)}{R_T} - \frac{1}{2a}\nabla^2_{x_2} \\ &\quad - \frac{Z_T}{x_2} - \frac{1}{2b}\nabla^2_{s_1} - \frac{Z_p}{s_1}, \\ V_i &= \frac{Z_P Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_P}{s_2} + \frac{1}{r_{12}} - \frac{(Z_P-1)(Z_T-1)}{R_T}, \\ &\approx Z_T\left(\frac{1}{R} - \frac{1}{x_1}\right) + Z_P\left(\frac{1}{R} - \frac{1}{s_2}\right) + \left(\frac{1}{r_{12}} - \frac{1}{R}\right). \end{aligned} \tag{3}$$

When the aggregates P and T are far apart, they interact through a residual Coulomb potential $\frac{(Z_P-1)(Z_T-1)}{R_T}$. According to the prescriptions of collision theory [22], this asymptotic potential has to appear in the initial channel Hamiltonian (H_i). However, the initial perturbation potential V_i is obtained by subtracting the asymptotic potential from the total interaction potential between projectile and target. So, in the initial channel V_i decreases much faster than the Coulomb interaction at large internuclear distance ($\vec{R}$). In the exit channel, the target is a bare ion. Thus, H_f and V_f can be written as

$$\begin{aligned} H_f &= -\frac{1}{2\mu_f}\nabla^2_{R_p} + \frac{Z_T(Z_P-2)}{R_P} - \frac{1}{2b}\nabla^2_{s_1} \\ &\quad -\frac{1}{2b}\nabla^2_{s_2} - \frac{Z_p}{s_1} - \frac{Z_p}{s_2} + \frac{1}{r_{12}}, \\ V_f &= \frac{Z_P Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} - \frac{Z_T(Z_P-2)}{R_P} \\ &\approx \frac{2Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2}, \end{aligned} \tag{4}$$

where

$$\mu_i = \frac{(1+M_P)(M_T+1)}{(2+M_P+M_T)}, \quad \mu_f = \frac{M_T(2+M_P)}{(2+M_P+M_T)},$$
$$a = \frac{M_T}{1+M_T}, \quad b = \frac{M_P}{1+M_P}.$$

The prior form of the scattering amplitude may be written in the form

$$T^{(-)}_{if} = \langle\psi^-_f|V_i|\psi_i\rangle. \tag{5}$$

Here the wave function in the initial channel is given by

$$\psi_i(\vec{R}_T,\vec{x}_2,\vec{s}_1) = \phi_T(\vec{x}_2)\phi_P(\vec{s}_1)\chi^+_i(\vec{R}_T),$$

where $\phi_T(\vec{x}_2)$ and $\phi_P(\vec{s}_1)$ are the target bound state and the projectile bound state wave functions, respectively. $\chi^+_i(\vec{R}_T)$ is the Coulomb distorted wave for the relative motion of P and T in the center-of-mass frame of the whole system which satisfies the equation

$$\left[-\frac{1}{2\mu_i}\nabla^2_{R_T} + \frac{(Z_P-1)(Z_T-1)}{R_T} - \frac{k_f^2}{2\mu_i}\right]\chi^+_i(\vec{R}_T) = 0. \tag{6}$$

Solving this equation, we find

$$\chi_i^+(\vec{R}_T) = e^{-\frac{\pi}{2}\alpha_3}\Gamma(1+i\alpha_3)e^{i\vec{k}_i\cdot\vec{R}_T} \times {}_1F_1\{-i\alpha_3;\ 1;\ i(k_iR_T - \vec{k}_i\cdot\vec{R}_T)\}, \quad (7)$$

where $\alpha_3 = \frac{(Z_P-1)(Z_T-1)}{v_i}$. Furthermore, $\vec{k}_i$ is the initial wave vector. The electron in the projectile is passive. The passive electron plays the role of screening the projectile ion. However, the interaction of the target ion with the screened projectile ion and that between the active electron and the projectile core are described by the Coulomb continuum wave functions in the final channel. The Coulomb continuum wave function in the final channel $\psi_f^{(-)}$ is given by

$$\psi_f^{(-)} = e^{\frac{\pi}{2}(\alpha_1-\alpha_2)}\Gamma(1+i\,\alpha_1)\Gamma(1-i\,\alpha_2) \times e^{i\vec{k}_f\cdot\vec{R}_p}\phi_f(\vec{s}_1,\vec{s}_2)\,{}_1F_1\{-i\alpha_1;\ 1;\ -i(v_fx_2+\vec{v}_f\cdot\vec{x}_2)\} \times {}_1F_1\{i\,\alpha_2;\ 1;\ -i(k_fR_T+\vec{k}_f\cdot\vec{R}_T)\}, \quad (8)$$

where

$$\alpha_1 = \frac{Z_T}{v_f}, \quad \alpha_2 = \frac{Z_T(Z_P-1)}{v_f}.$$

Here $\phi_f(\vec{s}_1,\vec{s}_2)$ is the bound-state wave function of the atomic system (Zp; e_1, e_2). The bound-state wave function of Li^+ or He, i.e., $\phi_f(\vec{s}_1,\vec{s}_2)$, may be written as [23] a set of two-electron hydrogenic configurations $\phi_{\lambda,\lambda'}(\vec{s}_1,\vec{s}_2)$.

