ELECTRON CAPTURE TO EXCITED STATES IN FAST COLLISIONS OF PROTONS WIHT ATOMS

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Abstract

The process of electon capture to arbitary excited state in fast proton-atom collision is considered. The initial bound state wave function is taken in one-parameter variational form which permits the calculation of the capture amplitude and the cross section to be done in closed analytical form. Some cross section calculations are performed for $p + He(1s^2) \rightarrow \rightarrow H(ns) + He^+(1s)$ reaction and comparison is made with the experimental data and other theoretical calculations.

1. Introduction

The electron capture to the excites states in heavy particle collisions has attracted recently great attention, as it has been shown that this process dominantly influences the structure of charge exchange cross section [1—3]. Poluektov and Presnyakov [4] have shown that this process is an important intermediate reaction channel which producess oscilations in the total cross section at low energies. At higher energies the charge exchange cross section varies smoothly with the impact energy which is an indication that the role of intermediate channels is small and the reaction proceeds via direct electron transitions. Nevertheless, there exists experimental evidence that the probability of the electron capture to excited states in ion-atom collisions at high energies is large enough and direct electron transitions to these states contribute considerably to the total capture cross section. Moreover, the cross sections of such processes have been mesured recently directly [2, 3] and these experimental data need theoretical interpretation.

In this work we shall study electron capture to excited states in proton-atom collisions at high energies. We shall restrict ourselves to the energy range where the first order perturbational method is applicable ($E \gtrsim 25$ KeV). We shall consider the case of light atoms where the one-parameter Slater type wave function has an integer effective principal quantum number which permits to carry out the calculations in closed form. The circumstance that the final state in this case is a hydrogenic one anable us to perform the sumation of the relevant matrix element over the angular and magnetic quantum numbers for a given principal quantum number.

In the next Section we give our theoretical derivations of the electron capture amplitude and the cross section, and in Section 3 we give some numerical results. Atomic units ($\hbar = m_e = e = 1$) will be used thrughout this work.

2. Derivation of the cross section expression

Let us consider one-electron capture process from an atom A in state „i" to a state (nlm) in fast collisions with protons, i.e. the reaction

$$p + A(i) \rightarrow H(\text{nlm}) + A^{+} \tag{1}$$

If with $\vec{r}_a$ and $\vec{r}_b$ we designate the position vectors of the „active" (i. e. transient) electron relative to the nucleus of atom A and the proton, then the interaction in the system can be represented in the form

$$V(\vec{r}_a, \vec{r}_b, \vec{R}) = -\frac{1}{r_b} + U(\vec{r}_a, \vec{R}) \tag{2}$$

where R is the internuclear distance, $-\frac{1}{r_b}$ is the electron-proton interaction and $U(\vec{r}_a, \vec{R})$ is the rest of the interaction in the system. It was shown by Oppenheimer [5] that the contribution of the second term in (2) to the transition matrix element is of order of magnitude $\frac{m}{M}$ where m is the electron mass and M is the reduced mass of the proton and ion A^{+}. In the case of reactios (1) we have always $M \gg m$, so that to the first order of magnitude in $\frac{m}{M}$, the transition amplitude for the process (1) is (see Ref. 6. p, 427);

$$F(\theta, \varphi) = -\frac{M}{2\pi} \int e^{i(\vec{q}\,\vec{r}_a - \vec{Q}\,\vec{r}_b)}\, \Psi_f(\vec{r}_b) \frac{1}{r_b} \Psi_i(\vec{r}_a)\, d\vec{r}_a\, d\vec{r}_b. \tag{3}$$

