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RADIATIVE RECOMBINATION OF COLD ELECTRON WITH PROTON AND DEUTERON

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The paper presents calculation of the radiative recombination (RR) cross-sections of cold electron with proton and deuteron via the two-step radiative recombination (TSRR) process. TSRR occurs in a virtual excited state which, to conserve momentum, decays to the ground state with the emission of a photon. The RR process due to the dipole interaction leading to the spontaneous photo-recombination (SRR), which is known for a long time, can not fully explain the recent experimental data. The radiative recombination is computed for TSRR channels using field theory and Coulomb gauge. Sum of the recombination rates from SRR and TSRR channels is compared with the experimental results.

1. Introduction

The radiative recombination (RR), the binding of a free electron with a proton (deuteron) accompanied by emission of radiation, plays an important role in astrophysical and fusion plasmas. The RR is one of the most fundamental processes in atomic physics and is connected to photo-ionization by the principle of detailed balance. Recombination of electron to proton with emission of radiation can also take place in the presence of a

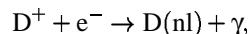
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third particle (electron or photon). The study of RR of electron with proton in the *spontaneous radiative recombination* (SRR) channel, in absence of a third particle, dates back to 1923 by Kramers [1] within a semiclassical approach. The quantum mechanical first-order perturbation theory for the process was devised by Gordon [2] and implemented by Stobbe [3]. The radiative recombination coefficients of hydrogenic atoms are also calculated in terms of oscillator strength [4] using the recalculated Gnat factor. Pajek and Schuch have studied RR as a time reversed photoionization process in a non-relativistic dipole approximation [5]. Analytical power-law fits to the rates of radiative recombination of H-like ions are available [6] over a wide range of temperatures from 3 to 10^9 K.

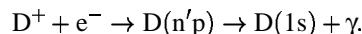
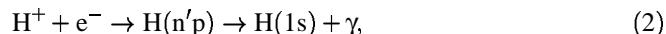
Experimentally [7,8] interest in RR of *supercool electron and proton into hydrogen atom* has been revived in the last several years due to the availability of electron and proton (deuteron) beams at sub-meV energies. The high value of the experimental data in CRYRING [8] on the recombination rates of proton (deuteron) and electron at sub-zero temperatures, in which possibility of the three-body recombination is reported negligible, however can not be explained by the existing theoretical results from SRR channel.

Since there is still scope for theory and speculation, we have assumed the presence of the *two-step radiative recombination* (TSRR) channel in RR over and above the usual SRR channel. The RR via TSRR channel occurs in two stages. Initially, the recombination takes place into a virtual excited state due to the Coulomb interaction. Subsequently, to conserve momentum, the virtual excited state decays to the ground state by dipole interaction, emitting photons of discrete energy. The TSRR is a second-order process. We have used field theory (FT) as in Ref. 9 to compute TSRR. Before applying the TSRR channel, we have tried it on SRR channel, for which theoretical results are available [3]. The field theoretic results on SRR are found comparable to those by Stobbe [3] for recombination into 1s and 2s+2p states of hydrogen atom. Since the result is mass independent, it is also true for deuteron. The sum total of the contributions from SRR and TSRR channels is found to partially explain the experimental results [8].

The physical processes leading to the SRR are



and those leading to the TSRR processes are



The photon emitted through SRR channel (1) has a continuous spectrum, while the spectrum emitted through TSRR channel is discrete.

2. Radiative recombination cross-sections

The initial state vector $|\Psi_i\rangle$ of the interacting system [9] of electron and proton having annihilation operators with momenta a_q and B_l , respectively, is

$$|\Psi_i\rangle = \exp\left(\frac{iE_it}{\hbar}\right) \int g_c(\vec{q}_1) \delta^3(\vec{q}_1 + \vec{l}_1 - \vec{P}_c) a_{q_1}^\dagger B_{l_1}^\dagger |0\rangle d^3\vec{q}_1 d^3\vec{l}_1. \quad (3)$$

The final state vector $|\Psi_f\rangle$ of the interacting system of electron, proton and photon is

$$|\Psi_f\rangle = \exp\left(\frac{iE_{ft}}{\hbar}\right) \int g_{nl}(\vec{q}_2) \delta^3(\vec{q}_2 + \vec{l}_2 + \vec{k}' - \vec{Q}_c) a_{q_2}^\dagger B_{l_2}^\dagger C_{k'}^\dagger |0\rangle d^3\vec{q}_2 d^3\vec{l}_2 d^3\vec{k}'. \quad (4)$$

