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CHARGE TRANSFER IN ENERGETIC Li^{2+} – H COLLISIONS

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Abstract. The total cross sections for charge transfer in $Li^{2+} - H$ collisions have been calculated, using the four-body first Born approximation with correct boundary conditions (CB1-4B) and four-body continuum distorted wave method (CDW-4B) in the energy range 10 - 5000 keV/amu. Present results call for additional experimental data at higher impact energies than presently available.

1. INTRODUCTION

The theoretical total cross sections for single electron capture in $Li^{2+} - H$ collisions are reported. Data for this process are of particular interest in fusion research. Heretofore there has been very little theoretical work especially for high impact energies. For $Li^{2+} - H$ collisions, previous theoretical work consists of calculations performed employing the following methods: three-body continuum distorted wave (CDW-3B) of the Belkić 1991, coupled-channel calculations in 'perturbative one-and-a-half-centre' (POHCE) formulation (Ford et al. 1982), modified continuum distorted wave (Crothers and Todd 1980), Oppenheimer-Brinman-Kramers approximation (Eichler et al. 1981). All quoted models reduced four-body problem to a three-body problem. Although some of these three-body models show a satisfactory agreement with experimental data, these methods completely neglect dynamic (i.e. collisional) correlations.

A substantially different approaches to the problem of high-energy electron capture from one- and multielectron atoms by hydrogen-like projectiles have recently been undertaken by Mančev, who introduced the four-body corrected first Born approximation (CB1-4B) approximation (Mančev 1995, 1996) and four-body Continuum Distorted Wave (CDW-4B) method (Mančev 2007). Different quantum-mechanical four-body methods for high-energy ion-atom collisions have recently been extensively discussed in review paper of Belkić et al. (2008).

Four-body treatments allow one to study the effects of the electron-electron correlation in single capture. Along this line the CDW-4B and CB1-4B approximations are utilized for investigating $Li^{2+} - H$ collisions, since the evidence of correlation effects in this process has not been previously assessed.

Atomic units will be used throughout unless otherwise stated.

2. THEORY

We examine single electron capture in collision between hydrogen-like projectiles:

$$(Z_P, e_1) + (Z_T, e_2) \longrightarrow (Z_P, e_1, e_2) + Z_T. \tag{1}$$

The parentheses $(\ldots)$ symbolize the bound states. 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). Further, let us denote by $\vec{R}$ the position vector of the Z_T with respect to Z_P. The vector of the distance between the two active electrons (e_1 and e_2) is denoted by $\vec{r}_{12} = \vec{x}_1 - \vec{x}_2 = \vec{s}_1 - \vec{s}_2$. In the entrance channel, it is convenient to introduce $\vec{r}_i$ as a the position vector between the center of mass of (Z_P, e_1) and target system. Symmetrically in the exit channel, let $\vec{r}_f$ is the position vector of the center of mass of (Z_P, e_1, e_2) system relative to Z_T. The transition amplitudes in the prior (-) and post (+) forms in the CDW-4B theory can be written as (Mančev 2007):

$$\begin{aligned} T_{if}^{+(CDW-4B)} &= N^{-*}(\nu_T)N^{+}(\nu_P)\int\int\int d\vec{x}_1 d\vec{x}_2 d\vec{R}\, e^{i\vec{\alpha}\cdot\vec{s}_2 + i\vec{\beta}\cdot\vec{x}_2}\varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2) \\ &\times F(i\nu_P, 1, ivs_2 + i\vec{v}\cdot\vec{s}_2)\left\{Z_T\left(\frac{1}{R} - \frac{1}{x_1}\right)\varphi_f^*(\vec{s}_1, \vec{s}_2)F(i\nu_T, 1, ivx_2 + i\vec{v}\cdot\vec{x}_2)\right. \\ &\left. - \nabla_{s_2}\varphi_f^*(\vec{s}_1, \vec{s}_2)\cdot\nabla_{x_2}F(i\nu_T, 1, ivx_2 + i\vec{v}\cdot\vec{x}_2)\right\}, \end{aligned} \tag{2}$$