$$\varphi_{\lambda,\lambda'}(\vec{s}_1,\vec{s}_2) = \sum_{\lambda\leqslant\lambda'} a^f_{\lambda\lambda'}\,\varphi^f_{\lambda\lambda'}(\vec{s}_1,\vec{s}_2),$$

where $\phi^f_{\lambda\lambda'}$ is a configuration with the same symmetry as ϕ_f.

$$\phi^f_{\lambda\lambda'}(\vec{s}_1,\vec{s}_2) = N_f\{R_{n_\lambda l_\lambda}(s_1)R_{n_{\lambda'}l_{\lambda'}}(s_2)Y^{LM}_{l_\lambda l_{\lambda'}}(\hat{s}_1,\hat{s}_2) + (-1)^\delta R_{n_{\lambda'}l_{\lambda'}}(s_1)R_{n_\lambda l_\lambda}(s_2)Y^{LM}_{l_{\lambda'}l_\lambda}(\hat{s}_1,\hat{s}_2)\}\,. \quad (9)$$

Here the constant

$$N_f = \frac{1}{\sqrt{2}} \quad \text{for} \quad \lambda\neq\lambda'$$
$$= \frac{1+(-1)^{L+S}}{4} \quad \text{for} \quad \lambda=\lambda' \text{ and } \delta=L+S-l_\lambda-l_{\lambda'}.$$

$\hat{s}_k(k=1,2)$ is the direction of the vector $\vec{s}_k$; $R_{n_\lambda l_\lambda}(s_k)$ and $Y^{LM}_{l_\lambda l_{\lambda'}}(\hat{s}_1,\hat{s}_2)$ are radial hydrogenic function and spherical harmonics, respectively.

The transition amplitude in the post form can be written as

$$T^{(+)}_{if} = \langle\psi_f|V_f|\psi_i^+\rangle, \quad (10)$$

where ψ_f is the wave function in the final channel which is given by $\psi_f = \phi_f(\vec{s}_1,\vec{s}_2)\chi_f^-(\vec{R}_P)$. $\phi_f(\vec{s}_1,\vec{s}_2)$ is the final bound-state wave function and $\chi_f^-(\vec{R}_P)$, the Coulomb distorted wave in the exit channel, is given by

$$\chi_f^-(\vec{R}_P) = e^{-\frac{\pi}{2}\alpha_3}\Gamma(1-i\alpha_3)e^{i\vec{k}_f\cdot\vec{R}_p} \times {}_1F_1\{i\alpha_3;\ 1;\ -i(k_fR_P+\vec{k}_f\cdot\vec{R}_P)\}, \quad (11)$$

where $\alpha_3 = \frac{Z_T(Z_P-2)}{v_f}$. $\vec{k}_f$ is the final wave vector. Here, the passive electron in the projectile plays the role of screening the projectile ion in the initial channel. However, the interaction of the active electron and the target ion with the screened projectile ion are described by the Coulomb continuum wave functions. So, the wave function in the initial channel may be given by

$$\psi_i^+ = e^{\frac{\pi}{2}(\alpha_1-\alpha_2)}\Gamma(1-i\alpha_1)\Gamma(1+i\alpha_2)e^{i\vec{k}_i.\vec{R}_T}\phi_i(\vec{x}_2,\vec{s}_1) \times {}_1F_1\{i\alpha_1;1;i\,(v_is_2+\vec{v}_i\cdot\vec{s}_2)\} \times {}_1F_1\{-i\alpha_2;\ 1;\ ia(k_iR_P-\vec{k}_i\cdot\vec{R}_P)\}, \quad (12)$$

where $\alpha_1 = \frac{(Z_P-1)}{v_i}$, $\alpha_2 = \frac{Z_T(Z_P-1)}{v_i}$.

