PRAMANA
—journal of
physics

Vol. 50, No. 6,
June 1998
pp. 563–572

A field theoretic approach to the atomic collision problems

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Abstract. It is an endeavour to make field theoretic approach available to the domain of electronic and atomic collision physics. The capacity of QED is demonstrated in explaining atomic collision phenomena in Coulomb gauge and depending on energy, in relativistic Lorentz gauge. Feynman diagrams are used to calculate bound state collision problems in atomic physics.

Keywords. Field theory; atomic collisions.

PACS Nos 34.80; 82.30

1. Introduction

The talk is organized into two parts. In part I we shall discuss field theory in the context of its application in atomic collision problems. Part II will include the calculations of (a) charge signature on ionization-excitation of He by proton and antiproton in Lorentz gauge and (b) radiative recombination of cold electron and proton into hydrogen atom at subzero temperature in Coulomb gauge.

2. Part I – Field theory in bound state problems

Regarding the origin and growth of field theory one can say – where as quantum conditions govern the properties of extremely small bits of matter, relativistic conditions govern the properties of matter travelling at extremely high speed. Their difficult marriage produced what is known as field theory, a sickly child that eventually grew into the robust standard model of elementary particle physics. We are constrained by relativity and quantum mechanics to speak of a funny language of quantum field theory that is used to describe interactions between particles and fields.

In this connection we find that we do not have the right to talk about the complete description of nature. Our description of nature is organized by the distance scale. Newtonian mechanics for instance, is fine to something like billionth of a centimeter. After the advent of QED – we have complete description of nature at distances greater than 10^{-16} cm. After QCD we have complete description of nature below 10^{-16} cm, where elementary particles like proton and neutron begin to show structure. I like to state that *elementarity* of a particle is strongly energy dependent. In the collision theory any matter subjected to the energy opaque to its structure, can be treated as elementary. Thus a nucleus will behave like an elementary particle below its binding energy. One can take the liberty to represent a nucleus as Fermi-particle or a Bose-particle depending on its resultant spin. In atomic physics, bare ions can be represented by Feynman directed line.

Use of field theory in bound state problems in atomic physics may be justified on the following grounds. With the increase in precision in the measurements of various atomic collision processes, application of sophisticated theories are needed to explain experimental findings. Traditionally QED is used to study collision phenomena between free particles. The application of the gauge invariant language of quantum electrodynamics (QED) in collisions of atoms/molecules, with leptons or ions, though rarer, is most general. In the low energy limit QED exhibits classical behaviour. But because of the fully covariant treatment from the onset one may expect to get different results in QED technique as compared to the result obtained by extending the classical result to the relativistic limit. In quantum mechanical collision theory particles are assumed to be free if the interaction vanishes at $t = \pm\infty$. In principle by free particle it is meant that there is no interaction between particle and quantized electromagnetic field [1]. A bound particle in atomic physics is one which is under the influence of the Coulomb field of the nucleus. Bound particles in the presence of the external electromagnetic field have all the characteristics of the free particles as regards equal-time commutators and anticommutators of the field operators [1]. A composite system of particles in QED is represented by a string of field operators (e.g. creation operators) operating on particle vacuum and multiplied by the solution of the Schrödinger equation in momentum space [2]. For interaction between particles, bound or free, one may take for the interaction matrix the free particle interaction Hamiltonian operated between the initial and the final state vectors obtained in a field theoretic way. The interaction Hamiltonian is written either in Coulomb gauge or in Lorentz gauge. Very high energy ion beams now being available, Feynman diagrams are found to be convenient tools for calculating the high energy atomic collision processes. One can represent a nucleus by a Feynman directed line assuming it to be an elementary particle. Bound electrons are also represented by Feynman directed lines, and the information that these are bound will be contained in the state vectors. We have used the field theoretic technique in Coulomb gauge to calculate low energy processes like excitation [3], ionization [4], muon catalysed fusion [5] and recombination [6]. Feynman technique is used to calculate double ionization [7], charge transfer [8], transfer ionization [9] etc., due to high energy collisions. Since detailed discussion of the technique is beyond the scope of this talk, we present in part II two examples on the application of the field theory.

