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QED APPROACH TO HIGH ENERGY DOUBLE ELECTRON CAPTURE

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Double-electron capture from He and H_2 by fully stripped Li^{3+} ion in $1s^2$ and $2s^2$ states in high-energy (above 1 MeV) collision is done in a field theoretic way. Most of the double capture is found to occure in $1s^2$ state. H_2 stands out as a better candidate compared to He in delivering electrons. A good agreement is obtained for capture into $1s^2$ state from He with existing theoretical and experimental results. Auger decay probability from $2s^2$ state leading to transfer ionisation is discussed.

1. Introduction

Very recently there were several attempts towards theoretical calculation of double charge transfer[1,2,3]. Most of the works in the high energy region are based on continuum intermediate state method (CIS) or continuum distorted wave (CDW) approximation. The phenomena of double-electron capture from He by heavy ions are being studied experimentally and theoretically[4] to ascertain the nature of correlation between the electrons.

Although the theoretical results in the framework of (CIS) and (CDW) approximations give good experimental fit, yet as more and more high energy ion beam are becoming available there is scope for QED treatment of the collision events. Single electron capture, and capture and ionisation in high energy Li^{3+} and He collision is studied in QED technique in our previous paper[5]. Present paper contains an extension of the QED approach to double electron capture in $1s^2$ and higher orbital ^1S states, in similar encounters of Li^{3+} with He and H_2. The current-

-current interaction between the projectile and a target electron is taken similar to that in single electron capture. It is the overlap integral between the initial and the final interacting systems, which determines the different competing processes like transfer ionisation and double capture. To justify Auger induced transfer ionisation, we have invoked electron correlation effects in the wave functions. The object of the present paper is to calculate, in the high energy region, double electron capture cross-sections for the following processes

$$A^{Z+} + B \rightarrow A^{(Z-2)+}(1s^2) + B^{2+} \quad (1)$$

$$\rightarrow A^{(Z-2)+}(2s^2) + B^{2+} \quad (2)$$

$$A^{Z+} = Li^{3+} \quad \text{and} \quad B = He \text{ and } H_2,\ H_2^{2+} = 2H^+.$$

Results for double capture cross section in the ground state of Li^+ agree fairly well with the experiment of Shah and Gilbody[6] and other theoretical results with He as target. For both the targets, the capture into Li^+ ($1s^2$) state is exothermic and eventually there is energy gain by the projectile. However, double electron capture into the $2s^2$ state is endothermic for He and exothermic for H_2. Further, the double capture probability into L-shell of Li^+ is 10^{-5} smaller in order compared to that into the K-shells for both the targets. Fast projectiles do not change their velocity much in the capture or transfer ionisation processes. So double capture cross sections are computed for projectiles in the forward direction and are shown in Table 1 and Figs. 1 and 2. A comparative study of the cross sections,

TABLE 1.

$Li^{3+} + He$					$Li^{3+} + H_2$		
Energy (MeV)	FT	°1 s^2 CDWA	Expt	°2 s^2 FT	Energy (MeV)	°1 s^2 FT	°2 s^2 FT
	(10^{-16} cm^2)			(10^{-22} cm^2)		(10^{-16} cm^2)	(10^{-22} cm^2)
1.0	4.11^{-2}	—	—	1.639	1.0	17.23^{-2}	7.20
1.12	3.9^{-2}	3.37^{-2}	5.04^{-2}	—	1.2	10.52^{-2}	1.38
1.4	1.8^{-2}	2.97^{-2}	2.03^{-2}	3.49^{-1}	1.4	6.72^{-2}	7.83^{-1}
1.6	1.076^{-2}	—	—	1.91^{-1}	1.6	4.50^{-2}	4.76^{-1}
1.75	7.8^{-3}	9.54^{-3}	8.9^{-3}	—	1.8	3.11^{-2}	3.06^{-1}
2.0	4.73^{-3}	—	—	7.05^{-2}	2.0	2.22^{-2}	2.05^{-1}
2.191	2.75^{-3}	2.75^{-3}	3.1^{-3}	4.63^{-2}	2.2	1.62^{-2}	1.62^{-1}
2.5	2.045^{-3}	—	—	2.65^{-2}	2.5	1.06^{-2}	8.78^{-2}
2.8	1.3^{-3}	6.35^{-4}	1.05^{-3}	1.61^{-2}	2.8	9.26^{-3}	7.55^{-3}
3.0	1.02^{-3}	—	—	1.19^{-2}	3.0	5.65^{-3}	4.35^{-2}