$C_{k'}$ is the annihilation operator for photon of momentum \vec{k}' . \vec{P}_c and \vec{Q}_c are the CM momenta of the initial and the final systems, respectively. The virtual-intermediate state vector in the TSRR channel is

$$|\Psi_I\rangle = \exp\left(\frac{iE_{It}}{\hbar}\right) \int g_{n'l'}(\vec{q}_3) \delta^3(\vec{q}_3 + \vec{l}_3 - \vec{p}_{c'}) a_{q_3}^\dagger B_{l_3}^\dagger |0\rangle d^3\vec{q}_3 d^3\vec{l}_3. \quad (5)$$

$g_c(\vec{q}_1)$ in (3) is the Fourier transform in momentum space of the Coulomb distorted solution $\phi_i(\vec{x}_1, \vec{x}_2)$ of the Schrödinger equation of free electron in the field of proton in the initial state [Eq. (36) in Ref. 9]:

$$(H_0 + v)\phi_i(\vec{x}_1, \vec{x}_2) = E_i\phi_i(\vec{x}_1, \vec{x}_2)$$

v is the Coulomb interaction providing distortion to the plane wave, E_i is the positive eigenvalue of $(H_0 + v)$, H_0 is the free particle Hamiltonian for electron and proton, and $g_{n'l'}(\vec{q}_3)$ and $g_{nl}(\vec{q}_2)$ in (4) and (5) are the Fourier transforms in momentum space of the bound state solutions $\phi_f(\vec{x}_1, \vec{x}_2)$ and $\phi_I(\vec{x}_1, \vec{x}_2)$ of the Schrödinger equations in the final and intermediate states, respectively [Eq. (37) in Ref. 9]:

$$(H_0 + v')\phi_{f,I}(\vec{x}_1, \vec{x}_2) = E_{f,I}\phi_{f,I}(\vec{x}_1, \vec{x}_2).$$

E_f and E_I are the negative eigenvalues of $(H_0 + v')$ in the final and intermediate states, respectively, and v' is the interaction potential in the bound state.

The interaction Hamiltonian between the electron and the electromagnetic radiation field is

$$H_1 = \frac{e}{mc} \vec{p} \cdot \vec{A}(\vec{x}) + \frac{e^2}{2mc^2} \vec{A}^2(\vec{x}) = H'_1 + H''_1. \quad (6)$$

\vec{p} is the momentum operator and \vec{A} is the vector potential:

$$\vec{A}(\vec{x}) = \sum_k \sqrt{\frac{2\pi\hbar c^2}{\omega_k}} \vec{u} \{ C_k \exp(-i\vec{k} \cdot \vec{x}) + C_k^\dagger \exp(i\vec{k} \cdot \vec{x}) \}. \quad (7)$$

\vec{u} is the polarisation vector, \vec{k} is the photon momentum and C is the annihilation operator for photon. For single photon emission, we consider the first term, H'_1 , of the interaction H_1 in (6). The Coulomb attraction H_2 between electron and proton (deuteron) for the formation of the virtual intermediate state in the TSRR channel is

$$H_2 = \int \frac{\rho(\vec{x})\sigma(\vec{x}')}{|\vec{x} - \vec{x}'|} d^3\vec{x}d^3\vec{x}'. \quad (8)$$

$\rho(\vec{x})$ and $\sigma(\vec{x}')$ are the charge densities of electron and proton (deuteron), respectively:

$$\rho(\vec{x}) = -e \phi^*(\vec{x})\phi(\vec{x})$$

$$\sigma(\vec{x}) = e \theta^*(\vec{x})\theta(\vec{x}).$$

$\phi(\vec{x})$ and $\theta(\vec{x})$ are the field operators for electron and proton, respectively:

$$\phi(\vec{x}) = \sum_f \int \kappa_f a_s^\dagger \exp(i\vec{s} \cdot \vec{x}) d^3\vec{s}$$

$$\theta(\vec{x}) = \sum_{f'} \int \lambda_{f'} B_{s'}^\dagger \exp(i\vec{s}' \cdot \vec{x}) d^3\vec{s},$$

where κ and λ are the Pauli spinors for electron and proton, respectively.