In (3) we have introduced the following notations

$$M = \frac{M_a M_b}{M_a + M_b}, \quad M_a = M_{A^+}, \quad M_b = M_p \tag{4}$$

$$\vec{q} = \frac{M_a}{M_a + 1}\vec{k}_i - \vec{k}_f, \quad \vec{Q} = \vec{k}_i - \frac{M_b}{M_b + 1}\vec{k}_f \tag{5}$$

where $\vec{k}_i$ and $\vec{k}_f$ are the relative momenta in the initial and final state. Ψ_i and Ψ_f are the electron wave functions in these states. We note that the integral in (3) is in fact a product of two unnormalized Fourier transforms

$$f_i(\vec{q}) = \int e^{i\vec{q}\,\vec{r}_a}\, \Psi_i(\vec{r}_a)\, d\vec{r}_a \tag{6a}$$

$$g_f(\vec{Q}) = \int e^{i\vec{Q}\,\vec{r}_b}\, \frac{1}{r_b}\, \Psi_f(\vec{r}_b)\, d\vec{r}_b. \tag{6b}$$

Taking this into account, the cross section for electron capture from state „i“ to a state (nlm) is found to be

$$\sigma(i\,|\,nlm) = \frac{M_i M_f}{(2\pi)^2}\,\frac{k_f}{k_i}\int_0^{\pi}\int_0^{2\pi} |\,f_i(\vec{q})\,|^2\, |\,g_f(\vec{Q})\,|^2 \sin\theta\, d\theta\, d\varphi \tag{7}$$

where

$$M_i = \frac{(M_a + 1)\,M_b}{M_a + M_b + 1}, \quad M_f = \frac{(M_b + 1)\,M_a}{M_a + M_b + 1}. \tag{8}$$

In order to perform the integration in (7) it is convenient to transform the integral into an integral over a plane in the $\vec{q}$ space. If we take the z-component of $\vec{q}$ in the direction of $\vec{k}_i$, then the components q_x, q_y and q_z are connected with the angles θ and φ by the relations [7]

$$q_x = -k_f \sin\theta\, \cos\varphi, \quad q_y = -k_f \sin\theta\, \sin\varphi, \quad q_z = \frac{M_a}{M_a + 1}k_i - k_f\cos\theta. \tag{9}$$

With this transformation, the integral in (7) can be transformed into a surface integral

$$\int L\,[q\,(\theta,\, \varphi)]\, \sin\theta\; d\theta\; d\varphi = \frac{1}{k_f^2}\int_S L(\vec{q})\, d\vec{S} \tag{10}$$

where the equation of the surface S is

$$q_x^2 + q_y^2 + q_z^2 = k_f^2 - \left(\frac{M_a}{M_a + 1}\right)^2 k_i^2 + 2k_f q \frac{M_a}{M_a + 1}. \qquad (11)$$

We can now esealy transform the integral over $d\vec{S}$ into an integral over $dq_x\, dq_y$ and get the expression

$$\sigma(i \mid nlm) = \frac{1}{(2\pi)^2} \frac{1}{k_i k_f} \int\int_{-\infty}^{+\infty} |f_i(\vec{q})|^2 \, |q_f(Q)|^2 \, dq_x\, dq_y. \qquad (12)$$

At large energies we have $k_i \approx k_f = v$, where v is the relative velocity of the colliding patricles. In the case of reaction (1) the final state wave functions $\Psi_f = \Psi_{nlm}$ are well known, and their unnormalized Fourier transforms q_{nlm} can be found esealy.

Moreover, for given principal quantum number n, the following summation rule holds for these Fourier transforms [8]

$$\sum_{l=0}^{n-1} \sum_{m=0}^{l} |q_{nlm}(Q)|^2 = \frac{2^4 \pi}{n^3} \frac{1}{(Q^2 + n^{-2})^2}. \qquad (13)$$

Using this formula we can average the cross section $\sigma(i \mid nlm)$ over the quantum numbers l and m of the final state and for the averaged cross section obtain

$$\sigma(ikn>) = \frac{4}{\pi v^2 n^3} \int\int_{-\infty}^{+\infty} |f(\vec{q})|^2 \frac{dq_x\, dq_y}{(Q^2 + n^{-2})^2}. \qquad (14)$$