Superscripts are powers of ten.

Cross section for double electron capture from He and H_2 into $1s^2$ and $2s^2$ states, respectively, of Li^{3+} and projectile moving in the forward direction. Experimental data for capture into all (n, 1) states by Shah and Gilbody[6] and theoretical data for capture into $1s^2$ by Ghosh et al.[2] in CDWA for He target are included along with the present field theoretic (FT) calculation.

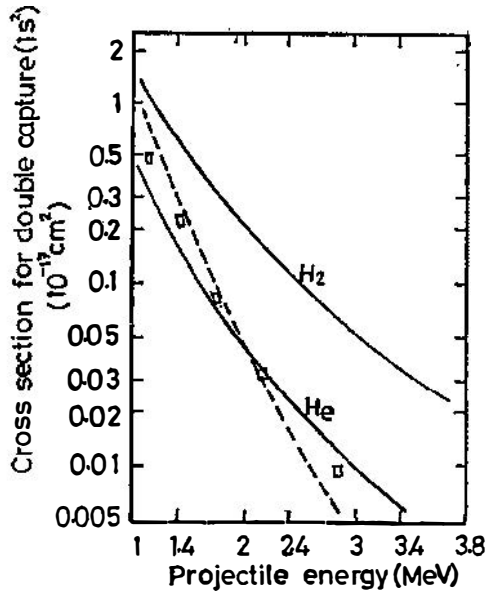

Fig. 1. Double capture cross-section into $1S^2$ state for the reaction $Li^{3+} + H_2(He) \rightarrow Li^+(1S^2) + 2H^+(He^{2+}) + 166.991$ eV (118.25 eV). Theoretical calculation: — Present theory for H_2 and He, – – –– CDWA by Ghosh et al.[2] for He. Experimental results: □ with He target by Shah and Gilbody for capture into all possible (nl) states.

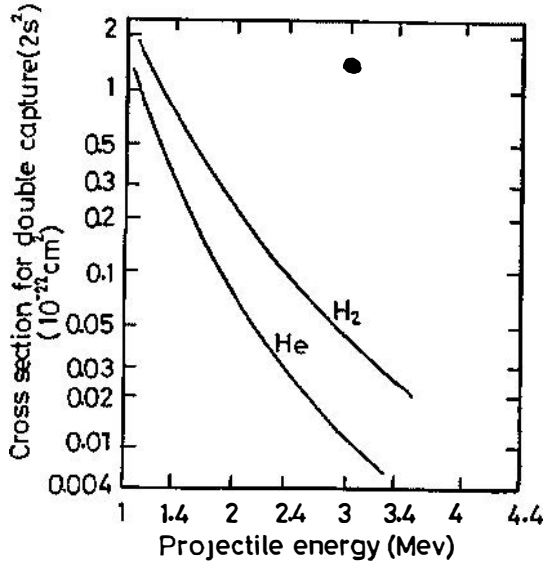

Fig. 2. Double capture cross-section into $(2S^2)$ state for the reaction $Li^{3+} + H_2(He) \rightarrow$ $\rightarrow Li^+(2S^2) + 2H^+(He^{2+}) + 17.589$ eV (—29.156 eV). —— Present calculation.

of all the reaction processes, between H_2 and He targets indicate that contributions from H_2 is much higher than that from He. This may be because the electrons in H_2 are loosely bound compared to those in He.