3. Part II

3.1 *Use of Lorentz gauge and Feynman diagram to calculate ionization-excitation of He by proton* (P^{*}) *and antiproton* (P^{-})

$$\mathrm{He} + P^{+}(P^{-}) \rightarrow \mathrm{He}^{+}(nl) + P^{+}(P^{-}) + e^{-}. \tag{1}$$

Single ionization of He by energetic charged particles is well understood as long as He^{+} remains in the ground state [10]. However when the He^{+} goes to the excited state the situation becomes quite fascinating. Several theories exist to explain double ionization (DI) by charged particles, but the quantal calculation on IE [11, 12] is still rare. McGuire

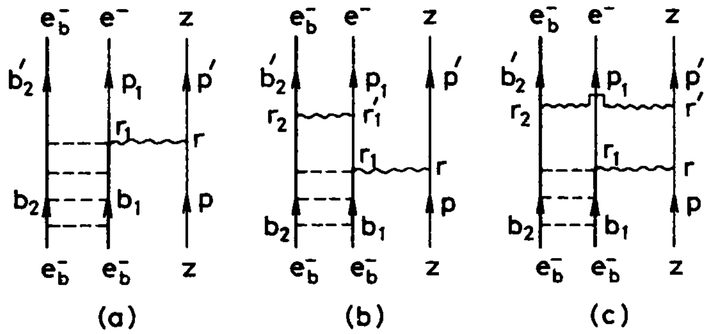

Figure 1. Feynman diagram for ionization-excitation of He by projectiles of charge Z. e_b^- represents bound electron. e^- is the ionized electron. (**a**) Shake-up mechanism, (**b**) two-step-one mechanism, (**c**) two-step-two mechanism.

[13] and Ford and Reading [14] have suggested that IE, being a two-electron process like DI, can be treated by the same model calculation as DI. McGuire has identified collision mechanisms responsible for DI. These are the shake-up (SU) process and the two-step (TS) process. In the present work we shall compute the SU and TS processes in a field theoretic way.

The high energy charged projectile interacts with the electron cloud of the He atom ejecting one electron and leaving behind He^+ in an excited state. Feynman diagrams representing SU mechanism (figure 1a) corresponds to ejection of electron due to the current – current interaction between one of the bound electrons and the fast projectile, and excitation of the second electron due to change in the Coulomb field of the nucleus. The correlated wave function [15] takes care of the Coulomb effect. In principle, SU mechanism arises out of the static correlation between the two bound electrons. The second order Feynman diagram with one virtual photon exchange and the corresponding second order S-matrix giving the SU amplitude can be identified with the first order Born term as given by McGuire. Under TS process there are two fourth-order Feynman diagrams namely two-step-1(TS1) and two-step-2 (TS2). The TS1 mechanism (figure 1b) arises out of the dynamic correlation between the ejected electron and the bound electron. In the TS1 mechanism virtual photon exchange between the projectile and the atom causes ejection of one of the electron. The ejected electron in turn exchanges a virtual photon with the remaining bound electron raising it to the excited state. The TS2 mechanism (figure 1c) is a case of double collision between the projectile and the He atom. Projectile exchanges two virtual photons with the target causing simultaneous ionization and excitation. TS amplitudes can be identified with the second order Born terms in matter-radiation field coupling. Unlike McGuire's TS amplitudes, present TS amplitudes cannot be taken as the products of S-matrices for single ionization and excitation. TS1 and TS2 both contain two virtual photon propagators and one particle propagator. The particle propagator in the TS1 amplitude is an electron propagator necessary for dynamic correlation between the outgoing electron and the bound electron which is excited. In the TS2 process the particle propagator is the projectile propagator essential for double collision causing simultaneous ionization and excitation. As such, because of the anticommutative and covariant nature of the algebra, contributions from the TS1 and TS2 terms, and the term due to interference between SU and TS, will be at variance with that obtained from usual quantum mechanical methods. The SU and the TS1 amplitudes contain Z (projectile charge), while the TS2 amplitude contains Z^2 as factor. The interference of TS2 with SU and TS1, which is proportional to Z^3, causes differences in IE of He by protons and antiprotons.