In the binding energy of the electron in its initial state is $-\gamma^2/2$, then the vectors $\vec{q}$ and $\vec{Q}$ (which are in fact momentum transfers) have the following projections

$$\vec{q} = \left\{q_x,\ q_y,\ \left[\frac{v}{2} - \frac{\gamma^2 + n^{-2}}{2v}\right]\right\} \qquad (15a)$$

$$\vec{Q} = \left\{q_x,\ q_y,\ \left[\frac{v}{2} + \frac{\gamma^2 - n^{-2}}{2v}\right]\right\} \qquad (15b)$$

so that the energy conservation is preserved

$$q^2 + \gamma^2 = Q^2 + n^{-2}. \qquad (16)$$

Now, to carry out the integration in (14) one should calculate the Fourier transform $f(\vec{q})$ of the initial state wave function. In one-electron approximation the simpliest wave functions are the Slater type one-parameter variational wave functions [9], given by

$$\Psi_i(\vec{r}) = \frac{(2\gamma)^{n^*+1/2}}{[(2n^*)!]^{1/2}} r^{n^*-1} e^{-\gamma r} Y_{lm}(\theta, \varphi) \tag{17}$$

where γ is varitinal parameter, n^* is the effective principal quantum number and $Y_{lm}(\theta, \varphi)$ are normalized spherical harmonics. For $n^* = 1,2$ and 3 for $f_i(\vec{q})$ we obtain

$$f_{1s} = \frac{2^3 \pi^{1/2} \gamma^{5/2}}{(\gamma^2 + q^2)^2} \tag{18}$$

$$f_{2s} = \frac{2^3 \pi^{1/2} \gamma^{5/2}}{\sqrt{3}(\gamma^2 + q^2)} \left[\frac{4\gamma^2}{\gamma^2 + q^2} - 1 \right], \tag{19}$$

$$f_{2p} = i\, 2^5 \pi^{1/2} \gamma^{7/2} \frac{q}{(\gamma^2 + q^2)^3}, \tag{20}$$

$$f_{3s} = \frac{2^4 \pi^{1/2} \gamma^{9/2}}{3\sqrt{10}(\gamma^2 + q^2)^2} \left[\frac{48\gamma^2}{(\gamma^2 + q^2)^2} - \frac{4}{\gamma^2 + q^2} - 1 \right], \tag{21}$$

$$f_{3p} = -i\, 2^5 \left(\frac{2\pi}{15} \right)^{1/2} \gamma^{7/2} \left[\frac{q}{(\gamma^2 + q^2)^3} - \frac{6\gamma q}{(\gamma^2 + q^2)^4} \right]. \tag{22}$$

Using these expressions in (14) and the energy conservation relation (16), for the corresponding cross section we obtain

$$\sigma_{(1s|<n>)} = \frac{2^8 \pi \gamma^5}{5n^3 v^2 \beta^5}, \tag{23}$$

$$\sigma_{(2s|<n>)} = \frac{2^8 \pi \gamma^7}{3n^3 v^2 \beta^5} \left[\frac{16\gamma^2}{7\beta^2} - \frac{4}{3\beta} + \frac{1}{5\gamma^2} \right], \tag{24}$$

$$\sigma_{(2p|<u>)} = \frac{2^{12} \pi \gamma^7}{n^3 v^2} \left[\frac{q_z^2}{7\beta^7} + \frac{\Gamma\left(\frac{3}{2}\right)\Gamma(6.5)}{\beta^{6.5}\,\Gamma(8)} \right], \tag{25}$$

$$\sigma_{(3s|<n>)} = \frac{2^{11} \pi \gamma^9}{46n^3 v^2 \beta^5} \left[\frac{(16\gamma^2)^2}{\beta^4} - \frac{48\gamma^2}{\beta^3} - \frac{16(6\gamma^2 - 1)}{7\beta^2} + \frac{4}{3\beta} + \frac{1}{5} \right], \tag{26}$$

