Electron Capture Cross-sections in Proton-H (1s) Collision

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Capture cross sections of electron by proton in collision with ground state hydrogen atom into 1*s*, 2*s*, and 2*p* states are calculated in the framework of an impact parameter representation. The calculations are performed within the solution of the coupled differential equations arising from a two-state atomic-orbital close-coupling approach, in the impact energy range from 4 keV to 200 keV. The electronic wave function is expanded in terms of atomic orbitals in the fields of the target nucleus and the projectile with appropriate plane-wave electron translational factors. The agreement of the calculated cross sections with the available previous theoretical and experimental results is satisfactory.

1. Introduction

The scattering of protons from ground state hydrogen atoms has often been used as a benchmark system for theoretical investigations [1–7] and experimental measurements [8-13]. Cross sections due to excitation, ionization, and capture processes for this collisional system have many applications in plasma physics. Charge transfer theory for ion-atom collisions is a much developed research field. Nevertheless, a single suitable theory to deal with projectile energies ranging from low to high energies has not yet been found.

The earliest quantum calculations of electron capture cross sections were based on a simplified version of the first Born approximation [14, 15]. The two-center close-coupling method is based on expanding the scattering wave-function into a linear combination of traveling atomic orbitals localized on two nuclear centers to describe the electron of the colliding atomic system. Therefore, it allows for the movement of the electron cloud between the target and the projectile; that is, electron capture from the target atom is possible. The choice of orbitals depends on the physical process of interest, as well as on the computational effort, convergence, and so on. If one can include a complete basis set of orbitals, one might study the collision process with any kind of basis set. In practice, it is very difficult to include a complete basis set, as discussed by Kuang and Lin [16].

Olson [1] employed a three-dimensional Monte Carlo approach that uses a classical description of the hydrogen atom and the Coulomb forces among all particles to obtain the charge-transfer cross sections for collisions of proton or positive ions of higher electric charge with hydrogen atoms. Keim et al. [17] reported experimental and theoretical data for the degree of linear polarization of Lyman-α emission induced by proton and antiproton impact on atomic hydrogen, where a two-center extension of the basis generator method is used to solve the time-dependent Schrödinger equation. Tupitsyn et al. [18] developed a method for solving the time-dependent two-center Dirac equation to calculate the charge-transfer cross sections for the proton and ground state hydrogen atom collisions. The time-dependent Dirac wave-function is represented as a sum of atomic like Dirac-Sturm orbitals localized at the nuclei and the atomic orbitals are generated by numerical solution of the one-center Dirac and Dirac-Sturm equations by means of a finite-difference approach with the Coulomb potential taken as the sum of the exact reference-nucleus potential and of the other nucleus within the monopole approximation.

Winter [4] extended the work of Shakeshaft [19, 20] and determined electron transfer and excitation, as well as ionization cross sections in collisions between protons and ground state hydrogen atoms using two-center close-coupling Sturmian bases. Ferreira *et al.* [21] made calculations of the resonant cross sections for electron capture by proton from ground state hydrogen atoms in the impact parameter picture with a two-center atomic expansion. They used a two-state approximation with a continuum distorted wave basis, which ensured that Coulomb boundary conditions are met. The semi-classical close-coupling method [22] utilized a large basis of pseudo-states for expansion of the electronic part of the scattering wave-function. The Hamiltonian for the target is diagonalized using the orthogonal Laguerre basis resulting in negative and positive energy pseudo-states. This method is generalized to include the electron capture channels and is used to study the electron-capture process in proton-hydrogen collisions [23].

