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RATIO OF THE DOUBLE TO SINGLE ELECTRON CAPTURE CROSS SECTION BY HIGH ENERGY BARE PROJECTILE IN COLLISION WITH He

SUJATA BHATTACHARYYA

Gokhale College, Calcutta 700020, India

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Ratio of the double to single electron capture cross section in high energy bare projectile colliding with He atom is obtained in a Feynman technique. For Li^{3+} projectile the ratio is found to vary between 0.03 to 0.017 in the energy range 200 keV amu^{-1} to 300 keV amu^{-1}, while the corresponding experimental value lies between 0.04 to 0.02. Energy dependence on the ratio is discussed.

1. Introduction

Two-electron processes in the collision of He atom with bare projectile is the subject of extensive current research. This system contains minimum number of particles for a many-electron collision system. Furthermore, the strength of the electron-electron correlation in this system is relatively important because of the low He nuclear charge. Most of the measurements and calculations are on ionisation of He[1-7]. Data are available in the form of ratio R of the cross section for double to single ionization ($R = He^{++}/He^{+}$) or as the charge state fraction $F_2 = He^{++}/(He^{+} + He^{++})$. The study shows that there are two theoretical models that can accurately explain the physics in double ionisation in high energy ion-atom collisions[5]. Though we aimed at the ratio for double-electron to single-electron capture cross sections by the projectile, we want to be guided by those models for double ionisation of He while computing the ratio in Feynman technique.

In one model known as rearrangement mechanism (RM), the double-electron capture occurs, because, due to interaction of the fast projectile with one of the peripheral electron of He the other electron is shaken and both the electrons go to the first projectile while rearranging themselves in the new potential field. The second model is the two step process (TS) in which projectile interacts with both the electrons of the target simultaneously. As pointed out by many[1-5], the ratio of the double to single ionisation in rearrangement mechanism is independent of the projectile energy, while that in direct interactions (or TS mechanism) the ratio is proportional to $(Z/v_e)^2$. Direct interaction corresponds to a higher Born contribution. Semiclassically the high energy behaviour of the ionisation ratio was analysed as a combination of these two processes.

Since double electron capture is a two electron process like double ionisation, we were tempted to use the idea of RM and direct mechanism to compute double-electron capture cross section. In QED technique these are, respectively, second order and fourth order terms of the S-matrix expansion. One electron capture by Li^{3+} is already computed in a Feynman technique[7]. Double electron transfer can be treated in a similar way using second order S-matrix and rearrangement model. The direct interaction or two step model can be identified with the fourth order Feynman diagrams where there are two virtual photon exchanges between the projectile and target-electrons, along with the projectile propagator. The virtual photon propagators combined with the projectile propagator will make the contribution from the fourth-order term negligible compared to the contribution from second order S-matrix. As such we compute only the second order Feynman diagram for double-electron capture. The result thus obtained is found to agree fairly well with the experimental result of Shah and Gilbody[6].

2. *Theory*

Current-current interaction between bound electron and bare projectile is considered in co-variant Lorentz gauge to compute single capture and simultaneous capture and ionisation cross-sections[7] in the reaction between Li^{3+} and He atom. Single collision condition dominates the high energy capture reaction if projectile velocity is greater than orbital electron velocity. At such high energies it is tempting to invoke QED approach and assume that during one-electron capture the virtual-photon exchange, between the bound-electron of He target and Li^{3+} projectile, causes change in the potential field of the target nucleus. In the course of readjustment in the new potential field the second electron may suffer shake-up either to the continuum state or to the bound state of the projectile, giving rise to transfer ionisation (TI) or double capture (DC), respectively. However, the probability of the second electron to remain attached to He^+ is high and the corresponding process is single electron capture due to charge transfer (CT). In the rearrangement mechanism the double capture occurs due to static correlation i. e. correlation contained in the wave function[1]. In this paper we study the ratio of the cross section, σ_{DC}, for double electron-capture divided by the cross section, σ_{CT}, for single electron-capture. By taking the ratio (R) of a two-electron to one-electron capture cross sections the effect of one-electron transition mechanism tends to cancel so that the two-electron mechanism become more apparent.

