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Double electron capture cross-sections of the ground state in the collisions of He^{2+} and Li^{3+} with He

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Abstract. We investigate the problem of the double charge transfer cross-section of a helium atom by bare ions of helium and lithium at energies ranging from 60 to 200 keV/amu. The boundary corrected continuum intermediate state approximation (BCCIS) is used to calculate the capture cross-section in the ground state. The continuum state of each electron has been accounted for in the formalism. The present results are compared with existing theoretical and experimental results.

PACS. 34.70.+e Charge transfer

1 Introduction

Double charge transfer in collisions of fully stripped ions with atoms has attracted a great deal of both theoretical [1–5] and experimental works [6–8] for more than a decade. In most of the cases, the chosen target atom is the helium atom. In particular, studies on collisions of He^{2+} with He atom are important both from academic point of view as well as practical applications. From application point of view, this resonant double charge transfer process is one of the most important processes in the determination of transport properties of doubly charged ions in controlled high-temperature thermonuclear fusion plasma and the energy balance therein. Double electron capture cross-sections have been calculated quantum mechanically by McGuire and Weaver [9], Gayet et al. [1] and Ghosh et al. [2]. Adopting the same principle, Chatterjee and Roy [10] and Olson [11] have studied two electron capture in the framework of classical mechanics. Crother and McCarrol [12] have employed the continuum distorted wave (CDW) approximation with a view to include continuum-continuum coupling into the scheme with the continuum correlation between the active electrons adopted through the Pluvinage [13] wavefunction. Gravielle and Miraglia [3] have formulated the problem in the framework of the impulse approximation in such a way that double electron capture takes place through a singly excited state of the target atom. The four-body formulation (4B) is basically the extension of the 3-body formulation of collision problems in the framework of different approximations applied at high energies. Belkic [5] has calculated the double electron capture cross-sections in the ground state in collisions of He^{2+} and Li^{3+} with He atoms within the Coulomb-Born (CB) approximation in the energy range of 250–2000 keV respectively. This was subsequently extended to the boundary corrected continuum intermediate state (BCIS) approximation [4] originally proposed by Mandal et al. [14] into the four-body formalism of the He^{2+}+He collision. In doing so, he made a simplifying replacement of an exact on-shell coulomb wave for relative motion by an eikonal phase and as such, he failed to provide any cross-section data below a projectile energy of 700 keV. Gayet et al. [1] have calculated the double electron capture cross-sections for the abovementioned processes in the framework of a continuum distorted wave with an eikonal initial state (CDW-EIS) in the energy range of 0.4–30 MeV. They have calculated the two electron capture cross-sections in the ground, singly and doubly excited states. However, the results of Gayet et al. are lower by an order of magnitude in comparison with experimental observations. Under such circumstances, we are interested in studying such a double electron capture process in the collision of heavy ions with atoms in the framework of the BCCIS-4B theory. The essence of the theory lies in the fact that (i) it satisfies the correct boundary condition and (ii) the continuum state of each electron has been accounted for within the formalism.

The organization of the paper is as follows. The theoretical formulation is discussed in Section 2. The calculated results are discussed with graphs in Section 3. Finally it ends with some concluding remarks in Section 4. Atomic units are used unless otherwise stated.

2 Theoretical formalism

A collision diagram is shown in Figure 1. The total Hamiltonian of the whole system may be written in terms

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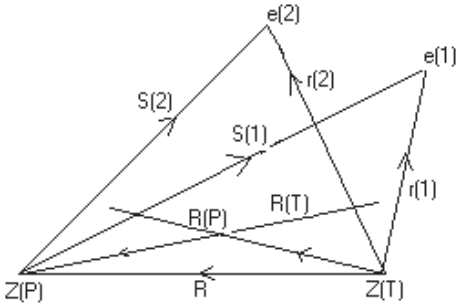

Fig. 1. Coordinate representation for the reaction of He^{2+}, Li^{3+} with a He atom.

of channel Hamiltonians (initial and final) and channel interactions (initial and final) in the form

$$H = \underbrace{H_0 - \frac{Z_T}{r_1} - \frac{Z_T}{r_2} + \frac{1}{r_{12}}}_{H_i} + \underbrace{\frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}}_{V_i} \quad \text{(1a)}$$