Here $\phi_i(\vec{x}_2,\vec{s}_1) = \phi_T(\vec{x}_2)\phi_p(\vec{s}_1)$. $\phi_T(\vec{x}_2)$ and $\phi_p(\vec{s}_1)$ are the hydrogenlike wave functions for the target and the projectile, respectively. The transition amplitudes in the prior and post forms for single-electron capture in the BCCIS-4B theory may be written as

$$T^{\text{BCCIS}(-)}_{if} = N\int\!\!\int\!\!\int d\vec{s}_1d\vec{x}_2d\vec{R}e^{i\vec{k}_i\cdot\vec{R}_T-i\vec{k}_f\cdot\vec{R}_p}\varphi^*_f(\vec{s}_1,\vec{s}_2)_1F_1\{i\alpha_1;\ 1;\ i(v_fx_2+\vec{v}_f\cdot\vec{x}_2)\}_1F_1\{-i\alpha_2;\ 1;\ i(k_fR_T+\vec{k}_f\cdot\vec{R}_T)\} \times\left\{Z_T\left(\frac{1}{R}-\frac{1}{x_1}\right)+Z_P\left(\frac{1}{R}-\frac{1}{s_2}\right)+\left(\frac{1}{r_{12}}-\frac{1}{R}\right)\right\}\varphi_i(\vec{x}_2,\vec{s}_1)_1F_1\{-i\alpha_3;\ 1;\ i(k_iR_T-\vec{k}_i\cdot\vec{R}_T)\}, \quad (13)$$

where

$$N = e^{\frac{\pi}{2}(\alpha_1-\alpha_2-\alpha_3)}\Gamma(1-i\alpha_1)\Gamma(1+i\alpha_2)\Gamma(1+i\alpha_3), \quad \alpha_1=\frac{Z_T}{v_f}, \quad \alpha_2=\frac{Z_T(Z_P-1)}{v_f}, \quad \text{and} \quad \alpha_3=\frac{(Z_P-1)(Z_T-1)}{v_i},$$

and

$$T^{\text{BCCIS}(+)}_{if} = N\int\!\!\int\!\!\int d\vec{s}_1d\vec{s}_2d\vec{R}e^{i\vec{k}_i.\vec{R}_T-i\vec{k}_f.\vec{R}_p}\varphi^*_f(\vec{s}_1,\vec{s}_2)\,{}_1F_1\{-i\alpha_3;\ 1;\ i(k_fR+\vec{k}_f\cdot\vec{R})\}\left(\frac{2Z_T}{R}-\frac{Z_T}{x_1}-\frac{Z_T}{x_2}\right)\varphi_i(\vec{x}_2,\vec{s}_1) \times {}_1F_1\{i\alpha_1;\ 1;\ i(v_is_2+\vec{v}_i.\vec{s}_2)\}\,{}_1F_1\{-i\alpha_2;\ 1;\ ia(k_iR_P-\vec{k}_i\cdot\vec{R}_P)\}, \quad (14)$$

where

$$N = e^{\frac{\pi}{2}(\alpha_1-\alpha_2-\alpha_3)}\Gamma(1-i\alpha_1)\Gamma(1+i\alpha_2)\Gamma(1+i\alpha_3), \quad \alpha_1=\frac{(Z_P-1)}{v_i}, \quad \alpha_2=\frac{Z_T(Z_P-1)}{v_i},$$

and

$$\alpha_3 = \frac{Z_T(Z_P - 2)}{v_f}.$$

Using the integral representation of confluent hypergeometric function, the technique of Fourier transform, a Feynman parametric integral such as $\frac{1}{a'b'} = \int_0^1 \frac{dx}{[a'x+(1-x)b']^2}$, and applying the Lewis integral [24], respectively, Eqs. (13) and (14) can be expressed in both prior and post forms as

$$T_{if}^{\mathrm{BCCIS}(\pm)} = 32C' N \frac{1}{2\pi i} \oint dt_3 t_3^{-i\alpha_3 - 1}(t_3 - 1)^{i\alpha_3} \lim_{\beta_1,\,\varepsilon_1 \to 0} D(\beta_1,\delta_2,\gamma_1,\gamma_2,\varepsilon_1) \int_0^1 \frac{dx}{\Delta} \int_0^\infty dy K, \tag{15}$$

where

$$K = -\frac{1}{A}\left(\frac{A}{A+B}\right)^{i\alpha_1}\left(\frac{A}{A+D}\right)^{-i\alpha_2} {}_2F_1\left\{i\alpha_1;\ -i\alpha_2;\ 1;\ \frac{P}{Q}\right\},\quad P = BD - AC,\quad Q = (A+B)(A+D),$$

$$\Delta^2 = \left\{\frac{\vec{k}_f}{2+M_p} - (1-b)\vec{k}_i\right\}^2 x(1-x) + \lambda_1^2 x + (1-x)\beta_1^2,$$

$\lambda_1 = \gamma_1' + \gamma_1$ for the prior form and

$$\Delta^2 = \left\{\frac{\vec{k}_f}{2+M_p} - \frac{\vec{k}_i}{1+M_T}\right\}^2 x(1-x) + \lambda_1^2 x + (1-x)\beta_1^2 \quad \text{for the post form.}$$