2. *Theory*

Current-current interaction between a bound electron and the bare projectile is considered to compute the cross section for the processes of double capture occurring in high energy ion-atom collisions. Virtual photon exchange during the process causes change in the potential field of the target nucleus. In the course of readjustment of the second electron in the new potential field of the target, the said electron may suffer shake-up either to the continuum or to the bound state of the projectile, giving rise to the transfer ionisation and double capture, respectively. With projectile velocity greater than Bohr orbital velocity of the target electron, the shake up mechanism dominates over independent removal of atomic (or molecular) electrons due to interaction of each of them with the fast nucleus. The transfer ionisation with He target is done in independent electron approximation[5]. For present calculation following the argument of McGuire et al.[7] it is assumed that due to static correlation second electron gets captured into the projectile after the capture of the first electron, to make the final-state rearrangement.

Second order S matrix for the process is given by

$$S_2 = \int\int (J_\mu^{e-} A_\mu)_y (J_\mu^{A+} A_\mu)_x \, \mathrm{d}y^4 \, \mathrm{d}x^4. \tag{3}$$

$J^{e-}(y)$ and $J^{A+}(x)$ are, respectively, the bound electron current and the bare projectile current. A is the four vector potential. In second order S matrix we are restricting ourselves to the lowest order perturbation theory as regards radiation field, yet we can obtain results accurate to all orders in Coulomb coupling by suitable choice of wave functions. To estimate the effect of this additional Coulomb coupling, the cross section is multiplied by the 'Sommerfeld factor'. However, for high energy projectile under consideration the correction to the cross section is negligible. We write the general matrix element for all the processes as (see Eq. (11) in Ref. 5)

$$M_r = \langle \Psi_r | S_2 | \Psi_i \rangle = G_r L_r \tag{4}$$

$r = 1, 2$ — corresponding to reaction processes (1) and (2), respectively. G_r is the momentum integral over the spinor part and L_r is the integral over the space part of the matrix element (see Appendix)

$$G_r = 2\pi \delta (E_i - E_r) \, e^2 z \sum_{\alpha,\beta} (u_\alpha (p') \, v_\mu \, u_\alpha (p)) \, (U_\beta (q_r) \, v_\nu \, U_\beta (q))/(4\pi^2 \, |q_r - q|^2) \tag{5}$$

$$L_r = \int\int \Phi_r (y, y_1) \, \Psi (y, y_1) \exp (\mathrm{i} (\vec{q}_r - \vec{q}) \cdot y) \, \mathrm{d}^3 y \, \mathrm{d}^3 y_1. \tag{6}$$

u and U are, respectively, the Dirac spinors for electron and the projectile with indicated momenta. For $r = 1$ and 2, $\Phi_r(y, y_1)$ is the hydrogen type product wave function of the Li^+ ion in $1s^2$ and $2s^2$ states, respectively. $\Psi(y, y_1)$ is the wave function of target (He or H_2) in the initial state. Since accounting for correlations between electrons is very important in describing the capture processes we have considered the Hartree-Fock orbital for each individual electron in $\Phi_r(y, y_1)$ and $\Psi(y, y_1)$. Double capture cross sections for reactions (1) and (2) in the forward direction are computed as below and shown in Table 1 and Figs. 1 and 2, respectively, for both the hydrogen molecule and helium atom

$$\frac{d\sigma_r}{d\Omega} = \int |M_r|^2 \frac{M^2}{|q|} dE/(2\pi)^3 \qquad r = 1, 2. \tag{7}$$

3. *Results and discussions*

Double capture of electrons by Li^{3+} from hydrogen molecule and helium atom are computed and shown in Figs. 1 and 2. Our result for double electron capture is found to agree fairly well with that of Shah and Gilbody[6] for He target and projectile Li^+ ($1s^2$) moving in the forward direction. As discussed in the introduction, similar result for H_2 is four time higher. But there is yet no result for H_2 in the high energy range to compare with. Double capture probability in $2s^2$ state is 10^{-4} to 10^{-5} times smaller compared to that in $1s^2$ state of Li^+. This result although smaller than the present day experimental error bar in double electron capture, yet one may hope to get capture cross section in L-shell with the improvement in the measurement in the state-selective processes.