(entrance channel)

$$= \underbrace{H_0 - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} + \frac{1}{s_{12}}}_{H_f} + \underbrace{\frac{Z_P Z_T}{R} - \frac{Z_T}{r_1} - \frac{Z_T}{r_2}}_{V_f} \quad \text{(1b)}$$

(exit channel)

where the total kinetic energy operator, H_0 may be written as

$$H_0 = -\frac{1}{2\mu_i}\nabla^2_{R_T} - \frac{1}{2a}\nabla^2_{r_1} - \frac{1}{2a}\nabla^2_{r_2} \quad \text{(2a)}$$

(entrance channel)

$$= -\frac{1}{2\mu_f}\nabla^2_{R_P} - \frac{1}{2b}\nabla^2_{s_1} - \frac{1}{2b}\nabla^2_{s_2} \quad \text{(2b)}$$

(exit channel).

Here μ_i, μ_f, a and b are the appropriate reduced masses associated with the relative coordinates $\vec{R}_T$, $\vec{R}_P$, $\vec{r}_i$ (i = 1, 2) and $\vec{s}_i$ (i = 1, 2) respectively. A transition amplitude may be defined as

$$T_{if}^{(-)} = \langle \psi_f^- | V_i | \psi_i \rangle, \quad \text{where} \quad \psi_i = e^{i\vec{K}_i\cdot\vec{R}_T}\varphi_i(r_1, r_2) \quad (3)$$

and the total scattering wave function in the exit channel satisfies the Schrödinger equation

$$H\psi_f^- = E\psi_f^-. \quad (4)$$

We can made the approximation,

$$\psi_f^- = \psi_f^{BCCIS(-)}. \quad (5)$$

There $\psi_f^{BCCIS(-)}$ is the approximate form of the total wave function of the whole collisional system in the on-shell approximation and may be written as

$$\psi_f^{BCCIS(-)} = N e^{i\vec{K}_f\cdot\vec{R}_P}\varphi_f(\vec{s}_1, \vec{s}_2) \times {}_1F_1\{i\alpha_1; 1; i(v_f r_1 + \vec{v}_f\cdot\vec{r}_1)\}\,{}_1F_1\{i\alpha_2; 1; i(v_f r_2 + \vec{v}_f\cdot\vec{r}_2)\} \times {}_1F_1\{-i\alpha_3; 1; i(K_f R_T + \vec{K}_f\cdot\vec{R}_T)\} \quad (6)$$

where $\alpha_1 = \alpha_2 = Z_T/v_f$ and $\alpha_3 = Z_P Z_T/v_f$.

So the transition amplitude for the two-electron transition may be written as

$$T_{if}^{BCCIS(-)} = A\int d\vec{r}_1 d\vec{r}_2 d\vec{R}\, e^{i\vec{K}_f\cdot\vec{R}_P}\varphi_f^*(\vec{s}_1, \vec{s}_2) \times {}_1F_1\{i\alpha_1; 1; i(v_f r_1 + \vec{v}_f\cdot\vec{r}_1)\}\,{}_1F_1\{i\alpha_2; 1; i(v_f r_2 + \vec{v}_f\cdot\vec{r}_2)\} \times {}_1F_1\{-i\alpha_3; 1; i(K_f R_T + \vec{K}_f\cdot\vec{R}_T)\} V_i e^{i\vec{K}_i\cdot\vec{R}_T}\varphi_i(\vec{r}_1, \vec{r}_2) \quad (7)$$

where A is a constant connected with the normalization of three confluent hypergeometric functions. In the case of a heavy particle collision, it has been shown [15] that

$${}_1F_1\{-i\alpha, 1; i(K_f R_T + \vec{K}_f\cdot\vec{R}_T)\} \approx {}_1F_1\{-i\alpha; 1; i(K_f R + \vec{K}_f\cdot\vec{R})\}. \quad (8)$$