$$\begin{aligned} T_{if}^{-(CDW-4B)} &= N^{-*}(\nu_T)N^{+}(\nu_P)\int\int\int d\vec{x}_1 d\vec{x}_2 d\vec{R}\, e^{i\vec{\alpha}\cdot\vec{s}_2 + i\vec{\beta}\cdot\vec{x}_2}\varphi_f^*(\vec{s}_1, \vec{s}_2) \\ &\times F(i\nu_T, 1, ivx_2 + i\vec{v}\cdot\vec{x}_2)\left\{\left[Z_T\left(\frac{1}{R} - \frac{1}{x_1}\right) + \frac{1}{r_{12}} - \frac{1}{s_2}\right]\varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2)\right. \\ &\left. \times F(i\nu_P, 1, ivs_2 + i\vec{v}\cdot\vec{s}_2) - \varphi_P(\vec{s}_1)\nabla_{x_2}\varphi_T(\vec{x}_2)\cdot\nabla_{s_2}F(i\nu_P, 1, ivs_2 + i\vec{v}\cdot\vec{s}_2)\right\}. \end{aligned} \tag{3}$$

The corresponding expressions for transition amplitudes in the CB1-4B approximation are given by (Mančev 1995, 1996):

$$\begin{aligned} T_{if}^{+(CB1-4B)} = \quad & Z_T\int\int\int d\vec{s}_1 d\vec{s}_2 d\vec{R}\, e^{i\vec{\alpha}\cdot\vec{s}_2 + i\vec{\beta}\cdot\vec{x}_2}\varphi_f^*(\vec{s}_1, \vec{s}_2) \\ & \times\left(\frac{2}{R} - \frac{1}{x_1} - \frac{1}{x_2}\right)\varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2), \end{aligned} \tag{4}$$

$$\begin{aligned} T_{if}^{-(CB1-4B)} = \quad & \int\int\int d\vec{s}_1 d\vec{x}_2 d\vec{R}\, e^{i\vec{\alpha}\cdot\vec{s}_2 + i\vec{\beta}\cdot\vec{x}_2}\varphi_f^*(\vec{s}_1, \vec{s}_2) \\ & \times\left(\frac{Z_T + Z_P - 1}{R} - \frac{Z_T}{x_1} - \frac{Z_P}{s_2} + \frac{1}{r_{12}}\right)\varphi_P(\vec{s}_1)\varphi_T(\vec{x}_2), \end{aligned} \tag{5}$$

where $\varphi_f(\vec{s}_1, \vec{s}_2)$ is the bound state wave function of the atomic system (Z_P, e_1, e_2), whose binding energy is ε_f. The hydrogen-like wave functions of the (Z_P, e_1) and

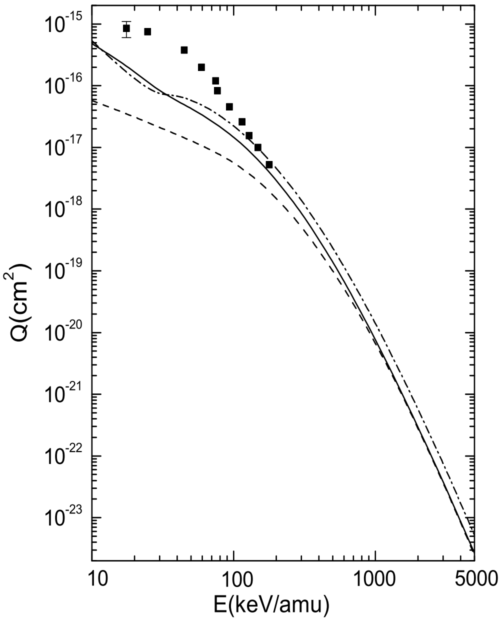

Figure 1: Total cross sections $Q(cm^2)$ as a function of laboratory incident energy $E(keV/amu)$ for charge transfer in $Li^{2+} - H$ collisions. The solid line represents the results of the prior form of the CDW-4B method, whereas singly chained curve is due to the the post version of the CDW-4B theory. The dashed curve represents the cross sections of the CB1-4B approximation. All computations have been performed using the two-parameter Silverman et al. (1960) wave function. Experimental data: ■ Shah et al. (1978).