Abdurakhmanov et al. [24] developed a fully quantum-mechanical two-center close-coupling approach to proton hydrogen scattering [25] to report the total capture cross sections for proton-hydrogen atom collisions. The formulation is based on the exact three body Schrödinger equation, where the total scattering wave-function is expanded in a two-center pseudo-state basis, which allows to include electron capture into bound and continuum states of the projectile. This leads to coupled-channel Lippmann–Schwinger equations for the transition amplitudes in the momentum-space. Agueny et al. [26] reported the cross sections for electron capture process in collisions between fully stripped hydrogen, helium and lithium ions and hydrogen atoms in the ground. They used the two-center atomic orbital close-coupling approach [27] with expanding the wave-function on states expressed as linear

combinations of Gaussian-type orbitals. Tseliakhovich et al. [28] introduced a formalism to obtain the cross sections for collisions between protons and hydrogen atoms being initially in the ground state, they developed a numerical code which directly solves the Schrödinger equation with variable resolution and utilizes a hybrid Spatial-Fourier grid. Kolakwaska et al. [2] calculated capture cross sections for collision of proton with ground state hydrogen atom by direct solution of the time-depending Schrödinger equation on a three-dimensional Cartesian lattice. The cross sections are obtained by projecting a time-evolved wave-function onto a lattice target states of hydrogen. Tong et al. [6] calculated the 2*s* and 2*p* charge transfer cross sections in proton-hydrogen atom collision by direct solution of the time-dependent Schrödinger equation using the split-operator method with a generalized pseudo-spectral method [29], where a classical trajectory approximation for the projectile is employed.

The present work is devoted to calculate the capture cross sections of electron by proton from atomic hydrogen in the ground state. The calculations are made in the impact parameter representation with a two-center atomic expansion.

2. Method

Capture of electron by proton from hydrogen atoms can be described in a two-center atomic-orbitals close-coupling approach. In the impact parameter formulation, an un-deflected (straight line, constant velocity) trajectory for the nuclei can be used. Choosing a coordinate system such that the relative velocity of the nuclei υ points along the *z*-axis and the inter-nuclear distance vector is given by $\mathbf{R}=\mathbf{b}+\boldsymbol{\upsilon}t$, where *b* is the impact parameter such that $\mathbf{b}\cdot\boldsymbol{\upsilon}=0$ and *t* is the time. Consider, $\mathbf{r}_T, \mathbf{r}_P$, and $\mathbf{r}$ are the electron position vectors with respect to the target nucleus *T*, to the projectile *P*, and to the center of mass of the nuclei, respectively. The two-center atomic-orbitals close-coupling approach is based on expanding the electronic wave-function around both the target nucleus and the projectile. That is, the electronic wave-function can be expressed in the expansion [30] as

$$\Psi(\mathbf{r},t)=\sum_k a_k(t)\phi_k^T(\mathbf{r}_T)\,e^{-i(\varepsilon_k^T t+\boldsymbol{\upsilon}\cdot r/2+\upsilon^2 t/8)} + \sum_j c_j(t)\phi_j^P(\mathbf{r}_P)\,e^{-i(\varepsilon_j^P t-\boldsymbol{\upsilon}\cdot r/2+\upsilon^2 t/8)} \qquad (1)$$

Here $\phi_n^T\,(\phi_n^P)$ are the eigenstates of the electron in the field of the target nucleus (projectile), and $\varepsilon_n^T\,(\varepsilon_n^P)$ are the associated eigenstates. The terms $e^{-i(\pm\boldsymbol{\upsilon}\cdot r/2+\upsilon^2 t/8)}$ are the plane wave electronic translation factors, describe the motion of the target and projectile nuclei with respect to the center of mass of the nuclei.