In the present paper we find that for projectile energies from 1–3 MeV/amu, the total cross section for IE by antiprotons becomes greater than that by equivelocity protons by a factor of two, only when the maximum limiting value of the energy E_1 of the ejected electron is less than 39.5 eV. We have presented here the total cross section (TCS) for IE of He to $2p$-state, as well as the differential cross section (DCS) with respect to E_1.

For like-charge projectile (p^-, e^-), the present theory predicts decreasing cross section with increasing mass. In the absence of any theoretical calculation we have compared the present result with the existing experimental data [16, 17]. IE by electrons is also presented. The experimental data by the two groups [16, 17] do not agree among themselves. Fuelling *et al* and Pederson and Folkman had declared uncertainties to the extent of 10% and 20% respectively in their data.

The interaction S-matrix is computed between the initial and the final bound state vectors $|\Psi_i\rangle$ and $|\Psi_f\rangle$ respectively [18].

$$|\Psi_i\rangle = (2\pi)^{1/2}\exp(iR_0L_0)\phi_i(x,y,R)C^+_{b_1}C^+_{b_2}a^+_p|0\rangle, \tag{2}$$

$$|\Psi_i\rangle = (2\pi)^{1/2}\exp(iR_0L_0)\phi_i(x,y,R)C^+_{p_1}C^+_{p_2}a^+_{p'}|0\rangle, \tag{3}$$

where $\vec{r}_1 = \vec{r}_1 - \vec{R}$, $\vec{y} = \vec{r}_2 - \vec{R}$. $\vec{r}_1, \vec{r}_2$ and $\vec{R}$ are respectively the space coordinates of the two electrons and CM of the He atom. $L(L_0, \vec{L})$ and $R(R_0, \vec{R})$are the 4-momentum and the 4-coordinate respectively of the CM. C_{p_1}'s and a_p's are the annihilation operators of the electrons and charged projectiles respectively with $u(p_1)$ and $U(p)$ being the corresponding spinors.

The bound electron current at r_1 is

$$(J^e_\mu)_{r_1} = (\overline{\Psi}_e\gamma_\mu\Psi_b)_{r_1}. \tag{4}$$

The projectile current at r is

$$(J^z_\nu)_r = (\overline{\Psi}_z\gamma_\nu\Psi_z)_r. \tag{5}$$

Ψ_e, Ψ_b, and Ψ_z are respectively the state vectors for ionized-electron, bound electron and the projectile of charge Z. $D(r - r_1)$ is the photon propagator. $S_e(r_2 - r_1')$ is the electron propagator in figure 1b, and $S_z(r' - r)$ is the projectile propagator in figure 1c. The S-matrices corresponding to different diagrams are given below [19].

$$S^{\rm su}_2 = Ze^2(J^e_\mu)_{r_1}D(r - r_1)(J^z_\nu)_r, \tag{6}$$

$$S^{\rm ts1}_4 = Ze^4(J^z_\nu)_r\overline{\Psi}_f\gamma_\mu S_e(r_1' - r_1)\gamma_\nu\Psi_f(J^e_\mu)r_2D(r - r_1)D(r_2 - r_1'), \tag{7}$$

$$S^{\rm ts2}_4 = Z^2e^4\overline{\Psi}_z\gamma_\mu S_z(r' - r)\gamma_\nu\Psi_z(J^e_\nu)r_2(J^e_\mu)r_1D(r - r_1)D(r' - r_2). \tag{8}$$

The probability amplitude for IE will be given by

$$M_{fi} = \langle\Psi_f|S^{\rm su}_2 + S^{\rm ts1}_4 + S^{\rm ts2}_4|\Psi_i\rangle. \tag{9}$$

The cross section for the process is given by

$$\sigma^z = \frac{M}{|p|}\int \left|M_{fi}^z\right|^2 \frac{d^3p'd^3p_1}{(2\pi)^6} = \frac{mM}{|\vec{p}|}\int C|W^z|^2|\vec{p}_1|dE_1 d\Omega. \tag{10}$$