Here A, B, C, and D in prior form (–) and post form (+) are given by

$$A^{\pm} = A_1^{\pm} y^2 + 2y(\beta^{\pm} A_1^{\pm} + A_{22}^{\pm} + A_{23}^{\pm}) + A_3^{\pm},\quad B^{\pm} = B_1^{\pm} y^2 + 2y(\beta^{\pm} B_1^{\pm} + B_{22}^{\pm} + B_{23}^{\pm}) + B_3^{\pm},$$

$$C^{\pm} = C_1^{\pm} y^2 + 2y(\beta^{\pm} C_1^{\pm} + C_{22}^{\pm} + C_{23}^{\pm}) + C_3^{\pm},\quad D^{\pm} = D_1^{\pm} y^2 + 2y(\beta^{\pm} D_1^{\pm} + D_{22}^{\pm} + D_{23}^{\pm}) + D_3^{\pm},$$

where in prior form, $\beta^- = \gamma_2$,

$$A_1^- = q_-^2 + (\delta_2 + \Delta + \varepsilon_1)^2 - 2\vec{q}_- \cdot \vec{v}_f t_1 - 2i\, v_f t_1(\delta_2 + \Delta + \varepsilon_1),$$
$$B_1^- = -2\vec{q}_- \cdot \vec{k}_f + 2\vec{v}_f \cdot \vec{k}_f t_1 - 2ik_i(\delta_2 + \Delta + \varepsilon_1) - 2v_f k_f t_1,\quad C_1^- = 2\vec{q}_- \cdot \vec{k}_i - 2\vec{v}_f \cdot \vec{k}_i t_1 - 2ik_i(\delta_2 + \Delta + \varepsilon_1) - 2v_f k_i t_1,$$
$$D_1^- = -2k_i k_f - 2\vec{k}_i \cdot \vec{k}_f,\quad A_{22}^- = \beta_2^-\{q_-^2 + (\Delta + \varepsilon_1)^2 + \gamma_2^2\},\quad B_{22}^- = -2\beta_2^-\{\vec{q}_- \cdot \vec{k}_f + ik_f(\Delta + \varepsilon_1)\},$$
$$C_{22}^- = 2\beta_2^-\{\vec{q}_- \cdot \vec{k}_i - ik_i(\Delta + \varepsilon_1)\},\quad D_{22}^- = -2\beta_2^-(k_i k_f + \vec{k}_i \cdot \vec{k}_f),$$
$$A_{23}^- = (\Delta + \varepsilon_1)P_{23}^-,\quad B_{23}^- = -ik_f P_{23}^-,\quad C_{23}^- = -ik_i P_{23}^-,\quad D_{23} = 0,$$
$$A_3^- = E_{11}^-\{q_-^2 + (\Delta + \varepsilon_1 + \gamma_2)^2\},\quad B_3^- = -E_{11}^-\{2\vec{q}_- \cdot \vec{k}_f + 2ik_f(\Delta + \varepsilon_1 + \gamma_2)\},$$
$$C_3^- = E_{11}^-\{2\vec{q}_- \cdot \vec{k}_f - 2ik_i(\Delta + \varepsilon_1 + \gamma_2)\},\quad D_3^- = -2E_{11}^-\{\vec{k}_i \cdot \vec{k}_f + k_i k_f\}.$$

The terms $\vec{q}_-$, β_2^-, P_{23}^- and E_{11}^- can be explicitly written as

$$\vec{q}_- = \vec{k}_f\left(1 - \frac{x}{2+M_T}\right) - (1 + bx - x)\vec{k}_i,\quad \beta_2^- = \delta_2 - iv_f t_1,$$

$$P_{23}^- = \left\{\frac{\vec{k}_f}{2+M_P} + (1-a)\vec{k}_i\right\}^2 + \delta_2^2 + \gamma_2^2 - 2\vec{v}_f \cdot \left\{\frac{\vec{k}_f}{2+M_P} + (1-a)\vec{k}_i\right\} t_1 - 2i\, v_f\, \delta_2\, t_1,$$