$$\sigma_{(3p|<n>)} = \frac{2^{13} \pi \gamma^7}{15n^3 v^2} \left\{ q_z^2 \left(\frac{1}{7\beta^7} - \frac{12\gamma}{8\beta^8} + \frac{36\gamma^2}{9\beta^9} \right) + \right.$$

$$\left. + \Gamma\left(\frac{3}{2}\right) \left[\frac{\Gamma(6.5)}{\beta^{6.5}\,\Gamma(8)} - \frac{12\gamma\,\Gamma(7.5)}{\beta^{7.5}\,\Gamma(9)} + \frac{36\gamma^2\,\Gamma(8.5)}{\beta^{8.5}\,\Gamma(10)} \right] \right\}, \tag{27}$$

where $\Gamma(x)$ is gamma function and $q_z{}^2$ and β have the following forms

$$q_z^2 = \frac{1}{4}\left[v^2 - 2(\gamma^2 - n^{-2}) + \frac{(\gamma^2 - n^{-2})}{v^2}\right] \tag{28a}$$

$$\beta = \frac{1}{4}\left[v^2 + 2(\gamma^2 - n^{-2}) + \frac{(\gamma^2 - n^{-2})^2}{v^2}\right]. \tag{28b}$$

For $\gamma = n = 1$ (proton-hydrogen atom collision, capture to the ground state) from (23) we obtain the well known Brinkman-Kramer formula [10].

It is of some interest to investigate the high energy asymptotic behaviour of the above cross sections. At high energies the parameters β and $q_z{}^2$ behave as v^2, so for $n^* s \rightarrow n$ andn^*p transitions we have

$$\sigma(n^* s | <n>) \underset{v \to \infty}{\sim} \frac{1}{n^3 v^{12}} + O(v^{-14}), \tag{29}$$

$$\sigma(n^* p | <n>) \underset{v \to \infty}{\sim} \frac{1}{n^3 v^{14}} + O(v^{-15}). \tag{30}$$

We see that she cross section for electon capture from a p-state decreases more rapidely than that for capture from an s—state. We also see shat in both cases the variation of the cross section with the principal quantum number of the final state is n^{-3}, which is a demostration of the known Oppenheimer's rule.

3. Electon capture to 2s and 3s states in fast proton-helium atom collisions

In the preseeding Section we have derived some general formulae for electron capture to an excited state in proton collisions with light atoms. Now we shall apply this results to proton-helium atom collisions with electron capture to $2s$ and $3s$ states. We shall treat the two electrons in the helium atom as distinguishable and for both of them capture probabillity is equal.

Therefore, the cross section for capture of either electron should be multipled by a factor of two. The one-parameter variational wave functon of the „active“ electron we take in the usual form [9[. The corresponding Fourier transform is

$$f_{He}(q) = N_{He} \frac{1}{(\gamma^2 + q^2)}, \quad N_{He} =: 2^3 \pi^{1/2} \gamma^{5/2}, \quad \gamma = 1{,}6872. \tag{31}$$

The Fourier transfrms $g(Q)$ corresponding to the hydrogenic $2s$ and $3s$ wave functions are

$$g_{2s}(Q) = N_2\left[\frac{1}{\alpha_2^2 + Q^2} - \frac{1}{(\alpha_2^2 + \mathrm{Q}^2)^2}\right], \quad N_2 = (2\pi)^{1/2}, \quad \alpha_2 = 1/2, \tag{32}$$

$$g_{3s}(Q) = N_3\left[\frac{1}{\alpha_3^2 + Q^2} + \frac{a}{(\alpha_3^2 + Q^2)^2} + \frac{b}{(\alpha_3^2 + Q^2)^3} + \frac{cq^2}{(\alpha_3^2 + Q^2)^3}\right] \tag{33}$$

$$N_3 = \frac{4}{3}\left(\frac{\pi}{3}\right)^{1/2}, \quad \alpha_3 = 1/3, \quad a = -\frac{4\alpha_3}{3}, \; b = \frac{4}{27}\left(2\alpha_3^2 + \frac{1}{9}\right),$$