C is a function of the incident projectile momentum and

$$|W^z|^2 = (Ze^2K_1 + Ze^4K_2 + Z^2e^4K_3)^2. \tag{11}$$

The three terms in W^z are contributions from the three mechanisms SU, TS1 and TS2 respectively [20]. K's contain the products of spinors and propagators. It is obvious from W^z that the cross section will contain a term proportional to Z^3 that will be responsible for any difference in the cross sections between the negative and the positive projectiles. The dominant contribution from W^z is

$$|W^z|^2 = (8m^2E_1^2X_2^2)^{-1}[Z^2X_2^2 + Z^2 12\pi e^2/\Delta_{nl} - Z^3 6\pi e^2/\{F_{nl}(\varepsilon_{1s}/E_1 - 1)\}],$$

where

$$X_2^2 = (\varepsilon_{1s} - \varepsilon_{nl})^2, \quad \Delta_{nl} = \varepsilon_{1s^2} - \varepsilon_{nl},$$

$$F_{nl} = \Delta_{nl} - \varepsilon_{1s} - \frac{E}{M}\left(1 - \frac{E_1 + \varepsilon_{1s}}{2E}\right)(E_1 + \varepsilon_{1s})$$

and E_1 is the energy of the ejected electron, E is the projectile energy, $\varepsilon_{1s^2} = 2\varepsilon_{1s} = 79.0\,\mathrm{eV}$.

By negative projectile, IE is found to be a factor of two, larger than that by the equivelocity positive projectile in the collision energy range 1–3 MeV/amu. The present result is shown in figures 2, 3 alongwith the existing experimental results [16, 17].

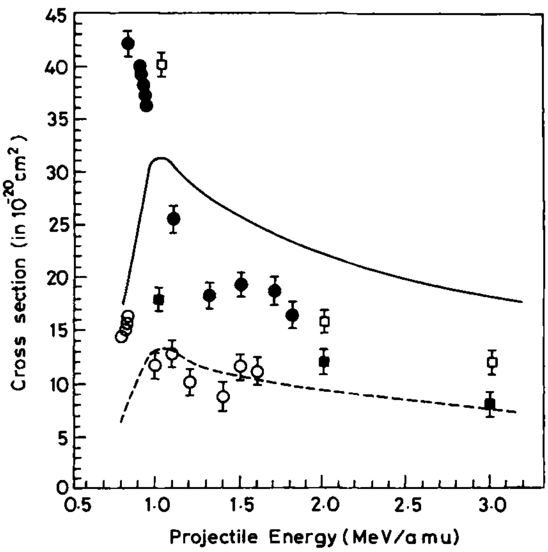

Figure 2. Total cross section for ionization-excitation of He to $2p$-state versus energy of the projectiles e^- and p^+. Present result: e^-, ———; p^+, - - - - - -. Experiment: Fuelling *et al* [16] $e^- \to \bullet$, $p^+ \to \circ$; Pedersen and Folkman [17] $e^- \to \square$, $p^+ \to \blacksquare$.

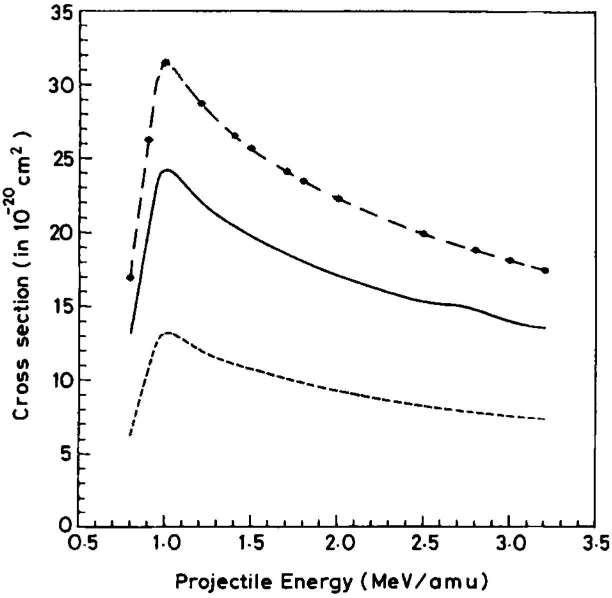

Figure 3. Same as in figure 2 for present result with projectiles. e^-, -*-; p^-, ——; p^+, - - -.