Most of the theoretical calculation on capture processes are centred around single capture cross section[7-9]. Only very recently have attempts been made[10-12] to calculate double capture cross section. Feynman diagrams for capture processes are shown (Fig. 1).

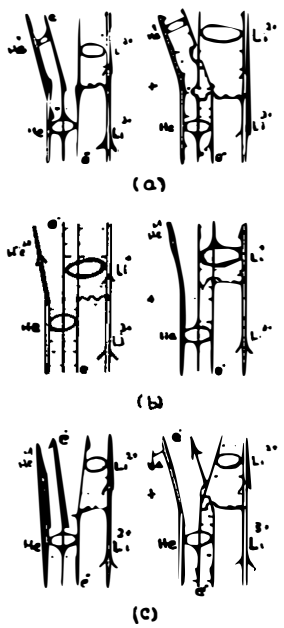

Fig. 1. Feynman diagrams for intersections of a projectile ion with two bound electrons causing (a) charge transfer (CT) (b) double capture (DC) and (c) transfer ionisation (TI), respectively, in the reactions

$$\mathrm{He} + \mathrm{Li}^{3+} \rightarrow \mathrm{He}^{+} + \mathrm{Li}^{2+}\,(\mathrm{CT})$$

$$\rightarrow \mathrm{He}^{2+} + \mathrm{Li}^{+}\,(\mathrm{DC})$$

$$\rightarrow \mathrm{He}^{2+} + \mathrm{Li}^{2+} + \mathrm{e}\,(\mathrm{TI}).$$

The horizontal broken lines with inset circles indicate bound system of electrons.

We wish to clarify that, while we are restricting ourselves to the lowest-order perturbation theory with regard to radiation field (order e^2, S matrix), we can obtain results accurate to all orders in Coulomb coupling by a suitable choice of the wave function. The Sommerfeld-Maue relativistic wave function is well suited to describing the incoming distorted-wave projectile. To estimate the effect of this additional Coulomb coupling over the second-order S-matrix particle-radiation-field coupling, we can multiply the cross section by the Sommerfeld factor[13].

Numerically, we find that, for energies above 100 keV amu^{-1}, this introduces a negligible correction in case of CT and DC. For lower energies, its effect on the cross section gradually increases. However, in the case of TI the emitted electron moves slowly in the combined Coulomb field of He^{2+} and Li^{2+} and the corresponding distortion effect is found to be quite appreciable.

TABLE 1.

E (keV amu^{-1})	200	250	313	400	429
FT	0.581	0.285	0.157	0.07	0.045
SG	0.479	0.274	0.148	—	—
MG	1.49	—	0.321	0.2	—

Cross section for charge transfer σ_{CT} (10^{-16} cm^2) in $He + Li^{3+} \rightarrow He^+ + Li^{2+}$. FT — Present calculation for capture into ground state, SG — The experimental result of Shah and Gilbody for single electron capture into all possible states[6], MG — The theoretical result by Mukherjee and group in CDM approximation[8].

TABLE 2.

E (keV amu^{-1})	200	250	313	400	429
ET	1.8^{-2}	7.8^{-3}	2.75^{-3}	1.3^{-3}	1.02^{-3}
SG	2.03^{-2}	8.9^{-3}	3.1^{-3}	1.05^{-3}	—
MG (CDW)	2.97^{-2}	9.54^{-3}	2.75^{-3}	6.35^{-4}	—
MG (CTS)	4.04^{-2}	1.34^{-2}	4.12^{-3}	1.05^{-3}	—

Cross section for double electron capture σ_{DC} (10^{-16} cm^2) in $He^+ + Li^{3+} \rightarrow He^{2+} + Li^+$. FT — Present result for capture into ground state, SG — Experimental by Shah and Gilbody for capture into all possible states, MG — Theoretical result by Mukherjee and group[12] in CDW approximation and CIS approximation, respectively.

TABLE 3.