Inserting the electronic wave-function $\Psi(\mathbf{r},t)$ into the time-dependent Schrödinger equation of the colliding system gives the first-order coupled differential equations for the amplitudes $a_k(t)$ and $c_j(t)$ as

$$i(\dot{A}+S\dot{C})=H\,A+KC, \qquad (2.a)$$

$$i(\dot{C}+S^{\dagger}\dot{A})=\bar{K}A+\bar{H}C, \qquad (2.b)$$

with the initial condition $a_k(-\infty)=\delta_{0k}$, $c_j(-\infty)=0$, where 0 refers to the initial state of the target atom. Where, *A* and *C* are the vectors of amplitudes $a_k(t)$ and $c_j(t)$ respectively, *S* is the overlap matrix ($S^{\dagger}$ is its transposed form), *H* and $\bar{H}$ are the direct coupling matrices, while *K* and $\bar{K}$ are the electron exchange matrices defined by the expressions

$$S_{kk'}=\int\tilde{\phi}_k^{T*}(\mathbf{r}_T,t)\tilde{\phi}_{k'}^{P}(\mathbf{r}_P,t)\,d\mathbf{r} \qquad (3.a)$$

$$H_{kk'}=\int\tilde{\phi}_k^{T*}(\mathbf{r}_T,t)\left[V^P(\mathrm{r}_P)+W(R)\right]\tilde{\phi}_{k'}^{T}(\mathbf{r}_T,t)\,d\mathbf{r} \qquad (3.b)$$

$$K_{kk'}=\int\tilde{\phi}_k^{T*}(\mathbf{r}_T,t)\left[V^T(\mathrm{r}_T)+W(R)\right]\tilde{\phi}_{k'}^{P}(\mathbf{r}_P,t)\,d\mathbf{r} \qquad (3.c)$$

$$\bar{H}_{kk'}=\int\tilde{\phi}_k^{P*}(\mathbf{r}_P,t)\left[V^T(\mathrm{r}_T)+W(R)\right]\tilde{\phi}_{k'}^{P}(\mathbf{r}_P,t)\,d\mathbf{r} \qquad (3.d)$$

$$\bar{K}_{kk'}=\int\tilde{\phi}_k^{P*}(\mathbf{r}_P,t)\left[V^P(\mathrm{r}_P)+W(R)\right]\tilde{\phi}_{k'}^{T}(\mathbf{r}_T,t)\,d\mathbf{r} \qquad (3.e)$$

$$S^{\dagger}_{kk'}=\int\tilde{\phi}_k^{P*}(\mathbf{r}_P,t)\tilde{\phi}_{k'}^{T}(\mathbf{r}_T,t)\,d\mathbf{r} \qquad (3.f)$$

Because of the eigenstates of the electron in the field of the target nucleus or the field of the projectile has position symmetry under reflection through the collision plane $(\boldsymbol{\upsilon},\mathbf{b})$, the eigenstates $\phi_{nlm}^{T,\mathrm{P}}(\mathbf{s})$ can be further expanded as [31, 32]:

$$\phi_{nlm}^{T,P}(\mathbf{s})=\frac{R_{nl}(s)}{\sqrt{2(1+\delta_{m,0})}}\left[(-1)^m Y_l^{-m}(\hat{\mathbf{s}})+Y_l^m(\hat{\mathbf{s}})\right],\ m\geq 0 \qquad (3)$$

Where, $R_{nl}(s)$ are the radial function and $Y_l^m(\hat{\mathbf{s}})$ are the spherical harmonics. This reduces the number of states and makes evaluation of the exchange matrix elements possible.

3. Calculations and Discussion

Application of the two-center atomic-orbitals close-coupling approach needs solving the coupled differential equations (2.a) and (2.b). The integration of these coupled differential equations over $z=\upsilon t$ is carried out from z = −500 to z = 500 au by using Maple 18 codes of the Bulirsch-Stoer method, for fixed values of the impact parameter at given impact energies. The corresponding capture cross sections into the state nlm can be obtained

by squaring the transition amplitudes and integrating over the impact parameter, i.e.,

$$\sigma_{nlm} = 2\int_0^{\infty} \left| c_{nlm}(\upsilon, b; z \to +\infty) \right|^2 b\, db$$

$$(\pi a_0^2 = 8.797 \times 10^{-17}\ \mathrm{cm}^2) \qquad (4)$$

In the present work, we employ a two-center atomic-orbital close-coupling method to calculate the cross sections for capture of electron into 1s, 2s, and 2p states in collisions between protons and H(1s) atom. We have considered atomic orbital bases, of the n=1 to 4 states, on each of the projectile and the atomic nucleus centers. The effectiveness of the calculations is examined by employing the two-state and three-state approximations [7].