$$C = -\frac{4}{27}.$$

With these expressions for $f(g)$ and $g(Q)$ the cross sections for capture to $2s$ and $3s$ hydrogenic states in $p + He\,(1s^2)$ collisions are

$$\sigma_{2s} = \frac{2N_{He}^2 N_2^2}{(2\pi v)^2}\left[\frac{1}{5\beta_2^5} - \frac{1}{3\beta_2^6} + \frac{1}{7\beta_2^7}\right], \tag{34}$$

$$\begin{aligned}\sigma_{3s} = \frac{2N_{He}^2 N_3^2}{(2\pi v)^2}\Bigg\{&\frac{1}{5\beta_3^5} + \frac{a}{3\beta_3^6} + \frac{a^2 + 2b}{7\beta_3^7} + \frac{ab}{4\beta_3^8} + \frac{b^2}{9\beta_3^9} + \\ &+ q_z^2\left(\frac{2c}{7\beta_3^7} + \frac{ac}{4\beta_3^8} + \frac{2bc}{9\beta_3^9} + q_2^2\,\frac{c^2}{9\beta_3^9}\right) + \\ &+ \Gamma\left(\frac{3}{2}\right)\left[\frac{2c\,\Gamma(6.5)}{\beta_3^{6.5}\,\Gamma(8)} + \frac{2ac\,\Gamma(7.5)}{\beta_3^{7.5}\,\Gamma(9)} + \frac{2bc\,\Gamma(8.5)}{\beta_3^{8.5}\,\Gamma(10)} + \right. \\ &\left. + \frac{2c^2 {q_z}^2\,\Gamma(8.5)}{\beta_3^{8.5}\,\Gamma(10)}\right] + \frac{c^2\,\Gamma(5/2)\,\Gamma(7.5)}{\beta_3^{7.5}\,\Gamma(10)}\Bigg\}\end{aligned} \tag{35}$$

where

$$\beta_i = \frac{1}{4}\left[v^2 - 2(\gamma^2 - \alpha_i^2) + \frac{(\gamma^2 - \alpha_i^2)^2}{v^2}\right], \quad (i = 2, 3) \tag{36a}$$

$$q_z^2 = \frac{1}{4}\left[v^2 + 2(\gamma^2 - \alpha_3^2) + \frac{(\gamma^2 - \alpha_3^2)^2}{v^2}\right]. \tag{36b}$$