Projectile velocity dependence for double capture for the energy range under consideration are mainly due to four-momentum transfer factor $|q_r - q|^{-4}$ and the incident flux v^{-1}. In the present case, the overall velocity dependence is v^{-9} and the projectile charge dependence is Z^2. With the increase in energy, the negative exponent of velocity goes to 13.

3.1. *Auger induced transfer ionisation (ATI)*

Transfer ionization in ion-atom collision is known to occur due to projectile emission of the prompt Auger electron after double capture in the excited state[8,9,10]. Auger spectroscopy or radiative decay rate may be used to study state-selective double capture in $Li^{3+} + He\,(H_2)$ collisions. An estimate of the Auger emission probability (M_A) from Li^+ ($2s^2$) state is obtained by invoking static Coulomb interaction between the bound electrons in the field of the nucleus. Eventually the selection rules

$$\Delta l = 0, \qquad \Delta s = 0, \qquad \Delta I = 0$$

are satisfied. The KLL Auger emission width in the emitter rest frame comes out to be of the order 10^2 a. u. A probability for ATI may be obtained by taking the product of the probabilities for double capture in $2S^2$ state (M_2) and that for

Auger decay (M_A). Although Auger induced transfer ionisation is α^2 order small compared to direct transfer ionisation[5], yet ATI may lead to some insight into the electron correlation effects in state selective double capture processes. A detailed study on this is left for future communication. As a rough estimate we obtained, the ATI cross-section for a 2.2 MeV projectile to be of the order $8 \cdot 10^{-5}$ a. u., whereas corresponding direct transfer ionisation cross-section is $7 \cdot 10^{-2}$ a. u., from He target.

In conclusion I like to state that in QED technique[5,11,12], ion-atom charge transfer in high energy collisions can be dealt in a very compact form. In the case of high velocity bare projectile the virtual photon propagator and the overlap integral L_r mainly determine the interaction processes. In the case of H_2 molecule the results are much higher because the electrons are loosely bound compared to that in He. Further the nuclear part of the molecular wave function contained in the overlap integral also contributes to the cross sections. With the increase in projectile velocity above Bohr velocity in the target atom, contribution from spinor part also increases.

Appendix

For $r = 1$, and 2

$$|M_r|^2 = |G_r|^2 L_r^2 \tag{1A}$$

$$|G_r|^2 = 4\pi^2 Z^2 e^4 (TT^*)_r / ((4\pi^2)^2 |q_r - q|^4) \tag{2A}$$

q is 4-momentum vector.

$$L_r = \int\int \Phi_r(y, y_1) \Psi(y, y_1) \exp(i\vec{y} \cdot (\vec{q}_r - \vec{q}))\, d^3y\, d^3y_1 \tag{3A}$$

$$\Phi_1(y, y_1) = \Phi_{Li^+(1s^2)}(y, y_1) = \Phi_{Li^+(1s)}(y)\, \Phi^*_{Li^+(1s)}(y_1)$$

$$\Phi_2(y, y_1) = \Phi_{Li^+(2s)}(y)\, \Phi_{Li^+(2s)}(y_1) \tag{4A}$$

$$\Psi(y, y_1) = \Phi_{He(1s)}(y)\, \Phi_{He(1s)}(y_1) \text{ for He atom} \tag{5A}$$

$$= N(R)\, 2(1 + \lambda)\, \Psi_{H(1s)}(y)\, \Psi_{H(1s)}(y_1)/(2S + 2) \text{ for } H_2 \text{ molecule.} \tag{6A}$$

$N(R)$ is the nuclear part and the remaining portion is the electronic part of the molecular wave function. The trace part (TT^*) is given by

$$(TT^*)_r = (1/4)(2/M^2)\{(E_r a + M)(Ea + M) + M^2 + 2Ma(E_r E)^{1/2}\} \tag{7A}$$

4-momentum transfer of the projectile Li^{3+}, $(q_r - q)$ is given by

$$|q_r - q|^4 = 4M^2((E_r + E)a + E_r E a^2/M - 2a(E_r E)^{1/2})^2. \tag{8A}$$

All quantities are in atomic units.

