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CHARGE-TRANSFER CROSS SECTION IN THE Li-Li$^+$ SYSTEM

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ABSTRACT: This work deals theoretically with the charge exchange cross section computed for the system Li-Li$^+$ assuming a very low electric field. The calculations are performed quantum mechanically within the Chapman-Enskog model [1]. The calculation starts by constructing the ion-atom potential and, with this system, the collisional dynamics are determined by the molecular Σ_g^+ and Σ_u^+ states [2] . The gerade and ungerade potential-energy curves are shown in Fig. 1. The potentials are further used to solve the radial wave equation and therefore to determine the phase shifts. These phase shifts have been used to compute the elastic and charge-transfer cross sections. For illustration, the charge-transfer cross section for the scattering at low energies in the Σ_g^+ and Σ_u^+ states are presented in fig. 2.

KEYWORDS: charge-transfer cross-section, lithium

1. Introduction

The interaction between an atom and ion of the same element leads to have gerade and ungerade states of the diatomic molecular ion, only the two lowest electronic states of the molecular ion are considered in this interaction, in these systems the collisional dynamics are determined by the molecular Σ_g^+ and Σ_u^+ states.

The present paper is concerned with collision of neutral atom-ion systems in the ultralow energy. The calculation of potentials using *ab initio* data, The potential are further used to solve the radial wave equation and therefore to determine the phase shifts, these phase shifts have been used to compute elastic and charge-transfer cross section

2. Construction of potential

The interaction potential which is pertained to this collision is shown in figure1; for the example Li-Li+. In the Σ_g^+ and Σ_u^+ states. These potentials curves have been used *ab initio* data available in literature, at small inter-nuclear separation R, the potential curves were approximated with short-range potential of the form

$$V(R) = a \exp(-b/R) \qquad (1)$$

In long-distances, we have introduced dispersion terms is given, in atomic units by R. Côté and A. Dalgarno [3]

$$V(R) \sim V_{dis}(R) \pm V_{exch}(R) \qquad (2)$$

The dispersion term is given in atomic units

$$V(R) = -1/2\,[C_4/R^4 + C_6/R^6 + C_8/R^8] \qquad (3)$$

Where C_4, C_6, C_8 are the dipole, quadruple and octopole polarisabilities of neutral atom[4], the exchange term was performed using treatment of Tony C Scott et al [5] and takes the form

$$V_{exch}(R) = (A^2_{n,s}/4)\,(4/e)^{1/\alpha}\,(R/2)^{2\gamma+1}\exp(-R\alpha_{n,s}) \qquad (4)$$

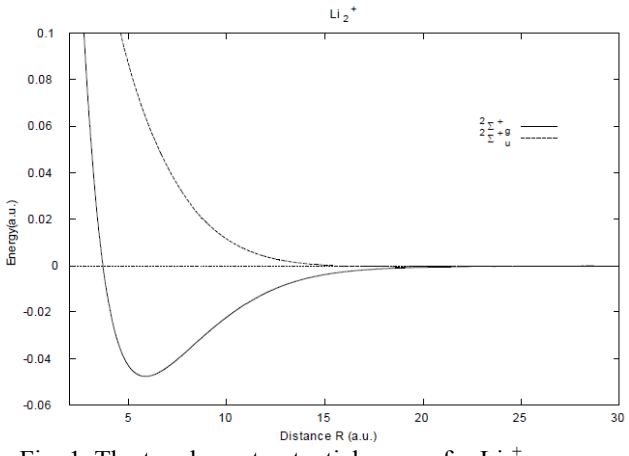

Fig. 1. The two lowest potential curves for Li_2^+.

3. Elastic and transfer- charge cross sections

The scattering of Li by Li$^+$ may be described by the appropriate solution of differential equation

$$[d^2/dR^2 + k^2 - 2\mu V_{g,u} - l\,(l+1)/R^2]U^{g,u}_{E,l} \qquad (5)$$

$V_{g,u}$, are the potentials as a function on inter-nuclear distance R for either the Σ_g^+ and Σ_u^+ states of Li_2^+, μ is the reduced mass, $k = (2\mu E)^{1/2}/\hbar$. $U^{g,u}{}_{E,l}$ is the nuclear wave function behaves asymptotically

$$U^{g,u}{}_{E,l} = \sin(kR - l\pi/2 + \eta_l^{g,u}) \quad (6)$$

For large values of l, the phase shift $\eta_l^{g,u}$ can be approximated by

$$\eta_l^{g,u} = \mu\pi C_4 k^2/8\hbar^2 L^3 \quad (7)$$

The elastic cross section given is by [6]

$$\sigma_{el} = \tfrac{1}{2}[\sigma^g{}_{el+}\ \sigma^u{}_{el}] \quad (8)$$

These cross section can be calculated from the phase shifts scattering along the Σ_g^+ and Σ_u^+

$$\sigma_{el} = 4\pi/k^2 \sum_{l=0}^{\infty} (2l+1) \sin^2 \eta_l^{g,u} \quad (9)$$

We will obtain the charge-transfer cross section of the form

$$\sigma_{ch} = \pi/k^2 \sum_{l=0}^{\infty} (2l+1) \sin^2 (\eta_l^g - \eta_l^u) \quad (10)$$

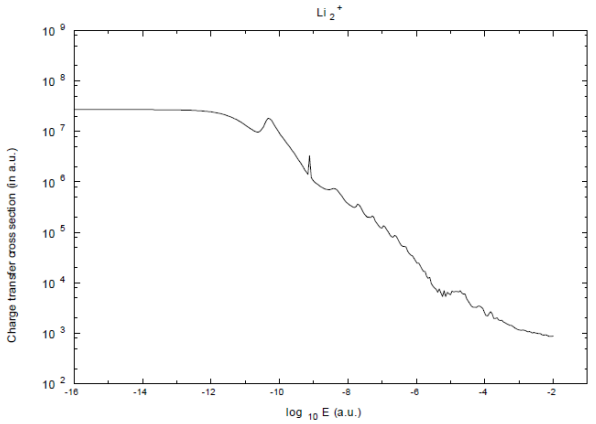

Fig. 2. Charge-transfer cross section as a function of the collision energy.

Our result are found is reasonably good with the theoretical result. In Fig. 2, we have presented the charge-transfer cross section result for Li-Li^+ system. The nature of the curve is simply monotonically decreasing with the increase of energy.

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