The S-matrix for the two-body radiative recombination is

$$S = 1 + H_1 + H_2 + H_1 H_1 + H_1 H_2 + H_2 H_2 + \text{higher order terms.} \quad (9)$$

The interaction terms H_1 and $H_1 H_2$ are responsible for SRR and TSRR channels. The first of H_1 in (6) gives rise to the SRR channel (1) and the corresponding amplitude is given by

$$M_s = \langle \Psi_f | (e/mc) \vec{p} \cdot \vec{A}(\vec{x}) | \Psi_i \rangle. \quad (10)$$

The amplitude for the TSRR channel is given by

$$M_T = \frac{\langle \Psi_f | H'_1 | \Psi_I \rangle \langle \Psi_I | H'_1 | \Psi_i \rangle}{E_i - E_I + i\eta}. \quad (11)$$

2.1. Spontaneous radiative recombination (SRR)

Summing over the photon polarization directions, and using the dipole approximation, the SRR amplitude (10) becomes

$$M_s = \bar{C} \langle \Psi_f | C_k^\dagger p | \Psi_i \rangle \sin \theta,$$

where

$$\bar{C} = \frac{e}{mc} \sqrt{\frac{2\pi\hbar c^2}{\omega}},$$

and θ is the angle between \vec{p} and \vec{k} . Taking photon momentum in the direction of z -axis,

$$M_s = \bar{C} \frac{im}{\hbar} (E_A - E_i) \langle \Psi_f | C_k^\dagger z | \Psi_i \rangle \sin \theta. \quad (12)$$

$E_A = E' - \epsilon_{nl}$, E' is the kinetic energy of the atom formed in the final state and ϵ_{nl} is the nl -state binding energy. Further,

$$E_A - E_i = \hbar\omega.$$

$\hbar\omega$ is the energy of the emitted photon in the SRR channel. The vacuum expectation value of the creation and annihilation operators in (12) gives the products of Dirac's delta functions as follows:

$$\langle 0 | C_{k'} B_{l_2} a_{q_2} C_k^\dagger a_{q_1}^\dagger B_{l_1}^\dagger | 0 \rangle = \delta^3(\vec{k}' - \vec{k}) \delta^3(\vec{l}_2 - \vec{l}_1) \delta^3(\vec{q}_2 - \vec{q}_1).$$

Integrating (12) over the momentum δ -function and transforming to the coordinate space, we get

$$M_s = \frac{\pi}{2} \bar{C} \left(\frac{-im}{\hbar} \right) \hbar\omega \int \Phi_{nl}(\vec{r}) r \cos \theta \Phi_c(r) \sin \theta d^3 \vec{r}. \quad (13)$$

Φ_{nl} is the bound state of the hydrogen atom in the nl -state. The distorted plane wave of the incident electron is

$$\Psi_c(\vec{r}) = F_c(\xi) \exp(i \vec{p} \cdot \vec{r}), \quad (14)$$

where $F_c(\xi) = \sqrt{2\pi m e^2 \xi / (\hbar^2 p)}$ is the Sommerfeld factor, $\xi (=1)$ is the charge of the target, and \vec{p} is the momentum of the electron relative to the target. The cross-section for SRR into the nl -state is

$$\sigma_{nl}^s(E_i) = \frac{m}{p} \frac{2\pi}{\hbar} \int \delta(E_i - E_f) | M_s |^2 d^3 \vec{k} d^3 \vec{p}' \frac{1}{(2\pi)^6}. \quad (15)$$

\vec{k} and \vec{p}' are the momenta of the photon and the atom, respectively. Writing

$$d^3 \vec{p}' = 4\pi m \sqrt{2mE'} dE',$$

$$d^3 \vec{k} = \frac{\omega^2}{c^3} d\omega \sin \theta d\theta d\phi,$$

the expression for the cross-section in (15) is integrated over dE' using the δ -function. As the limit of integration over ω is from 0 to $(E_i + \varepsilon_{nl})/\hbar$, after phase-space integration, we obtain

$$\sigma_{nl}^s(E_i) = \frac{\sqrt{2}\xi}{15c^3p^2} I_{nl}^2 \int_0^{(E_i + \varepsilon_{nl})/\hbar} \omega^3 \sqrt{E'} d\omega. \quad (16)$$