Using the integral representation of the confluent hypergeometric function, the transition matrix element may be written as

$$T_{if}^{BCCIS(-)} = \frac{N}{(2\pi\, i)^3}\lim_{\varepsilon\to 0}\Theta\left(\varepsilon, \delta_1, \delta_2, \lambda_1, \lambda_2\right) \times \oint dt_1\, t_1^{i\alpha_1 - 1}(t_1 - 1)^{-i\alpha_1}\oint dt_2\, t_2^{i\alpha_2 - 1}(t_2 - 1)^{-i\alpha_2} \times \oint dt_3\, t_3^{-i\alpha_3 - 1}(t_3 - 1)^{i\alpha_3} J \quad (9)$$

where N is some constant originating from the initial and final bound state wave functions and the normalization of confluent hypergeometric function. $\Theta\left(\varepsilon, \delta_1, \delta_2, \lambda_1, \lambda_2\right)$ is the parametric differential operator used to generate the appropriate wave functions. Here the explicit form of J may be written as

$$J = \int d\vec{r}_1 d\vec{r}_2 d\vec{R}\, e^{i\vec{K}_i\cdot\vec{R}_T}\, e^{-i\vec{K}_f\cdot\vec{R}_P}\, e^{it_1\vec{v}_f\cdot\vec{r}_1} e^{it_2\vec{v}_f\cdot\vec{r}_2} \times e^{it_3\vec{K}_f\cdot\vec{R}}\frac{e^{-\beta_1 r_1}}{r_1}\frac{e^{-\beta_2 r_2}}{r_2}\frac{e^{-\lambda_1 s_1}}{s_1}\frac{e^{-\lambda_2 s_2}}{s_2}\frac{e^{-\lambda_3 R}}{R} \quad (10)$$

where $\beta_1 = \delta_1 - it_1 v_f$, $\beta_2 = \delta_2 - it_2 v_f$, and $\lambda_3 = \varepsilon - it_3 K_f$.

Taking the Fourier transform of terms involving r_1, r_2, s_1, s_2 and R and using the properties of the delta function,

J may be reduced to

$$J = \frac{16}{\pi} \times \int \frac{d\vec{q}_1 d\vec{q}_2}{(q_1^2+\lambda_1^2)(q_2^2+\lambda_2^2)\{|\vec{q}_1-\vec{p}_1|^2+\beta_1^2\}\{|\vec{q}_2-\vec{p}_2|^2+\beta_2^2\}} \times \frac{1}{\{|\vec{q}_1+\vec{q}_2-\vec{p}_3|^2+\lambda_3^2\}} \quad (11)$$

where $\vec{p}_1 = \vec{p} - t_1\vec{v}_f$, $\vec{p}_2 = \vec{p} - t_2\vec{v}_f$, $\vec{p}_3 = \vec{K}_i + t_3\vec{K}_f - b\vec{K}_f$, and $\vec{p} = \vec{K}_i/(2+m_T) + \vec{K}_f/(2+m_P)$.

The integral equation (11) is calculated by using the Feynman parameterization technique such as

$$\frac{1}{(q_1^2+\lambda_1^2)\ \{|\vec{q}_1-\vec{p}_1|^2+\beta_1^2\}} = \int_0^1 \frac{dx}{\{|\vec{q}_1 - x\vec{p}_1|^2+\Delta^2\}^2} \quad (12)$$

where $\Delta^2 = \beta_1^2 x + \lambda_1^2(1-x) + x(1-x)p_1^2$.

Using the simple analytical result of the two-denominator integral in the form [16,17], we can calculate the $\vec{q}_1$ integration,

$$\int \frac{d\vec{q}_1}{\{|\vec{q}_1 - x\vec{p}_1|^2+\Delta^2\}^2\ \{|\vec{q}_1+\vec{q}_2-\vec{p}_3|^2+\lambda_3^2\}} = \frac{\pi^2}{\Delta}\frac{1}{\left\{|\vec{q}_2-\vec{p}_3+x\vec{p}_1|^2+(\lambda_3+\Delta)^2\right\}}. \quad (13)$$

Therefore equation (11) becomes

$$J = 16\pi \int_0^1 \frac{dx}{\Delta} \times \int \frac{d\vec{q}_2}{(q_2^2+\lambda_2^2)\ \{|\vec{q}_2-\vec{p}_2|^2+\beta_2^2\}\ \{|\vec{q}_2-\vec{p}_2'|^2+\Delta_1^2\}} \quad (14)$$

where $\vec{p}_2' = \vec{p}_3 - x\vec{p}_1$ and $\Delta_1 = \lambda_3 + \Delta$.