$a = 27.2/(0.5 \cdot 10^6)$ conversion factor for relativistic energy into atomic unit.

Z = charge of $Li^{3+} = 3$, M = mass of Li^{3+}

Mass of proton = 1836, mass of electron = 1.

For He target and double capture

$$L_r = S_r^B K_r^B \quad B = He$$

$$S_1^B = N_{Li^+(1s)} N_{B(1s)} 8\pi (Z_B + Z_{Li^+})/\{(Z_B + Z_{Li^+})^2 + (\vec{q}_{1B} - \vec{q})^2\}^2 \qquad (9A)$$

$$K_1^B = S_1^B \text{ with } (\vec{q}_{1B} - \vec{q}) = 0 \qquad (10A)$$

$$S_2^B = N_{Li^+(2s)} N_{B(1s)} 8\pi (21_B^3 - 7Z_{Li^+} 1_B^2 + (q_{2B} - q)^2 (21_B + Z_{Li^+}))/(1_B^2 + (q_{2B} - q)^2)^3 \qquad (11A)$$

$$K_2^B = S_2^B \text{ with } (q_{2B} - q) = 0$$

$1_B = Z_B + Z_{Li^+}/2$, N's are the normalising constants of the suffixed wave functions. q_{rB} is the projectile momentum after reaction (r) with target B. q is the initial projectile momentum.

For double capture with H_2 target,

$$L_r = S_r^B . K_r^B . (2(1 + \lambda)/(2S + 2)) N(R_e) \exp(i\vec{R} \cdot (\vec{P}_H + \vec{Q}_H)) d^3R, \quad B = H_2. \qquad (12A)$$

Contribution from the nuclear part is

$$N(R_e) (2\pi)^3 \delta^3 (\vec{P}_H + \vec{Q}_H).$$

Delta function balances the relative motion of the two molecular nuclei. For lowest vibrational state the equilibrium separation between the nuclei is

$$R_e = 2.12 \text{ a. u. and}$$

$$N(R_e) = (\alpha/\pi)^{1/2}/R_e, \qquad \alpha = 0.578 (1.836/2)^{1/2}, \qquad \beta = 1.19$$

$$\lambda = 1/6, \qquad S = (1 + \beta R_e + \beta_2 R_2/3) \exp(-\beta R_e).$$

For double capture E and E_r are, respectively, the initial and final projectile energies

$$E_r = E + \Delta_r.$$

For capture into $1s^2$ state $\Delta_1 = 118.25$ eV with He
$= 166.991$ eV with H_2.

For capture into $2S^2$ state $\Delta_2 = -29.156$ eV with He
$= 17.589$ eV with H_2.

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QED PRISTUP VISOKOENERGETSKOM DVOSTRUKOM UHVATU ELEKTRONA

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Originalni znanstveni rad

Teorijski je proučavan dvostruki uhvat elektrona sa He i H_2 od strane potpuno ogoljelog Li^{3+} u $1s^2$ i $2s^2$ stanju pri visokoenergetskom (> 1 MeV) sudaru. Za većinu dvostrukih uhvata nađeno je da se pojavljuju u $1s^2$ stanju. H_2 je bolji kandidat nego He za otpuštanje elektrona. Dobro slaganje s postojećim teorijskim i eksperimentalnim rezultatima je dobiveno za uhvat u $1s^2$ stanje. Diskutirana je vjerojatnost Augerova raspada sa $2s^2$ stanja koja vodi na prelaznu ionizaciju.