From energy conservation relation $E' = E_i + \varepsilon_{nl} - \hbar\omega$, the overlap integral I_{nl} is

$$I_{nl} = \int \Phi_{nl}(r) r \exp(i \vec{p} \cdot \vec{r}) d^3r.$$

For monochromatic beams of ions and electrons, the recombination rate via SRR channel into different nl -states, with relative velocity v_i , is given by

$$\alpha_s = \sum_{nl} \langle \sigma_{nl}^s(E_i) v_i \rangle. \quad (17)$$

For the relative collision energy E_i , the energy spectrum of the photons is given by

$$\frac{d\sigma(\omega)}{d\omega} = \frac{\xi\omega^3}{30c^3p^2} \sqrt{2(E_i + \varepsilon_{nl} - \hbar\omega)} I_{nl}^2. \quad (18)$$

2.2. Two-step radiative recombination (TSRR) rate

From Eq. (11), the amplitude for TSRR can be written as

$$M_T = \frac{M_1 M_2}{E_i - E_I + i\eta}, \quad (19)$$

where

$$M_1 = \langle \Psi_f | H'_1 | \Psi_I \rangle \quad \text{and} \quad M_2 = \langle \Psi_I | H_2 | \Psi_i \rangle. \quad (20)$$

M_2 is the amplitude for capture of electron by proton (deuteron) into the virtual excited $n'l'$ -state and M_1 is the amplitude for the decay of the virtual excited $n'l'$ -state into nl -state due to dipole interaction. The TSRR cross-section for recombination into the nl -state via $n'l'$ -state becomes

$$\sigma_{n'l'}^T(E_i) = \frac{2\pi}{\hbar} \int \delta(E_i - E_f) \frac{m}{\hbar|\vec{p}|} |M_T|^2 \frac{d^3\vec{k} d^3\vec{p}'}{(2\pi)^6}. \quad (21)$$

Since the transition rate $\tau_{n'l' \rightarrow nl}$ from $n'l'$ -state to nl -state is given by

$$(\tau_{n'l' \rightarrow nl})^{-1} = \frac{2\pi}{\hbar} \int \delta(E_i - E_f) |M_1|^2 \frac{d^3\vec{k}}{(2\pi)^3}, \quad (22)$$

the TSRR cross-section (17) can be written as

$$\sigma_{n'l'}^T(E_i) = (\tau_{n'l' \rightarrow nl})^{-1} \frac{m}{\hbar |\vec{p}|} \int |M_2|^2 \frac{d^3 \vec{p}'}{(2\pi)^3}. \quad (23)$$

To compute M_2 , the interaction potential H_2 in (8) is first written in momentum space [9]:

$$H_2 = -e^2 \int \delta(\vec{s}_1 - \vec{s}_2 + \vec{s}_1' - \vec{s}_2') \frac{2}{|\vec{s}_1 - \vec{s}_2|} \kappa_r^* \kappa_r \lambda_{r'}^* \lambda_{r'} a_{s_1}^\dagger a_{s_2} B_{s_1'}^\dagger B_{s_2'} d^3 \vec{s}_1 d^3 \vec{s}_2 d^3 \vec{s}_1' d^3 \vec{s}_2'. \quad (24)$$

Substituting in (20) from (3), (5) and (24), after some calculations, we get

$$M_2 = -e^2 \delta^3(\vec{P}_c - \vec{Q}_c) \int \frac{g_{n'l'}(\vec{q}_3) g_c(\vec{q}_1)}{(\vec{q}_1 - \vec{q}_3)^2} d^3 \vec{q}_1 d^3 \vec{q}_3.$$

Using the Bethe integral and transforming into coordinate space, we get

$$M_2 = -e^2 \delta^3(\vec{P}_c - \vec{Q}_c) J_{n'l'}, \quad (25)$$

where

$$J_{n'l'} = \int \frac{\Phi_{n'l'}(r) \Psi_c(r)}{|r|} d^3 \vec{r}. \quad (26)$$

Integrating over $d^3 \vec{p}'$, and using the atomic unit, we get from (23) for the TSRR cross-section

$$\sigma_{n'l'}^T(E_i) = (\tau_{n'l' \rightarrow nl})^{-1} \frac{e^4}{(2\pi)^3} \frac{m}{|\vec{p}|} J_{n'l'}^2 \frac{8\pi m \sqrt{2}}{3} \frac{\sqrt{(E_i + \epsilon_{nl})^3}}{(E_i - E_l)^2}. \quad (27)$$