$$E_{11}^- = P_{23}^- + 2\delta_2\gamma_2 - 2iv_f\gamma_2 t_1,$$

and in post form, $\beta^+ = \delta_2$,

$$A_1^+ = q_+^2 + (\gamma_2 + \Delta + \varepsilon_1)^2 + 2\vec{q}_+ \cdot \vec{v}_i t_1 - 2iv_i(\gamma_2 + \Delta + \varepsilon_1)t_1,\quad B_1^+ = 2\vec{q}_+ \cdot \vec{k}_i - 2ik_i(\gamma_2 + \Delta + \varepsilon_1),$$
$$C_1^+ = -2\vec{q}_+ \cdot \vec{k}_f - 2\vec{v}_i \cdot \vec{k}_f t_1 - 2ik_f(\gamma_2 + \Delta + \varepsilon_1) - 2v_i k_f t_1,\quad D_1^+ = -2\vec{k}_i \cdot \vec{k}_f - 2k_i k_f,$$
$$A_{22}^+ = \lambda_2^+\{q_+^2 + (\Delta + \varepsilon_1)^2 + \delta_2^2\},\quad B_{22}^+ = \lambda_2^+\{\vec{q}_+ \cdot \vec{k}_i - 2ik_i(\Delta + \varepsilon_1)\},$$
$$C_{22}^+ = \lambda_2^+\{\vec{q}_+ \cdot \vec{k}_f - 2ik_f(\Delta + \varepsilon_1)\},\quad D_{22}^+ = -2\lambda_2^+\{\vec{k}_i \cdot \vec{k}_f + k_i k_f\},$$
$$A_{23}^+ = (\Delta + \varepsilon_1)P_{23}^+,\quad B_{23}^+ = -ik_i P_{23}^+,\quad C_{23}^+ = -ik_f P_{23}^+,\quad D_{23}^+ = 0,$$
$$A_3^+ = E_{11}^+\{q_+^2 + (\delta_2 + \Delta + \varepsilon_1)^2\},\quad B_3^+ = 2E_{11}^+\{\vec{q}_+ \cdot \vec{k}_i - ik_i(\delta_2 + \Delta + \varepsilon_1)\},$$
$$C_3^+ = -2E_{11}^+\{\vec{q}_+ \cdot \vec{k}_f + ik_f(\delta_2 + \Delta + \varepsilon_1)\},\quad D_3^+ = -2E_{11}^+\{\vec{k}_i \cdot \vec{k}_f + k_i k_f\}.$$

The terms $\vec{q}_+$, λ_2^+, P_{23}^+, and E_{11}^+ can be explicitly written as

$$\vec{q}_+ = \vec{k}_f\left(1-\frac{x}{2+M_P}\right) - \vec{k}_i\left(1-\frac{x}{1+M_P}\right), \quad \lambda_2^+ = \gamma_2 - i\,v_i\,t_1,$$

$$P_{23}^+ = \left\{\frac{\vec{k}_f}{2+M_P} + \frac{\vec{k}_i}{1+M_T}\right\}^2 + \delta_2^2 + \gamma_2^2 - 2\vec{v}_i\cdot\left(\frac{\vec{k}_f}{2+M_P} + \frac{\vec{k}_i}{1+M_T}\right)t_1, \quad E_{11}^+ = P_{23}^+ + 2\delta_2\gamma_2 - 2i\,v_i\,\delta_2\,t_1.$$

Here the constant C' originates from the initial and final bound-state wave functions. $D(\beta_1,\delta_2,\gamma_1,\gamma_2,\varepsilon_1)$ is a parametric differential operator used to generate the excited-state wave functions. δ_2, γ_1 and γ_1', γ_2 are the orbital component of the initial and final bound-state wave functions. Finally, the total cross sections in prior form ($Q_{if}^{(-)}$) and post form ($Q_{if}^{(+)}$) are given by

$$Q_{if}^{(\pm)}(\pi a_0^2) = \frac{\mu_i\mu_f}{4\pi^2}\frac{k_f}{k_i}\int\left|T_{if}^{\mathrm{BCCIS}(\pm)}\right|^2 d\Omega, \qquad (16)$$

where $d\Omega$ is the solid angle around $\vec{k}_i$.

The transition amplitude contains three-dimensional integrals such as Lewis, Feynman, and a complex contour integration. The final real form of this complex contour integration (in t_3) in Eq. (15) may be written [25] as

$$\frac{1}{2\pi i}\oint dt_3 t_3^{-i\alpha_3-1}(t_3-1)^{i\alpha_3} f(t_3)\,dt_3,$$

$$t_3 \to \tau = \frac{e^{\pi\alpha_3}-e^{-\pi\alpha_3}}{2\pi i}\int_0^\infty\left\{\left[e^{i\alpha_3\tau}\phi\left(\frac{1}{e^\tau+1}\right)\right.\right.$$
$$\left.\left. + e^{-i\alpha_3\tau}e^{-\tau}\phi\left(\frac{1}{e^{-\tau}+1}\right)\right]\Big/\left(1+e^{-\tau}\right)\right\}d\tau + f(0), \quad (17)$$

where $e^\tau = (1-t_3)/t_3$, τ being the transformed integration variable, and $\phi(t_3) = f(t_3) - f(0)$.