E (keV amu^{-1})	200	250	313	400	429
FT	0.03098	0.0274	0.0175	0.0186	0.0226
SG	0.0482	0.0324	0.0209	—	—
MC CDW	0.0199	—	8.56^{-3}	3.18^{-3}	—
MC CIS	0.0271		0.0128	5.25^{-3}	

Ratio of the double to single capture cross sections σ_{DC}/σ_{CT} in collision between Li^{3+} and He atom. FT — Present field theoretic result, SG — Experimental results of Shah and Gilbody, MG — Theoretical results of Mukherjee and group in continuum distorted wave (CDW) and continuum intermediate state (CIS) approximations[8,12].

The reactions under consideration are

$$Li^{3+} + He \rightarrow Li^{2+} + He^{+} \qquad (CT)$$

$$\rightarrow Li^{+} + He^{2+}. \qquad (DC)$$

Ratio of double electron-capture (σ_{DC}) to single electron-capture (σ_{CT}) is

$$R = \sigma_2/\sigma_1 \qquad (1)$$

where

$$\sigma_2 = \sigma_{DC}, \qquad \sigma_1 = \sigma_{CT}$$

$$\sigma_K = \int |M_k|^2 \frac{M}{|q|} \frac{d^3 q_k}{(2\pi)^3}$$

for $K = 1, 2$ corresponding to single and double capture, respectively. The amplitude

$$M_k = \langle \Psi_k | S_2 | \Psi_i \rangle. \qquad (2)$$

The second-order S-matrix is given by the following current-current interactions:

$$S_2 = \int\int (J_\mu^{e^-} A_\mu)_y (J_\nu^{Li^{3+}} A_\nu)_x \, d^4x \, d^4y + \text{term for other electron.} \qquad (3)$$

$A_\mu(y)$, $A_\nu(x)$ are the vector potentials of the radiation field and contributes to the virtual photon propagator in the process.

$J_\mu^{e^-}(y)$ is the bound electron current at the vertex y and $J_\nu(x)$ is the bare ion correct at the vertex x

$$J_\mu^{e^-}(y) = \left(\frac{m_e^2}{E_{p_1}^R E_{p_1}^R}\right)^{1/2} \sum_r (V_{e^-(Li^{3+})}^{r+}(P_1') \gamma_\mu V_{e^-(\alpha)}^{r}(P_1))_y \, a^+(P_1') \, a(P_1) \qquad (4)$$

where E^R indicates the relativistic energy of the system. $V_{e-(Li^{3+})}(P_1)$ is the Dirac spinor for an electron bound to Li^{2+} and $V_{e-(\alpha)}(P_1)$ is that for the electron bound to a helium atom; a are the electron annihilation operators. The projectile current is similarly given by

$$J_\nu^{Li^{3+}}(x) = \left(\frac{M^2}{E_q^R E_{q_k}^R}\right)^{1/2} \sum_S (U_S^+(q_k) \gamma_\nu U_s(q_k))x \exp[-i(q - q_k)x] \, B^+(q_k) \, B(q) \qquad (5)$$

where U and B are, respectively, the spinors and annihilation operators for the ions. M is the mass of the projectile ion Li^{3+}; q, q_k are four-momenta of the Li-ion before and after interaction. We write the state vectors of the bound system in a field-theoretic way[14-16]. The initial state vector for the system of He atom and projectile ion is given by

$$|\Psi_i\rangle = L_i(y, y_1) \, a^+(P_1) \, a^+(P_2) \, B^+(q) \, C^+(l_\alpha) |0\rangle. \qquad (6)$$

The final-state vector is given by

$$|\Psi_k\rangle = L_k(y, y_1)\, a^+(P_1')\, a^+(P_2')\, B^+(q_k)\, C^+(l_\alpha)\, |0\rangle \tag{7}$$

where: $L_i(y, y_1)$ is the wave function of the electrons in He ($1s^2$), $L_1(y, y_1)$ is product of the wave functions of the electrons in He^+ (1s) and Li^{2+} (nl) after single capture, $L_2(y, y_1)$ is the wave function of the electrons in Li^+ ($nl, n\,l$) state after double capture.