The recombination rate α_T^T due to the TSRR process is obtained from Eq. (17)

$$\alpha_T = \sum_{n'l'} \langle \sigma_{n'l'}^T(E_i) v_i \rangle. \quad (28)$$

3. Results and discussions

We calculate the SRR cross-section $\sigma_{nl}^s(E_i)$ for recombination of the super cool electrons and protons (deuterons) into the first and the second Bohr orbits of hydrogen atom. The TSRR cross-section is computed for recombination into the ground state via 2p and 3p virtual intermediate states. Usually, atom formation is said to be complete if recombination occurs to the ground state. All the computations are done in atomic units where $e = m = \hbar = 1$, and $c = 1/137$.

The SRR cross-section (16) for recombination into the ground state becomes

$$\sigma_s^{ls}(E_i) = \bar{A} (8\sqrt{\pi})^2 \frac{(E_i + \epsilon_{ls})^{9/2}}{2E_i} \left(\frac{3 - 2E_i}{(1 + 2E_i)^3} \right)^2, \quad (29)$$

where $\bar{A} = 0.0507\sqrt{2}/(15 c^3)$. The SRR cross-section into the excited level ($n = 2$) is calculated for both 2s and 2p states:

$$\sigma_s^{2s}(E_i) = \bar{A} \frac{8\pi}{2E_i(0.25 + 2E_i)^8} [(E_i + \varepsilon_{2s})^{9/2} (4E_i + 4E_i^2 + 9/16)^2], \quad (30)$$

$$\sigma_s^{2p}(E_i) = \bar{A} \frac{2\pi}{4E_i^2(0.25 + 2E_i)^8} [(E_i + \varepsilon_{2p})^{9/2} (16E_i^2 - 10E_i)^2]. \quad (31)$$

The present results for the SRR cross-sections into the 1s state and sum of the SRR cross-sections into 2s and 2p states are shown in Fig. 1, along with the results by Stobbe [3].

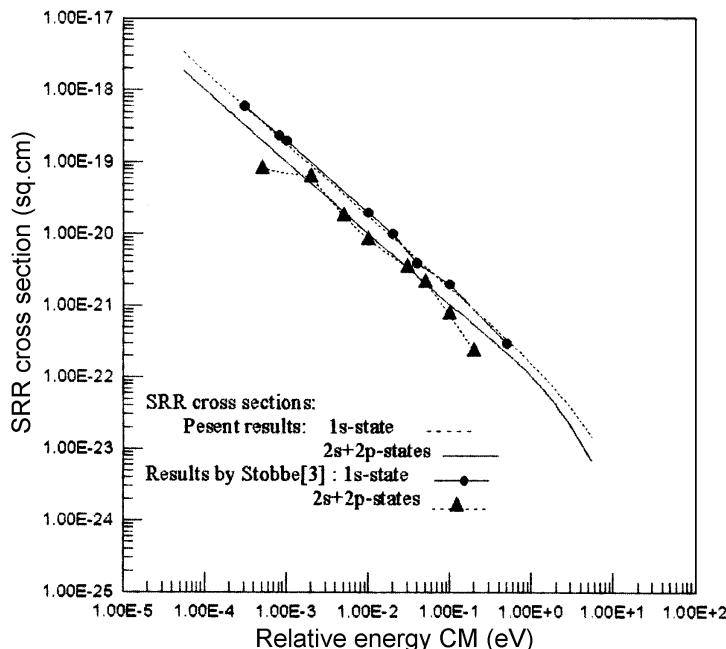


Fig. 1. Spontaneous radiative recombination (SRR) cross-section of electron to proton(deuteron) versus relative collision energy for capture into 1s state and 2s + 2p states from present work and from theoretical results by Stobbe [3].