The real two-dimensional integration in y and τ is finally carried out numerically. To evaluate the double integral (y and τ), we first perform the y integration by the Gauss quadrature method with different fixed values of τ, which are the Gauss Laguerre quadrature points required for the subsequent τ integration. The Feynman integral has been evaluated numerically with the 48-point Gauss-Legendre quadrature method. Finally, integration over the scattering angles has been performed with the 48-point Gauss-Legendre quadrature method. However, it may be mentioned that cross sections have finally been evaluated with an accuracy of 0.1%.

III. RESULTS AND DISCUSSION

The total single-electron capture cross sections for the process of the scattering between two hydrogenlike atomic systems were obtained by summing over all contributions (ground state ($1s^2$), singly excited states $1s2s$, $1s2p$) from individual shells and subshells up to $n = 2$, except the H + H collision as the H^- ion does not have any stable excited states. So only one state is to be taken into account in the capture process. The variation of single-electron capture cross sections of ground-state hydrogenlike ions by the impact of different projectile ions as a function of the incident energy ranging from 20 to 5000 keV/amu is plotted in Figs. 1–4, respectively using both prior and post forms of BCCIS-4B approximation. Post-prior discrepancy does not exceed 20% for all interactions above 70 keV/amu. Numerical computations are carried out for the following reactions:

$$\mathrm{H} + \mathrm{H} \to \mathrm{H}^-(1s^2) + \mathrm{H}^+, \qquad (18)$$
$$\mathrm{He}^+ + \mathrm{He}^+ \to \mathrm{He} + \mathrm{He}^{2+}, \qquad (19)$$
$$\mathrm{He}^+ + \mathrm{H} \to \mathrm{He} + \mathrm{H}^+, \qquad (20)$$
$$\mathrm{Li}^{2+} + \mathrm{H} \to \mathrm{Li}^+ + \mathrm{H}^+. \qquad (21)$$

The present results obtained for the reaction (18) are presented in Fig. 1 in both forms of BCCIS-4B approximation. Our computed results for total single-electron capture cross sections have also been compared with the measurements of McClure [26], Schryber [27], and Hill *et al.* [28] and with the theoretical results of Mancev [10] obtained by CB1-4B method, the continuum-intermediate-states approximation (CIS) of Banyard and Shirtcliffe [12], the CDW method of Moore and Banyard [29] using the Hartree-Fock (HF) function, the first Born approximation of Mapleton [30], and the couple-state results of Wang *et al.* [31]. The agreement between

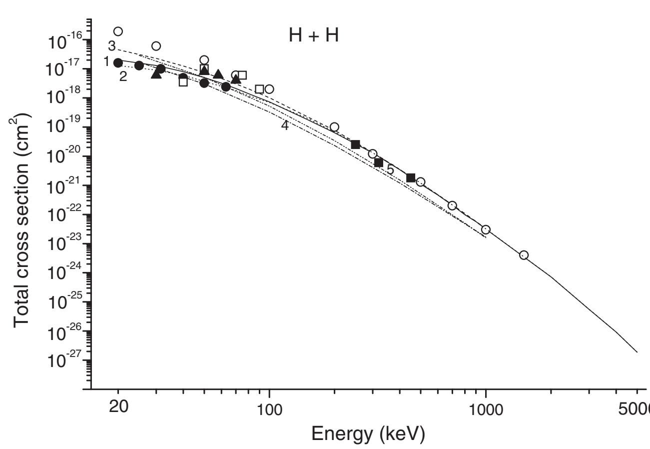

FIG. 1. Total cross sections (in cm^2) as a function of the incident energy E (keV) for reaction H + H($1s$)→H^- + H^+. Theory: (solid line, 1) present results (prior form of BCCIS-4B); (dotted line, 2) present results (post form of BCCIS-4B); (dashed line, 3) CB1-4B results of Mancev [10]; (dash-dotted line, 4) CIS-HF results of Banyard and Shirtcliffe [12]; (dash-dot-dotted line, 5) CDW-HF results of Moore and Banyard [29]; (open circle) first Born results of Mapleton [30]; (open square) couple state results of Wang *et al.* [31]. Experiments: (●) results of McClure [26]; (■) results of Schryber [27]; (▲) results of Hill *et al.* [28].

