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ELECTRON CAPTURE FROM HYDROGEN NEGATIVE IONS BY FAST PROTONS

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Abstract: A generalization of the continuum distorted wave method of Cheshire is made for proton — negative ion electron capture collisions. The attractive Coulomb interaction of the partners in the initial state is fully taken into account in this method. For reasons of simplicity of derivations, the generalization is given on the $p+H^-$ system. The cross section for this reaction is calculated in continuum distorted-wave-Born approximation.

1. Introduction

It became clear, in the last few years[1, 2], that the continuum distorted wave method of Cheshire[3] is one of the most adequate theoretical approaches to high-energy ion-atom collisions. This is a consequence of the inclusion of the coupling between the discrete and continuous states of the system in the Cheshire's method.

So far the Cheshire's method has been applied to ion-atom charge exchange collisions of a positive structurcless ion with a neutral atom. In this paper we shall generalize this method to charge collisions involving a positive and a negative ion. In this case the Coulomb interaction in the initial channel plays a very important role, and we shall show how this interaction can be fully taken into account by the continuum distorted wave method. For definiteness, we shall consider the reaction

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$$H^+ + H^- (1\,s^2) \rightarrow H(n\,l) + H(n'\,l'), \tag{1}$$

but as we shall see later, the results are valid also for more general situations. We shall calculate the cross section of the reaction (1) in the energy range above 25 keV where the continuum distorted wave approximation (CDWA) is supposed to be valid. Unfortunately, in this energy range there are no experimental data for this reaction. However, for the inverse reaction there exists a measurement by Mc Clure[4] and a comparison between our theory and his results has been published elsewhere[5].

2. General theoretical considerations

We shall treat the problem with the impact parameter method, describing the relative motion of the protons by

$$\vec{R} = \vec{\rho} + \vec{v}\,t, \tag{2}$$

where $\vec{R}$ is the position vector of the incident proton in respect to the nucleus of H^-, $\vec{v}$ is the relative velocity and ρ is the impact parameter. If $\vec{x}_i$ $(i = 1, 2)$ and $\vec{s}_i$ are the position vectors of the two electrons with respect to the nucleus of H^- and the incident proton, respectively, then the following relations are evident

$$\vec{s}_i = \vec{x}_i - \vec{R}, \qquad (i = 1, 2)$$

$$\vec{r}_i = \frac{1}{2}(\vec{x}_i + \vec{s}_i) = -\frac{1}{2}\vec{R} + \vec{x}_i = \frac{1}{2}\vec{R} + \vec{s}_i. \tag{3}$$

In this work we choose $\vec{R}$, $\vec{r}_1$ and $\vec{r}_2$ as independent variables. So we are led to the time-dependent Schrödinger equation (atomic units are used)

$$\left(H - i\frac{\partial}{\partial t}\right)\Psi(\vec{r}_1, \vec{r}_2, t) = 0, \tag{4}$$

with the Hamiltonian

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{x_1} - \frac{1}{s_1} - \frac{1}{x_2} - \frac{1}{s_2} + \frac{1}{x_{12}} + \frac{1}{R} \tag{5}$$

The solutions of the equation (4) should satisfy appropriate boundary conditions. In the final state we have two non-interacting H atoms. The corresponding channel Hamiltonian is

$$H_f = H - V_f = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{x_1} - \frac{1}{s_1}. \tag{6}$$

As V_f decreases at infinity faster than R^{-1}, the final wave function can be written as

$$\Phi_f(\vec{r}_1, \vec{r}_2, t) = \varphi_{nl}(\vec{s}_1)\,\varphi_{n'l'}(\vec{x}_2)\exp\{-i(\varepsilon_{nl} + \varepsilon_{n'l'})t - \\ -\frac{i}{2}\vec{v}\,\vec{r}_2 + \frac{i}{2}\vec{v}\,\vec{r}_1 - \frac{i}{4}v^2 t\} \equiv \Omega_f(\vec{r}_1, \vec{r}_2, t), \tag{7}$$

where φ_{nl} and ε_{nl} are the eigen-functions and eigen-energies of hydrogen atom in state *nl*. The above asymptotic wave function satisfies the equation

$$(H_f - i\frac{\partial}{\partial t})\,\Phi_f(\vec{r}_1, \vec{r}_2, t) = 0. \tag{8}$$