The TSRR cross-sections $\sigma_{n'l'}^T(E_i)$ for the formation of atom in the ground state are computed with 2p and 3p as the virtual intermediate states. It should be noted that only the magnetic quantum number $m = 0$ contributes. From (24), the TSRR cross-section is obtained. Since the overlap integral

$$J_{2p} = \frac{2\pi i |\vec{p}|}{(1/4 + 2E_i)^2}$$

and $E_I = E_i + \epsilon_{nl}$, TSRR via the 2p state is given by

$$\sigma_{2p}^T(E_i) = \tau_{2p \rightarrow 1s}^{-1} \frac{8\pi\sqrt{2}}{3} \frac{(E_i + \epsilon_{1s})^{3/2}}{2\pi\epsilon_{2p}^2 (0.25 + 2E_i)^4}. \quad (32)$$

The overlap integral takes the form

$$J_{3p} = 8\pi i N_1 p(p^2 - 1/9) \sqrt{2\pi/p} (N_3 + p^2)^{-3},$$

where

$$N_1 = 2\sqrt{2/\pi}/27 \quad \text{and} \quad N_3 = 1/3.$$

The cross-section for TSRR via 3p state is given by

$$\sigma_{3p}^T(E_i) = \tau_{3p \rightarrow 1s}^{-1} \frac{8\pi\sqrt{2}}{3} \frac{(E_i + \epsilon_{1s})^{3/2}}{\epsilon_{3p}^2} 16N_1^2 \frac{(2E_i - 1/9)^2}{(2E_i + 1/9)^6}. \quad (33)$$

The TSRR cross-section is plotted with respect to collision energies E_i in Fig. 2.

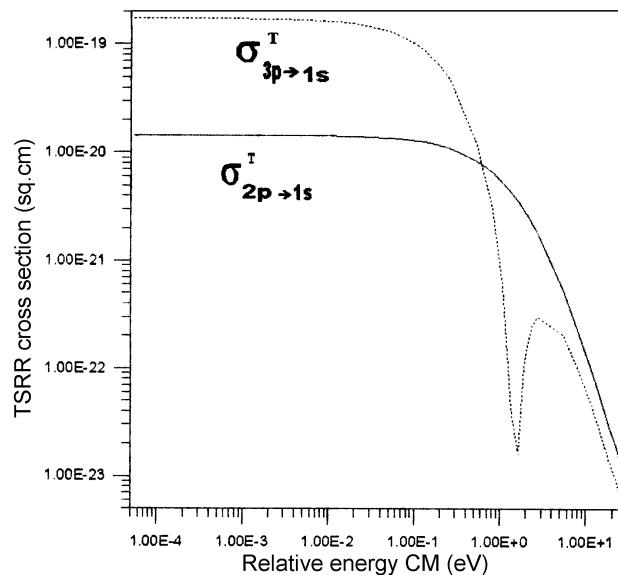


Fig. 2. Two-step radiative recombination (TSRR) cross-section of electron to proton (deuteron) for recombination into the ground state via intermediate states 2p and 3p versus relative collision energy from the present work.

To justify the use of field theoretic (FT) technique in calculating TSRR cross-section, we have applied it first to calculate SRR cross-sections in dipole approximation. Present results for SRR into 1s and 2s states vary inversely as the relative collision energy E_i , as long as E_i is less than the binding energies in the respective states. For capture into the

1s state, present result is similar to that of Stobbe (see Fig. 1). The sum of the capture cross-sections into 2s and 2p states also compares well with that by Stobbe. The TSRR cross-sections into the ground state via 2p and 3p states are shown in Fig. 2. The emitted photons have frequencies $(\epsilon_{1s} - \epsilon_{2p})/\hbar$ and $(\epsilon_{1s} - \epsilon_{3p})/\hbar$, respectively, in the case of TSRR via 2p and 3p as the virtual intermediate states. The emitted photons in the SRR channel have continuous spectrum having frequencies $\omega \leq (E_i - \epsilon_{nl})/\hbar$. In the collision energy range 10^{-5} to 10^{-1} eV, the TSRR cross-section is found to be independent of energy. The cross-sections for SRR into the first and second Bohr orbits are greater than those by TSRR channel into the ground state, as long as $E_i < 10^{-3}$ eV. As energy increases above 10^{-3} eV, the TSRR cross-section dominates the RR process.