Applying the Lewis integral representation [17] we can express equation (14) as

$$J = 32\pi^3 \int_0^1 \frac{dx}{\Delta} \int_0^\infty \frac{dy}{a'y^2+2b'y+c'} \quad (15)$$

where,

$$a' = |\vec{p}_2' - \vec{p}_2|^2 + (\Delta_1+\beta_2)^2$$
$$b' = \lambda_2 a + \beta_2\left(\lambda_2^2+p_2^2+\Delta_1^2\right) + \Delta_1\left(\lambda_2^2+p_2'^2+\beta_2^2\right)$$
$$c' = \left\{p_2^2+(\lambda_2+\Delta_1)^2\right\}\left\{p_2'^2+(\lambda_2+\beta_2)^2\right\}.$$

We have simplified the terms a', b' and c' in such a way that each term comes out to be a linear function of t_2 and t_3 only. So we can express equation (15) as

$$J = 32\pi^3 \int_0^1 \frac{dx}{\Delta} \int_0^\infty \frac{dy}{A+Bt_2+Ct_3+Dt_2t_3}. \quad (16)$$

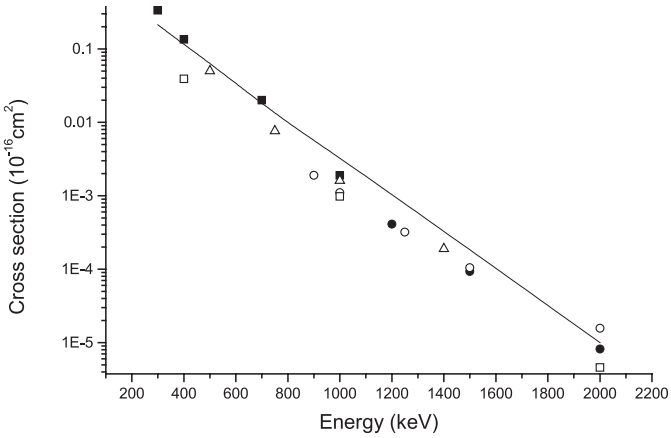

Fig. 2. Variation of the double charge transfer cross-sections as a function of energy for the interaction He^{2+}+He($1s^2$). Theory: (—) present results; (□) results of Gayet et al. [1]; (△) results of Gravielle and Miraglia [3]; (○) results of Belkic [5]. Experiment: (■) results of DuBois [6]; (●) results of de Castro et al. [7].

Finally, from equation (9), we may find

$$T_{if}^{BCCIS(-)} = 32\pi^3 N \lim_{\varepsilon\to 0} \Theta(\varepsilon, \delta_1, \delta_2, \lambda_1, \lambda_2) \times \frac{1}{2\pi i}\oint dt_1 t_i^{i\alpha_1-1}(t_1-1)^{-i\alpha_1} \int_0^1 \frac{dx}{\Delta}\int_0^\infty dy K \quad (17)$$

where

$$K = \frac{1}{(2\pi i)^2}\oint dt_2\, t_2^{i\alpha_2-1}\,(t_2-1)^{-i\alpha_2} \times \oint dt_3\, t_3^{-i\alpha_3-1}\,(t_3-1)^{i\alpha_3}\,\frac{1}{A+Bt_2+Ct_3+Dt_2t_3}. \quad (18)$$

Now the complex contour integration of equation (18) may be evaluated by applying Cauchy's residue theorem to obtain a general term in the form

$$K = -A^{i\alpha_2-i\alpha_3-1}(A+B)^{-i\alpha_2}(A+C)^{i\alpha_3} \times {}_2F_1\left(i\alpha_2, -i\alpha_3; 1; \frac{BC-AD}{(A+B)(A+C)}\right). \quad (19)$$