In what follows, the results are plotted in the impact energy region from 4 to 200 keV and discussed. In addition, we compare our results (solid curves) with the previous theoretical work of Tseliakhovich et al. [28] (dot curves) and Agueny et al. [26] (dashed curves) as well as the experimental measurements [9, 11, 13]. Measurements of Morgan et al. [9] for capture of electron into 2p state and Chong and Fite [11] for capture of electron into 2s state are based on a modulated crossed-beam technique. Hill et al. [13] used a tungsten-tube furnace to provide a target of highly dissociated hydrogen for incident protons or equi-velocity deuterons to measure capture cross sections into 2s state.

Fig. 1 illustrates the cross section for capture of electron into the 1s state in collision between proton and H (1s) atom as function of the impact energy. There seems to be a systematic shift between the present results and those of Tseliakhovich et al. [28] and Agueny et al. [26], which increase as the energy decreases. It is easy to see that the calculations of Tseliakhovich et al. [28] and Agueny et al. [26] are very close while the present calculations give higher cross sections. However, over the impact energy range the electron capture cross section rapidly diminishes.

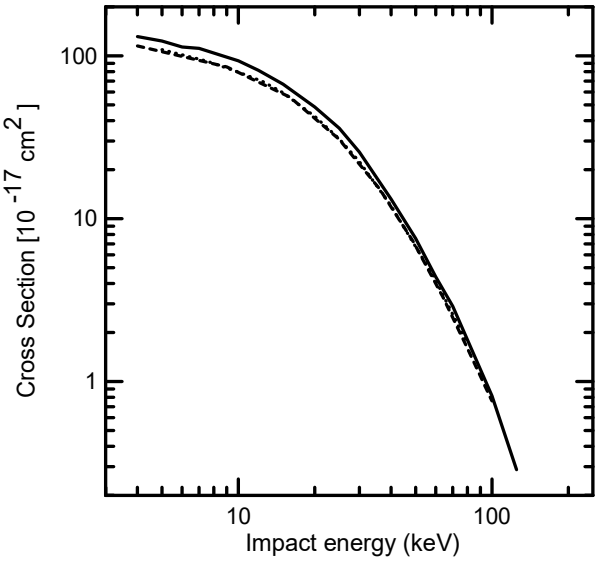

Fig. 1 Cross section for capture of electron into 1s state in collision between proton and H(1s) atom as function of the impact energy: Solid curve, present results; dot curve, Tseliakhovich et al. [28]; dashed curve, Agueny et al. [26].

In Fig. 2 we show the impact energy dependence of the cross sections for the electron capture into the 2*s* state in collision between proton and H (1s). The curves show maximum peaks near the matching velocity, at 25 keV impact energy, because of the large overlap of the electron cloud between the projectile and target. It is observed that our calculated cross sections are greater than those of Tseliakhovich et al. [28] and Agueny et al. [26] as well as the experimental measurements of Hill et al. [13] and Chong and Fite [11]. However, all the calculations are very close at impact energies above 60 keV and a systematic shift between the present results and previous ones can be noticed.