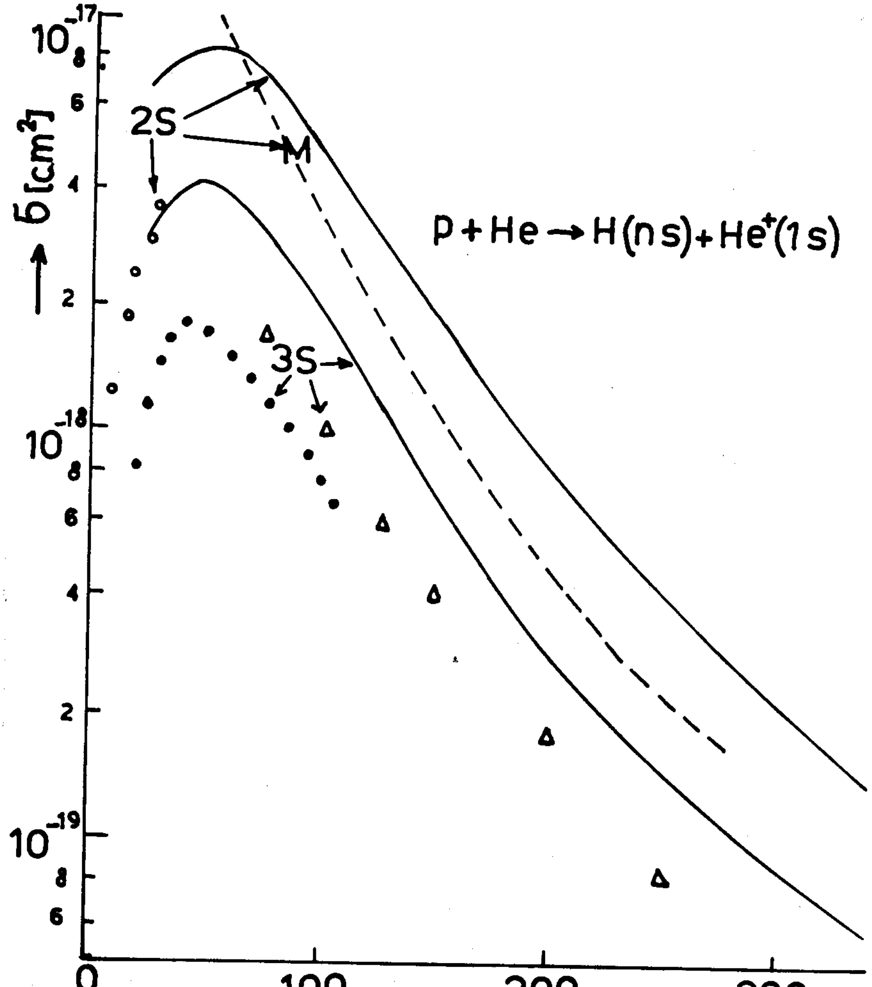

FIG. 1

Electron capture to $2s$ and $3s$ states in p — He collisions. Ful curves represent present results; curve M — calculations of Mapleton [11] for $2s$; ○ — experimental results of Jaecks et al [2] for $2s$ and ●, △ — experimental results for $3s$ of Hughes et al [3] and Ford and Thomas [1], respectively.

Using (34) and (35) we have computed the cross sections σ_{2s} and σ_{3s} in the proton energy range of 25 KeV to 300 KeV. The results of the calculations are• on Fig. 1 (ful lines). The dashed curve M on the figure is the result of Mapleton [11] for capture to $2s$ state. In his calculations the term $U(\vec{r}_a, \vec{R})$ in the interaction (2) was also included. The experimental data for capture to $2s$ state are taken from Jaecks et al, [2], (open circles), and for $3s$ state are those of Ford and Thomas [1] (trianqles) and Hughes et al [3] (points). The comparison shows that the first order perturbational theory with neglected $U(\vec{r}_a, \vec{R})$ term in the interaction overestimates the capture cross section for a factor of about two to three in the considered energy region. In the energy range below 80 KeV the inclusion of the term $U(\vec{r}_a, \vec{R})$ leads to even higher cross sections (see curve M). The agreement between the theory and the experimental data can be improved not on the line of taking into account the interaction term $U(\vec{r}_a, \vec{R})$ but using more exact one-electrons wave-functions. Namely, the correlation effect between the two electrons in helium atom are too strong and the one-parameter variational wave function does not include much of this correlation. One can use for this purpose many-parameter variational wave function of the Hartree-Fock type, but then no more simple analytical formulae can be obtained. Our calculations of electron capture cross sections to $2s$ and $3s$ states demonstrate that even with the simplest variational wave functions one can obtain reliable results for electron capture to excited states.

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ЗАХВАТ НА ЕЛЕКТРОНОТ ВО ПОБУДЕНИ СОСТОЈБИ ПРИ БРЗИТЕ СУДИРИ НА ПРОТОНИТЕ СО АТОМИТЕ

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Апстракт

Се проучува процесот на електронскиот захват во побудени состојби при брзите судири на протоните со лесните атоми. Брановата функција на почетната состојба се зема во вид на еднопараметарска вариациона функција што овозможува амплитудата и пресекот на процесите да се пресметнат во аналитичка форма. Некои пресметнувања на ефикасниот пресек се извршени за реакцијата $p + He(1s^2) \rightarrow H(ns) + He^+(1s)$. Се врши споредување на добиените резултати со експерименталните податоци и другите теориски пресметнувања.