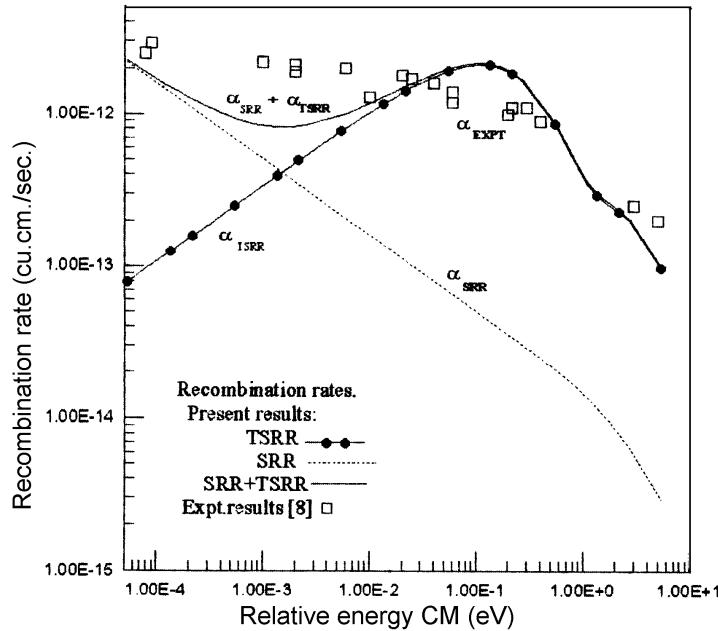


Fig. 3. Radiative recombination rates versus relative collision energy from the present work and from experimental results [8].

The only available experimental results [8] for the recombination rates (till the submission of the paper) for radiative formation of hydrogen isotope are from Schuch, Pajek and the group in Sweden. The experimental results [8] are shown in Fig. 3 along with the present theoretical calculations. In the experimental study of the rate coefficients, recombination may occur both via the SRR and TSRR channels. Eventually, it is natural that the experimental results will be closer to the sum of the coefficients ($\alpha_s + \alpha_T$) from the SRR and TSRR channels, than from the SRR channel alone.

4. Conclusion

Present paper is an attempt to show the importance of the TSRR channel on the radiative recombination process. Contributions from the SRR channel are well known on the RR process. Unlike the radiative recombination between ion (non-bare) and electron, where dielectronic recombination (DER) contributes to the recombination rate [6], in the present case of proton(deuteron)-electron radiative recombination, DER does not arise. Further, presence of a spectator electron, which might contribute to RR, is also ruled out in the experiment [8]. Hence, SRR and TSRR are the only possible channels open to RR in the experiment considered. The field-theoretic results for SRR to 1s and 2s states are comparable to the results by Stobbe. SRR to the p state fails to agree. The reason may be that in the present calculation, magnetic quantum numbers other than $m = 0$ do not contribute. Choice of exact Coulomb distorted wave $\Psi_c(r)$ in (14) might have improved the result, but at the cost of complicated calculations. For better agreement between theory and experiment, contributions to RR from TSRR via higher orbital and from SRR to excited states should be considered. The spectra emitted from the SRR and TSRR channels have completely different characteristics (continuous spectrum and discrete spectrum). There is no correlation between these two events. Eventually, from the physical point of view, one may doubt the possibility of interference between the two channels. As such, we have compared the sum of the rate coefficients from the SRR and the TSRR processes with the experimental data. However, it will be a good mathematical exercise to calculate the interference term. In conclusion, we like to say that the TSRR channel addresses itself, to some extent, to the high experimental values of the RR rate in the case of proton and electron for collisions at the sub meV energies.

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RADIJATIVNO VEZANJE HLADNOG ELEKTRONA S PROTONOM I S
DEUTERONOM

Izlaže se teorija dvostepene radijativne rekombinacije hladnog elektrona s protonom i s deuteronom. Dvostepena radijativna rekombinacija odvija se putem virtualnog uzbudenog stanja, a zbog očuvanja impulsa, sustav prelazi u osnovno stanje emisijom fotona. Primjenjuje se teorija polja i Coulombova sumjerljivost. Dugo poznat jednostepeni proces radijativne rekombinacije putem dipolnog međudjelovanja, koji opisuje spontanu fotorekombinaciju, ne uspijeva potpuno objasniti rezultate nedavnih mjerena. Zbroj udarnih presjeka za spontanu fotorekombinaciju i dvostepenu radijativnu rekombinaciju uspoređuje se s eksperimentalnim podacima.