Dirac solution for a bound electron is given by[17]

$$V_{e^-}^r(p)\, \Phi_{1s}(y) = N_0 (1 - \alpha Z \gamma_4 (\gamma_n)/2)\, u(p)\, \Phi_{1s}(y)$$

where N_0 is the normalisation factor, and $n = y/|y|$, $u(p)$ is the Dirac spinor for a free electron. Taking only the first term of this expansion since the second term is 1/137 smaller, we obtain for the matrix element

$$M_k = 2\pi\delta(E_i - E_k)\frac{e^2}{v^2} Z \left(\frac{m_e^2 M^2}{E_{p_1}^R E_{p_k}^R E_q^R E_{q_k}^R}\right)^{1/2} \int \frac{\exp[i(\vec{q} - \vec{q}_k)\cdot y]}{4\pi^2 (q - q_k)^2} \times$$

$$\times L(y, y_1)\, L_1(y, y_1)\, d^3y\, d^3y_1\, T_k \tag{8}$$

$$T_k = \sum_{r,s} (u_r^+(P_1'))\, \gamma_\nu u_r(P_1))\, (U_s^+(q_k)\, \gamma_\nu U_s(q)). \tag{9}$$

The relativistic energies are taken as

$$E_q^R = M + E_q\, (= q^2/(2M))$$

$$E_p^R = m_e + \varepsilon_{1s}\, (\text{orbital binding energy})$$

$$|M_k|^2 = (2\pi)^2 Z^2 e^4 (T_k^* T_k)\, I_k^2/(4\pi^2 (q - q_k)^2)^2. \tag{10}$$

$T_k T_k^*$ is the contribution from the trace part of the matrix.

Above 100 keV amu^{-1} the projectile velocity is greater than the orbital electron velocity and capture of electron occurs from the periphery of the atom and the target recoil momentum is almost negligible. The interaction time being much shorter than the rotational time of the electron, the bound electron spinor can be thought of as a zero momentum spinor. With this assumption the trace of the matrix becomes

$$T_k T_k^* = \frac{1}{4}(2/M^2)\, [(E_k a + M)(Ea + M) + M^2 + 2aM(EE_k)^{1/2}] \tag{11}$$

where $a = 54.4 \times 10^{-6}$ and all terms are in atomic units.

$$E_k = E_q + \Delta_k,$$

with Δ_k, the energy liberated during capture.

For ground state to ground state capture Δ_k is, respectively, 97.24 and 118.25eV for single and double capture from He by Li^{3+} ion. The four-momentum transfer of the projectile $(q - q_k)$ is given by

$$(q - q_k)^2 = 2M\,[(E_k + E)\,a + E_k E a^2/M - 2a\,(E_k E)^{1/2}]. \tag{12}$$

The overlap integral I_k is given by

$$I_k = \int\int L_i\,(y, y_1)\,L_k\,(y, y_1) \exp\,(-\mathrm{i}\,(\vec{q} - \vec{q}_k)\,y)\,\mathrm{d}^3y\,\mathrm{d}^3y_1. \tag{13}$$

3. *Results and discussion*

The ratio of the double-electron capture cross section to single-electron capture cross section is obtained as

$$R = R_1 R_2 R_3 \tag{14}$$

$$R_1 = (T_2 T_2^*)/(T_1 T_1^*), \quad R_2 = (I_2/I_1)^2, \quad R_3 = (q - q_1)^4/(q - q_2)^4.$$

Momentum transfer suffered by the projectile in one-electron capture $(q - q_1)$ is different from $(q - q_2)$ the momentum transfer due to two-electron capture. Eventually the trace part $T_k T_k^*$ arising out of the spin average and spin sum of the Dirac matrices are different for the two transfer processes. Moreover, the trace factors (11) contain non-linear combinations of E_i and E_k. Hence the factor R_1 of the ratio R is not energy independent. The overlap integrals I_1 and I_2 are the Fourier transform of the momentum transfer of the product wave functions and have different energy behaviour. Above analysis shows that all the three factors of the ratio R are projectile-energy-sensitive, however small. One may look to this as a QED behaviour which however is absent in the semiclassical calculation with rearrangement mechanism. However, the main deciding factor on the magnitude of R is R_2. As R_2 depends on the correlation between electrons in the wave functions of He and Li^+, one may extract R_2 and hence the electron-electron correlation factor by measuring R and calculating R_1 and R_3 of Eq. (14).