3.2 Use of QED in Coulomb gauge: Radiative recombination (RR) of cold electron with proton

Spontaneous radiative recombination (SRR) of electron with proton with the spontaneous emission of photon of continuous spectrum via the reaction channel

$$p^+ + e^- \rightarrow \mathrm{H}(1s) + \gamma \tag{12}$$

is known for a long time. Kramer [21] calculated the SRR cross section in 1923 in a semiclassical approach. The quantum mechanical first-order perturbation theory for the same problem was devised by Gordon [22] and implemented by Stobbe [23]. Same calculation also holds good for the formation of antihydrogen from antiproton and positron. Pajek and Schuch [24] have studied the process in a non-relativistic dipole approximation. Experimentally RR are being investigated in the range 10^{-4} to 1 eV by a group in Stockholm [25]. Experimental data are usually compared with Kramers' results at low energies applying correcting Gaunt factor. However, Kramers–Gaunt approach systematically yields results smaller than the experimental data [25].

To reduce the gap between the experimental and the theoretical results we have argued that the emitted photon can have both the continuous spectrum as well as discrete spectrum. A new channel

$$p^+ + e^- \rightarrow \mathrm{H}(np) \rightarrow \mathrm{H}(1s) + h\nu \tag{13}$$

namely two-step-radiative recombination (TSRR) channel (13) is considered over and above the existing SRR channel (12). In TSRR channel recombination occurs in an intermediate excited state and to conserve momentum it comes to the ground state with

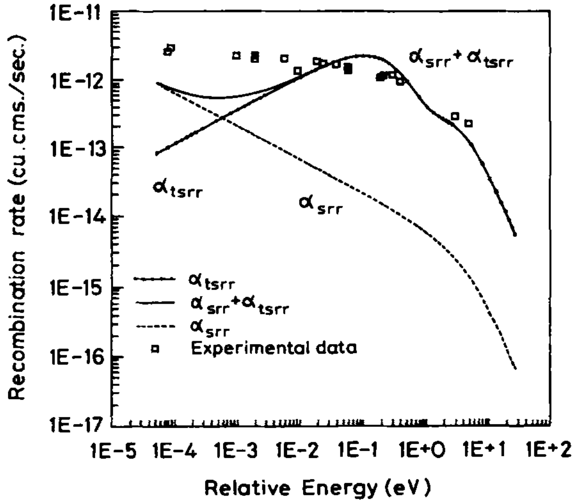

Figure 4. Radiative recombination rates $\alpha_{\rm srr}$ and $\alpha_{\rm tsrr}$ for SRR and TSRR processes respectively.

emission of a discrete photon. We have computed RR cross sections via both the channels in a field theoretic approach in Coulomb gauge. In the SRR channel dominant contribution comes from the recombination into $1s$ and $2s$ states and compares well with the results of Kramers–Gaunt–Stobbe. Recombination into $2p$ state is several order smaller than that into $1s$ state. Recombination via TSRR channel into $1s$ state with $2p$ and $3p$ as the intermediate state are computed. The sum of the contributions of the radiative recombination rates from SRR and TSRR channels are found to agree fairly well with those of the experimental results [25] (figure 4).

The state vectors of the interacting systems in the initial and in the final states are respectively [3]

$$|\Psi_i\rangle = \mathrm{e}^{-iE_it/\hbar}\int g_i(\vec{q}_1,\vec{l}_1)c^+_{q_1}a^+_{l_1}|0\rangle \mathrm{d}^3q_1\mathrm{d}^3l_1 \tag{14}$$

and

$$|\Psi_f\rangle = \mathrm{e}^{-iE_ft/\hbar}\int g_f(\vec{q}_3,\vec{l}_3)c^+_{q_3}a^+_{l_3}b^+_k|0\rangle \mathrm{d}^3q_3\mathrm{d}^3l_3\mathrm{d}^3k$$

where c^+_q, a^+_1 and b^+_k are the creation operators for electron, proton and photon respectively. g-functions are the Fourier transform in momentum space of the solutions of the Schrödinger equations of the interacting particles. For the TSRR channel the state vector at the intermediate state is

$$|\Psi_I\rangle = \mathrm{e}^{-iE_It/\hbar}\int g_I(\vec{q}_2,\vec{l}_2)c^+_{q_2}a^+_{l_2}|0\rangle \mathrm{d}^3q_2\mathrm{d}^3l_2. \tag{15}$$