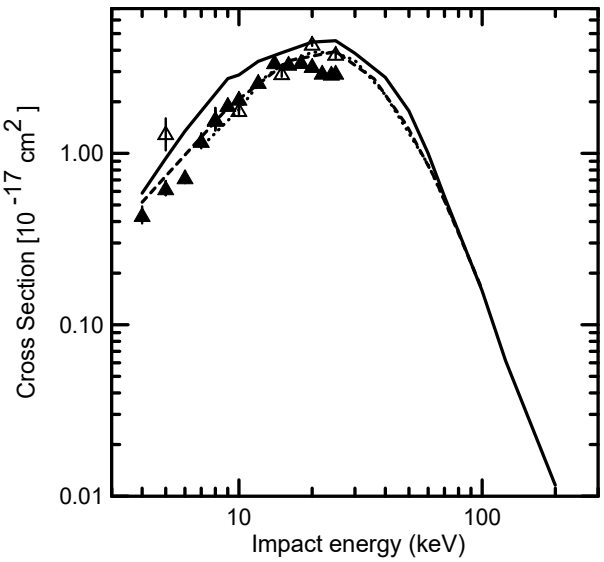

Fig. 2 Cross section for capture of electron into 2s state in collision between proton and H(1s) atom as function of the impact energy: Theoretical results: Solid curve, present results; dot curve, Tseliakhovich et al. [28]; dashed curve,

Agueny et al. [26]. Experimental data: Filled triangles, Hill et al. [13]; empty triangles, Chong and Fite [11].

Resulting plots of the 3*p* capture cross sections are given in Fig. 3. One can see that; the present cross sections are larger than those of Tseliakhovich et al. [28] over the impact energy range and are slightly larger than the results of Agueny et al. [26] at impact energies above 50 keV. It is seen that our results give good agreement with the experimental work of: Morgan et al. [9] at energies above 10 keV. Also, we can say that there is a systematic shift between the present results and the previous ones but in different directions. The curves show maximum peaks near the 15 keV impact energy.

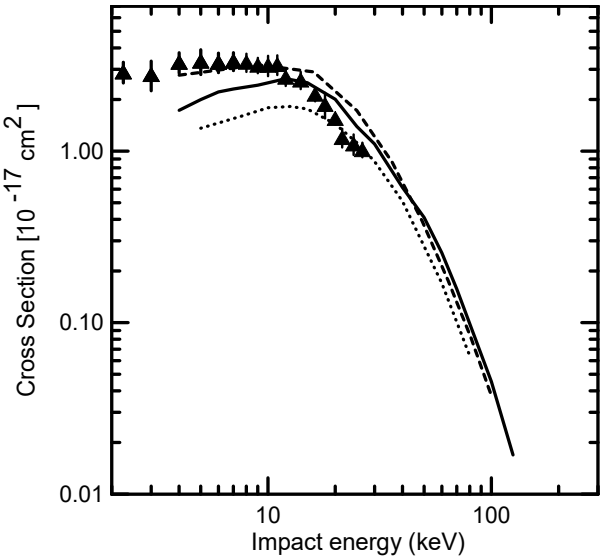

Fig. 3 Cross section for capture of electron into 2p state in collision between proton and H(1s) atom as functions of the impact energy: Theoretical results: Solid curve, present results; dot curve, Tseliakhovich et al. [28]; dashed curve, Agueny et al. [26]. Experimental data: Morgan et al. [9].

Finally, a comparison among our results for capture cross sections into 1s, 2s and 2p states show that cross sections for electron capture into the excited 2s and 2p states are much smaller than the 1s state especially at low impact energies. This may be due to the state-selective charge transfer effect, which represents the sensitivity of the magnitude of the capture cross section to the energy defect between the initial and final states of the collision system. It is also observed that the 2p state capture cross sections are smaller than the corresponding the 2s state results for impact energies above 8 keV. It is noticed that the 2s and 2p cross sections show max peaks while the 1s cross sections do not.

4. Conclusion

Calculations for cross sections for capture of electron into 1s, 2s, and 2p states in collisions between protons and H (1s) atoms are carried out in a two-center atomic-orbital close-coupling method. There seems to be a systematic shift between the present results and the previous ones, which increase as the energy decreases. At low collision energies the resonant reaction, capture into the 1*s* state, is more state-selective than the other reactions. Anyway, the agreement with the available previous theoretical and experimental results is satisfactory.

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