As a first step in the process, to avoid complexities, we computed I_k in independent electron model with screened nuclear charge and obtained the ratio, for the energy range 200 to 500 keV amu^{-1} where experimental data are partly available. The cross sections for electron transfer from ground state to ground state in single capture, double capture and their ratio are shown in Tables 1—3, respectively. Corresponding theoretical calculations by Mukherjee and his group[8,12] in continuum-distorted wave approximation (CDW) and continuum intermediate-state (CIS) approximation are presented for comparison.

In conclusion we like to say that in the high enregy region as long as the target-nucleus and the projectile interaction is not important the high energy ion-atom collisions leading to electron capture can be dealt with by taking S-matrix expansion between the properly chosen wave functions containing Coulomb-distortion and correlation. A formulation of this typical atomic collision problem in a gauge invariant language, that is similar to those describing most fundamental interactions in nature, has its own intrinsic appeal in highlighting the QED behaviour accompanying the collision processes.

References

1) J. H. McGuire, E. Salzborn and A. Müller, Phys. Rev. **A35** (1987) 3265;
2) J. P. Giese and E. Horsdal, Phys. Rev. Letts. **60** (1988) 2018;
3) E. Y. Kamber, C. L. Cocke, S. Cheng and S. L. Varghese, Phys. Rev. Letts. (1988) 2026;
4) T. J. M. Zouros, D. Schneider and N. Stolterfoht, Phys. Rev. **A35** (1987) 1963;
5) J. H. McGuire, Phys. Rev. Letts. **49** (1982) 1153;
6) M. B. Shah and H. B. Gilbody, J. Phys. **B18** (1985) 899;
7) S. Bhattacharyya, K. Rinn, E. Salzborn and L. Chatterjee, J. Phys. B**21** (1988) 111;
8) G. C. Saha, S. Datta and S. C. Mukherjee, Phys. Rev. **A34** (1986) 2809;
9) H. Suzuki, Y. Kajikawa, N. Toshima, T. Watanabe and R. Ryufuku, Phys. Rev. A**29** (1984) 525;
10) R. Gayet, R. D. Rivarola and A. Salin, J. Phys. B**14** (1981) 2412;
11) V. A. Sidorovich, V. S. Wikolrev and J. H. McGuire, Phys. Rev. A**31** (1985) 2193;
12) M. Ghosh, C. R. Mandal and S. C. Mukherjee, Phys. Rev. A**12** (19817) 2259;
13) I. Haris and C. M. Brown, Phys. Rev. **105** (1957) 1656;
14) S. Bhattacharyya, L. Chatterjee and T. Roy, Ind. J. Pure and Appl. Phys. **17** (1979) 825;
15) L. Chatterjee and S. Bhattacharyya, Phys. Scr. **32** (1985) 504;
16) S. Bhattacharyya, Fizika **19** (1987) 463;
17) A. I. Akhiezer and V. B. Berestetsky, *Quantum Electrodynamics* (N. Y. Interscience) 1965 Ch. 4, 5.

OMJER UDARNIH PRESJEKA ZA UHVAT DVA ELEKTRONA PREMA UHVATU JEDNOG PRI VISOKOENERGETSKOM SUDARU GOLOG PROJEKTILA S He

SUJATA BHATTACHARYYA

Gokhale College, Calcutta 700020, India

UDK 539.12

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Omjer udarnih presjeka za uhvat dva elektrona prema uhvatu jednog pri visokoenergetskom sudaru golog projektila s helijevim (He) atomom dobiven je Feynmanovom tehnikom. Za Li^{3+} projektil nađeno je da se omjer mijenja između 0,03 i 0,017 u području energije od 200 keV amu^{-1} do 300 keV amu^{-1}, dok odgovarajuće eksperimentalne vrijednosti leže između 0,04 i 0,02. Diskutira se energetska ovisnost omjera.