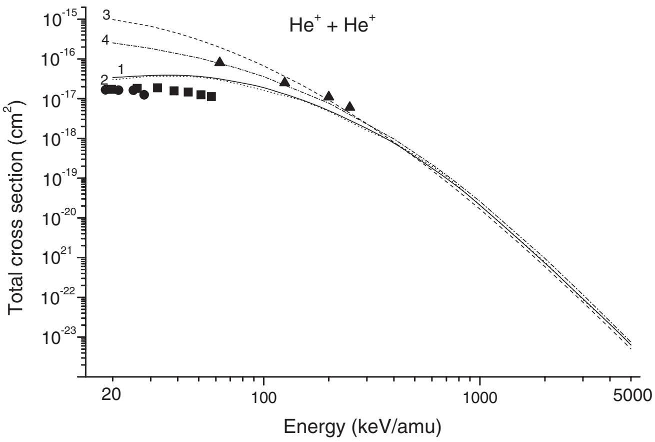

FIG. 2. Total cross sections (in cm^2) as a function of the incident energy E (keV/amu) for reaction $He^+ + He^+ \rightarrow He + He^{2+}$. Theory: (solid line, 1) present results (prior form of BCCIS-4B); (dotted line, 2) present results (post form of BCCIS-4B); (dashed line, 3) prior form of CDW-4B results of Mancev [19]; (dash-dotted line, 4) post form of CB1-4B results of Mancev [19]. Experiments: (■) results of Murphy *et al.* [34]; (•) results of Melchert *et al.* [35]; (▲) results of Schmidt-Bocking and Dorner [36] (data taken from Mancev [10]).

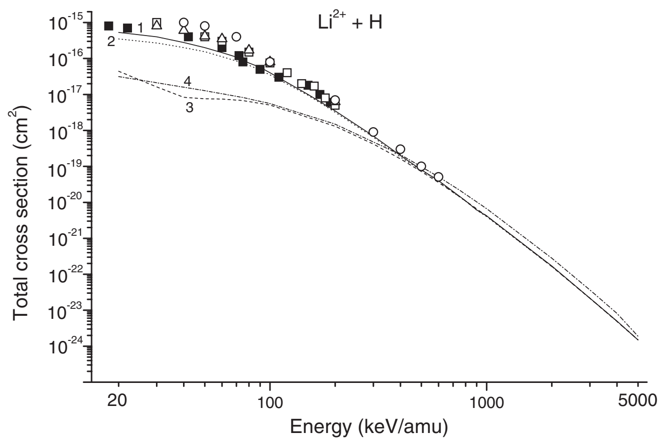

FIG. 4. Total cross sections (in cm^2) as a function of the incident energy E (keV/amu) for reaction $Li^{2+} + H(1s) \rightarrow Li^+ + H^+$. Theory: (solid line, 1) present results (prior form of BCCIS-4B); (dotted line, 2): present results (post form of BCCIS-4B); (dashed line, 3) prior form of CDW-4B results of Mancev [13]; (dash-dotted line, 4) post form of CB1-4B results of Mancev [19]; (open square) BCCIS-3B results of Purkait [6]; (open triangle) CTMC results of Purkait [6]; (open circle) results of Eichler *et al.* [4]. Experiments: (■) results of Shah *et al.* [40].

BCCIS-4B theory and experimental results [26–28] are found to be satisfactory in both low- and intermediate-energy ranges. Additional experimental results at higher impact energies are very much needed to provide a better test of our formalism. The CB1-4B results of Mancev [10] obtained by means of the Hylleraas wave function [32] for $H^-(1s^2)$ have a trend of departing from experimental data below 200 keV as collision energy decreases. This is expected because the formulation does not include intermediate continuum states which are very much important for the description of a charge transfer event. It is also observed that the present computed results using the Hylleraas wave function [32] agree with the theoretical results of Moore and Banyard [29], but agreement is not satisfactory with the CIS method of Banyard and Shirteliffe [12] using the HF function in the low-energy region. The reason may be attributed to the fact that the CIS method does not satisfy proper boundary conditions. However, the results of Mapleton [30] obtained by the two-parameter wave function of Chandrasekhar [33] in the first Born approximation overestimate the present findings at low energies. This feature is obvious because first Born approximation is valid at high energies. In Fig. 2, we have displayed the present results for another symmetric collision of He^+ with He^+ as a function of incident projectile energy. The present data are compared with the existing experimental results of Murphy *et al.* [34], Melchert *et al.* [35], Schmidt-Bocking and Dorner [36] [for the reverse reaction: $He^{2+} + He(1s^2) \rightarrow He^+(1s) + He^+(1s)$], and only the theoretical results of Mancev [19]. However, our calculated results are in better agreement with the experimental results [34,35] in comparison to other theoretical results [19], particularly at the lower side of the energy region under consideration, but agreement is poor with other experimental results [36] that have measured the cross sections for the reverse reaction. This discrepancy may be attributed to the principle of detail balancing. The theoretical results of Mancev using the CB1-4B [19] approximation agrees with the experimental results of Schmidt-Bocking and Dorner [36] (data taken from Ref. [10]), whereas the results obtained by the CDW-4B model [19] overestimate the experimental results [34–36] below 150 keV/amu. In the CDW-4B method, the electronic continuum intermediate states are included in both channels through the Coulomb waves but are not included in the CB1-4B method. However, the CDW-4B and CB1-4B