Interaction terms: S-matrix for the two body radiative recombination is

$$S = 1 + H_1 + H_2 + H_1H_1 + H_1H_2 + H_2H_2 + \cdots, \tag{16}$$

where H_1 is the interaction term between matter and electromagnetic field. H_2 is the Coulomb interaction term

$$H_1 = (e/mc)PA(x) + (e^2/2mc^2)A^2(x), \tag{17}$$

$$A(x) = \sum_{\sigma}(2\pi\hbar c^2/\omega k)^{1/2}u_\sigma\{c_k \exp(-ik.x) + c_k^+ \exp(ik.x)\}. \tag{18}$$

The Coulomb attraction H_2 between e^- and $P^+(D^+)$ to form the virtual intermediate excited state in the TSRR process is

$$H_2 = \int \{\rho(x)\sigma(x')/|x - x'|\}\mathrm{d}^3x\mathrm{d}^3x'. \tag{19}$$

$\rho(x), \sigma(x')$ are the charge densities for electron and proton respectively,

$$\rho(x) = -e\phi^*(x)\phi(x), \quad \sigma(x') = e\theta^*(x')\theta(x').$$

The electron and proton field operators are respectively

$$\phi(x) = \sum_r \int a_s^+\chi_r \exp(is.x)\mathrm{d}^3s, \quad \theta(x') = \sum_r \int B_{s'}^+\lambda_r \exp(is'.x')\mathrm{d}^3s'. \tag{20}$$

From (16) the lowest order perturbation responsible for SRR and TSRR are respectively H_1 and H_1H_2. The matrix element for the formation of atom at sub-zero temperature are given below.

Two-body radiative recombination:

(i) *SRR channel*: The amplitude M_{SRR} for SRR process calculated using dipole approximation

$$M_{\mathrm{SRR}}^{nl} = \langle\Psi_f|H_1|\Psi_i\rangle$$
$$= \underline{C}(-im/k)\hbar ck\langle\Psi_f|c_k^+P|\Psi_i\rangle \sin\theta. \tag{21}$$

θ is the angle between the relative momentum $\vec{p}$ between electron and proton, and momentum $\vec{k}$ of photon,

$$\underline{C} = (e/mc)(2\pi\hbar c^2/\omega)^{1/2}.$$

After integration over the momentum space

$$M_{\mathrm{SRR}}^{nl} = \underline{C}(-im/\hbar)\int \phi_{nl}(r)r\cos\theta\Psi_c(r)\sin\theta\mathrm{d}^3r. \tag{22}$$

$\phi_{nl}(r)$ is the wave function of electron in the bound state of the hydrogen atom. $\Psi_c(r)$ is the distorted plane wave of the electron

$$\Psi_c(r) = (2\pi me^2/\hbar^2 p)^{1/2}\exp(ip.r).$$

The SRR cross-section for the formation of hydrogen atom into nl-state

$$\sigma_{\mathrm{SRR}}^{nl}(E_i) = (m/p)\{(2\pi)^{-5}/\hbar\}\int \delta(E_i - E_f)|M_{\mathrm{SRR}}|^2\mathrm{d}^3k\mathrm{d}^3p'. \tag{23}$$

Cross sections are calculated for recombination into $1s, 2s$ and $2p$ states. The atom formation cross-section via SRR channel in $1s$-state is higher than that in the $2s$ and $2p$ states.