3 Results and discussions

The variation of the double electron capture cross-section as a function of the incident projectile energy is given in Figures 2 and 3. In all cases, the calculations have been carried out using the wavefunctions given by Lin et al. [18]. We have checked that, with the use of one, two and five parameter-variational wavefunctions of He by Lin et al. [18], the computed results agree within 7–10% at 200 and 1000 keV respectively. For this reason and due to lack of sufficient computational facilities, we have acquired all cross-sections with one parameter wavefunction

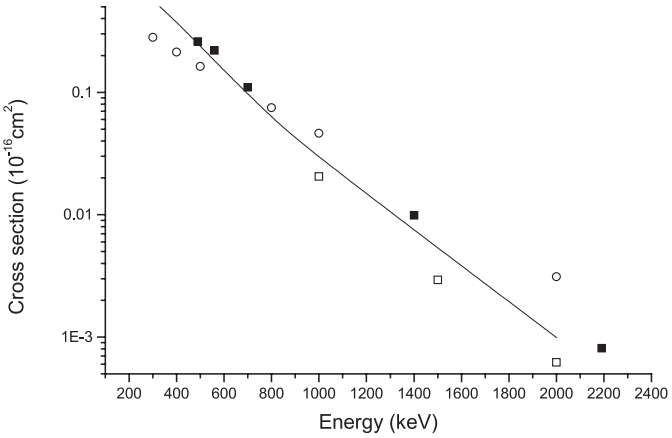

Fig. 3. Variation of the double charge transfer cross-section as a function of energy for the interaction Li^{3+}+He($1s^2$). Theory: (—) present results; (□) results of Gayet et al. [1]; (○) results of Belkic [5]; experiment: (■) results of Shah and Gilbody [8].

of He only. Here the three-dimensional integrals in the transition amplitude are Lewis, Feynman and a complex contour integration, which have been mentioned earlier. The Lewis integral and the Feynman integral are evaluated numerically with the 60-point and 48-point Gauss Legendre quadrature method respectively. The complex contour integration (t_1) in the final transition amplitude is transformed into a real one dimensional integral [19] from 0 to 1 which has been sub-divided into several parts and each sub-division is integrated using a 36-point Gauss Laguerre quadrature method which is reasonably accurate. Finally, integration over the scattering angles has been performed with the 44-point Gauss Legendre quadrature method which enable an accuracy of 1% for the integrated cross-sections to be obtained.

The variation of double charge transfer cross-sections with projectile energies are shown in Figure 2 for the He^{2+} ion and Figure 3 for the Li^{3+} ion along with the experimental results of de Castro et al. [7], DuBois [6], Shah and Gilbody [8] and the theoretical results of Graville and Miraglia [3], Belkic [4,5], Gayet et al. [1]. From Figure 2, we find that our theoretical results are in good agreement with the experimental results below 800 keV and at 2000 keV but is disagreement at 1200 keV. The results of the double electron capture cross-sections in the framework of the four-body version of the boundary corrected by the first Born (CB1) approximation are in disagreement below 1600 keV but agree well at high energy. Double electron capture cross-sections calculated by Gayet et al. [1] in the framework of the four-body continuum distorted wave (CDW-4B) approximation are in disagreement over an intermediate energy region but the divergence gradually diminishes as the projectile energy increases. From Figure 3 we can see that in the intermediate energy region, our results are favorable only with the experimental results of Shah and Gilbody [8], but above 900 keV, large discrepancies occur with both the theoretical results of Belkic [5] and Gayet et al. [1].

4 Concluding remarks

The theoretical findings in the framework of BCCIS-4B for double electron capture cross-sections in collisions of He^{2+}, Li^{3+} with He atoms have been found to be in reasonable agreement with other theoretical and experimental observations. The reasons for such success may be due to the following facts: (i) the total scattering wave function satisfies the proper boundary conditions, (ii) the perturbing potential falls faster than the coulomb potential and (iii) the intermediate continuum states of the two electrons have been taken into account. In this context it may be pointed that in such a formulation the dynamic correlation of the active electrons is absent in the process of two-electron transfer. Only the static correlation of the electron has been accounted for through the electron wave functions in the initial and final state respectively.

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