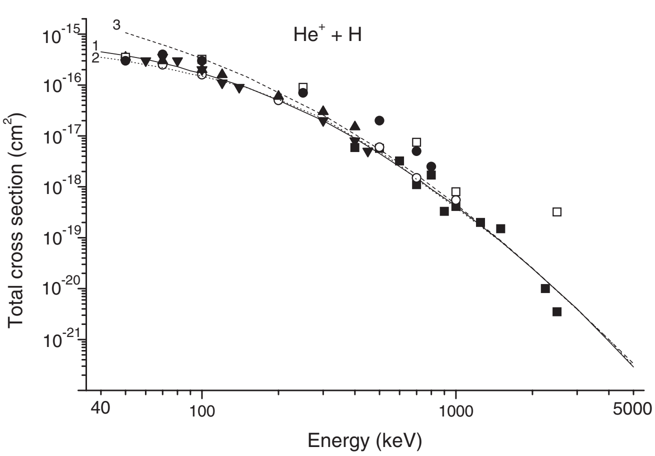

FIG. 3. Total cross sections (in cm^2) as a function of the incident energy E (keV) for reaction $He^+ + H(1s) \rightarrow He + H^+$. Theory: (solid line, 1) present results (prior form of BCCIS-4B); (dotted line, 2) present results (post form of BCCIS-4B); (dashed line, 3) CDW-4B results of Mancev [18]; (open square) CTMC results of Becker and MacKellar [13]; (open circle) CB1-4B results of Mancev [10]. Experiments: (▲) results of Olson *et al.* [7]; (▼) results of Shah and Gilbody [37]; (•) results of Phaneuf *et al.* [38]; (■) results of Hvelplund and Andersen [39].

approximation may not be accurate at low energies. We have also observed that the ground-state capture is dominant as for symmetric collision. This is expected because of energy resonance and velocity matching of the active electron in the initial and final states. We find from Figs. 1 and 2 the post-prior discrepancy is within 20% above 60 keV/amu for the H + H collision and throughout the whole energy region for the $He^+ + He^+$ collision.

Now, we shall study our computed results for the asymmetric reactions given by reactions (20) and (21). In Fig. 3, we have displayed the present results along with other available experimental and theoretical data for collision $He^+ + H$. From Fig. 3, it is evident that the present computed results show overall good agreement with the experimental results [7,37–39]. The results obtained by the CDW-4B approximation [18] overestimate the present computed results below 500 keV as the CDW-4B approximation may not be valid in the low-energy range. The CTMC results of Becker and MacKeller [13] overestimate all the available results to a significant extent because classical treatment of a two-electron collision system may not be accurate. It may be seen from Fig. 3 that the present results show good agreement with the theoretical results of Mancev [10] in the whole energy range. In such case the post-prior discrepancy is less than 20% above 70 keV/amu. For the $Li^{2+} + H$ collision, the present computed results in both forms are presented in graphical form in Fig. 4. We have compared our theoretical results with only the experimental results [40] and theoretical results [4,6,19]. It is evident that the present results show good agreement with the experimental results. However, a comparison of the CDW-4B and CB1-4B models of Mancev [19] with the measurements shows that the theoretical curves underestimate experimental data, especially at lower impact energy (less than 400 keV/amu). The results obtained by the method of three-body formalism of the BCCIS approximation in prior form and the CTMC method [6] have a similar trend with the present BCCIS-4B model. In both these methods [6], the interactions of the active electron in the target with incoming projectile ions have been taken by a suitable potential containing both a long-range part and a short-range part. However, such a BCCIS-3B model cannot yield any information about the relative significance of the role of the dynamic electron-electron correlation in collisions under study. As may be expected, the theoretical results of Eichler *et al.* [4] using the Oppenheimer-Brinkman-Kramers (OBK) approximation are not in agreement with the present results. We have observed that the maximum contribution of total capture cross sections occur at $n = 2$ state for $Li^{2+} + H$ collision in the low-energy range. The capture peak in the individual state may be explained in terms of the binding energy matching and the momentum distribution of the active electron in the initial and final state, respectively.

IV. CONCLUSIONS

We have calculated cross sections for the capture of $1s$ electrons by hydrogenlike projectile ions using the BCCIS-4B approximation in both the prior and post forms in the collision energy range of 20–5000 keV/amu. The present computed results are in satisfactory agreement with the experimental observations. The reasons for such success are the following: (i) The continuum state of the active electron has been taken into account properly; (ii) the boundary condition for the scattering wave function has also been satisfied; and (iii) the potential is faster falling than the Coulomb potential. In the presented four-body formalisms, the dynamic electron correlations are automatically included through the perturbation potentials. However, more experimental data covering higher energies is needed for the above-mentioned interactions both for the development of refined theory and their applications in other branches of physics.

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