(ii) *TSRR channel.* The matrix element for the two step process is

$$M_{\mathrm{TSRR}} = \frac{\langle \Psi_f | H_1 | \Psi_i \rangle \langle \Psi_i | H_2 | \Psi_f \rangle}{[E_i - E_I + i\eta]} = \frac{M_1^{1s} M_2^{nl}}{[E_i - E_I + i\eta]}, \tag{24}$$

where M_2^{nl} is the amplitude for Coulomb recombination into virtual intermediate state and M_1^{1s} is the spontaneous decay amplitude from the nl intermediate state into $1s$ state.

$$M_1^{1s} - \langle \Psi_f | H_1 | \Psi_I \rangle = \underline{C}(-im/\hbar) h\nu_{nl\to 1s} \int \Psi_{1s}(r) r \cos\theta \Psi_{nl}(lr) \sin\theta \mathrm{d}^3 r, \tag{25}$$

$$M_2^{nl} = \langle \Psi_I | H_2 | \Psi_i \rangle = -e^2 \delta^3 (P_i - Q_c) J_{nl}, \tag{26}$$

$$J_{nl} = \int [\Psi_{nl}(r) \Psi_c(r) / |r|] \mathrm{d}^3 r. \tag{27}$$

The cross section for the two step radiative recombination becomes

$$\sigma_{\mathrm{TSRR}}^{nl}(E_i) = (2\pi/\hbar) \int \delta(E_i - E_f)(m/\hbar |p|)(2\pi)^{-5} |M_{\mathrm{TSRR}}|^2 \mathrm{d}^3 k \mathrm{d}^3 p' = \tau_{nl\to 1s}^{-1} e^4 (2\pi)^{-3} (m/\hbar |p|) \int (E_i - E_I)^{-2} J_{nl}^2 \mathrm{d}^3 p', \tag{28}$$

where the decay rate $\tau_{nl\to 1s}^{-1}$ of $nl \to 1s$ state is given by

$$\tau_{nl\to 1s}^{-1} = (2\pi/\hbar) \int \delta(E_i - E_f) |M_1^{1s}|^2 (2\pi)^{-3} \mathrm{d}^3 k. \tag{29}$$

At relative energies less than 1 eV, the TSRR cross section via intermediate $3p$-state is one order higher than that via intermediate $2p$-state.

Recombination rate: For monochromatic beams of electron and proton with relative velocity v_i, the recombination rates α_{srr} and α_{tsrr} via SRR channel and TSRR channel respectively are given below.

$$\alpha_{\mathrm{srr}} = \langle \sigma_{\mathrm{SRR}}^{nl}(E_i) \cdot v_i \rangle, \quad \alpha_{\mathrm{tsrr}} = \langle \sigma_{\mathrm{TSRR}}^{nl}(E_i) \cdot v_i \rangle.$$

α_{srr} and α_{tsrr} are shown in figure 4 along with the experimental results. It is obvious from the diagram that the experimental data lie closer to the curve for the rate sum $\alpha_{\mathrm{srr}} + \alpha_{\mathrm{tsrr}}$. As the energy increases above 10 meV, α_{tsrr} dominates over α_{srr}.

4. Conclusion

The above two examples amply show the flexibility of QED in containing both the low and high energy collision phenomena in the atomic domain.

Unlike single ionization the IE of He depends on the charge signature of the projectile. The interference term of the TS2 amplitude with those of SU and TS1 which is proportional to z^3, causes difference in the cross sections by positive and negative projectiles. Further, as the mass term enters into the SU amplitude, IE by electron is different from that by antiproton. Present result agrees in principle with that of the experimental result [16, 17] and with the theoretical prediction of McGuire [12].

For the radiative recombination (RR) of cold electron with proton to form hydrogen or RR of cold positron with antiproton to form antihydrogen, present results from SRR and TSRR channels compare well with the experimental results which are higher than the existing predictions from SRR channel alone.

We like to conclude that the field theory, which can explain most of the fundamental processes in nature, provides a compact and elegant tool for calculating the atomic and ionic collision problems.

Acknowledgement

The author is grateful to K Pathak, S Mitra, A Roy and S K Bhattacharyya who rendered help in the numerical computations and in drawing the graphs. The work is supported by UGC, New Delhi through Project No. F.10-100/90(RBB-II).

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