(Z_T, e_2) systems are respectively denoted as $\varphi_P(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$. The corresponding binding energies are ε_P and ε_T. The momentum transfers $\vec{\alpha}$ and $\vec{\beta}$ are defined by $\vec{\beta} = -\vec{\eta} - \beta_z\hat{\vec{v}}$, $\vec{\alpha} = \vec{\eta} - \alpha_z\hat{\vec{v}}$, $\vec{\alpha} + \vec{\beta} = -\vec{v}$, $\alpha_z = v/2 - \Delta\varepsilon/v$, $\beta_z = v/2 + \Delta\varepsilon/v$, $\Delta\varepsilon = \varepsilon_P + \varepsilon_T - \varepsilon_f$. The transverse component of the change in the relative linear momentum of a heavy particle is denoted by $\vec{\eta} = (\eta\cos\phi_\eta, \eta\sin\phi_\eta, 0)$. The incident velocity vector $\vec{v}$ is chosen as $\vec{v} = (0, 0, v)$. The symbol ${}_1F_1(a, b, z)$ stands for the regular confluent hypergeometric function.

It should be recalled that both CDW-4B and CB1-4B models satisfy correct boundary condition according to principles of scattering theory (Belkić 2004). The proper connection between long-range Coulomb distortion effects and accompanying perturbation potentials are established. It must be emphasized that imposing the proper Coulomb boundary conditions in the entrance and the exit channels is of crucial importance for ion-atom collisions (Belkić 2008). Experience has shown that if this requirement is disregarded, serious problems may arise and such models are generally inadequate for description of experimental findings (Belkić 2008).

As shown (Mančev 2007), after analytical calculations performed by means of standard Nordsieck technique, the expressions for the total cross sections for the CDW-4B model can be reduced to a four-dimensional numerical integral. In the case of CB1-4B model (post version), the total cross sections are expressed (Mančev 1995) via a three-dimensional quadrature, whereas prior version of the CB1-4B approximation requires an additional three-dimensional integral due to term $1/r_{12}$ in the perturbation potential.

3. THE RESULTS OF THE NUMERICAL COMPUTATIONS

In this work, the explicit calculation of the matrix elements for single electron capture are carried out by using the two-parameter wave function of Silverman et al. (1960) for the final state of lithium ion: $\varphi_i(\vec{s}_1,\vec{s}_2) = N[e^{-\alpha_1 s_1-\alpha_2 s_2}+e^{-\alpha_2 s_1-\alpha_1 s_2}]/\pi$, where $N = \left[1/\alpha_1^3+1/\alpha_2^3+16/(\alpha_1+\alpha_2)^3\right]^{-1/2}$. Despite its very simple form in this function Silverman et al. (1960) the radial static correlations are taken into account to within nearly 90%.

Numerical computations of the total cross sections are presently carried out for the following charge exchange reaction:

$$Li^{2+}(1s)+H(1s)\longrightarrow Li^{+}(1s^2)+H^{+}. \tag{6}$$

The explicit computations of the total cross sections are carried out only for capture into the final ground state $1s^2$. In Fig. 1 we compare our theoretical results for prior (solid line) and post (dot-dashed line) CDW-4B cross sections, together with CB1-4B results (dashed line).

Our total cross sections are also compared with the experimental data of Shah et al. (1978). A comparison of the CDW-4B and CB1-4B models with measurements Shah et al. (1978) shows that the theoretical curves underestimate experimental data, especially at lower impact energies. Unfortunately the measurements of Shah et al. (1978) are limited up to 178 keV/amu, and this is only marginally within the considered range $10 \le E \le 5000 keV/amu$. However, we recall that CDW-4B and CB1-4B models are high-energy approximations and we expect better agreement at larger impact energies. New measurements for the considered reaction are needed for a better assessment of the validity of the CDW-4B and CB1-4B models.

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