In the entrance channel the situation is not so simple because of the presence of the Coulomb attraction. This interaction should be fully taken into account in the asymptotic wave function $\Phi_i\,(\vec{r}_1, \vec{r}_2, t)$, i. e. it is solution of the equation

$$(H_i - \frac{1}{R} - i\frac{\partial}{\partial t})\,\Phi_i(\vec{r}_1, \vec{r}_2, t) = 0, \tag{9}$$

with

$$H_i = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{x_1} - \frac{1}{x_2} + \frac{1}{x_{12}}. \tag{10}$$

The explicit form of Φ_i is

$$\Phi_i(\vec{r}_1, \vec{r}_2, t) = \Omega_i(\vec{r}_1, \vec{r}_2, t)\exp\{\frac{i}{v}\ln(vR - v^2|t|)\}, \tag{11}$$

$$\Omega_i = \varphi^-(\vec{x}_1, \vec{x}_2)\exp\{-i\varepsilon^- t - \frac{i}{2}\vec{v}\,\vec{r}_2 - \frac{i}{2}\vec{v}\,\vec{r}_1 - \frac{i}{4}v^2 t\},$$

where φ^- and ε^- are the wave function and the energy of the negative ion. So, the boundary conditions for the solutions of the equation (4) are

$$\lim_{t\to-\infty}\Psi_i^+ = \lim_{t\to-\infty}\Phi_i\,, \qquad \lim_{t\to+\infty}\Psi_f^- = \Phi_f\,. \tag{12}$$

Now the transition amplitude for reactions of the type (1) has the form

$$b(\rho) = \lim_{t\to\infty} \langle \Phi_f \mid \Psi_i^+ \rangle = \lim_{t\to-\infty} \langle \Psi_f^- \mid \Phi_i \rangle. \tag{13}$$

Introducing the distorted waves $\chi_{i,f}^{\pm}$ in an analogous manner as in Cheshire's work[3], from the second part of (13) one obtains

$$b(\rho) = -\mathrm{i} \int_{-\infty}^{+\infty} \mathrm{d}t \, \langle \Psi_f^- \mid (H - \mathrm{i}\frac{\partial}{\partial t})\, \chi_i^+ \rangle \tag{14}$$

where

$$\lim_{t\to-\infty} \chi_i^+ = \lim_{t\to-\infty} \Psi_i^+.$$

3. *The choice of wave functions*

The distorted wave function of the entrance channel we represent in the form

$$\chi_i^+ = \Omega_i(\vec{r}_1, \vec{r}_2, t)\, L_i(\vec{s}_1), \tag{15}$$

with

$$L_i(\vec{s}_1) = N(v)\, {}_1F_1(\frac{\mathrm{i}}{v}, 1, \mathrm{i}\, v\, s_1 + \mathrm{i}\, \vec{v}\vec{s}_1),$$
$$N(v) = \Gamma(1 - \frac{\mathrm{i}}{v}) \exp(\frac{\pi}{2v}). \tag{16}$$

Having in mind the equation which $L_i(\vec{s}_1)$ satisfies

$$(-\frac{1}{2}\nabla_1^2 - \frac{1}{s_1} + \frac{1}{2}(\vec{v}\,\nabla_1) - \mathrm{i}\frac{\partial}{\partial t})\, L_i(\vec{s}_1) = 0,$$

we obtain using (9) and (4)

$$(H - \mathrm{i}\frac{\partial}{\partial t})\,\chi_i^+ = -\frac{\mathrm{i}}{2}\,\Omega_i\,(\vec{v}\,\nabla_1)\, L_i - \nabla_1 L_i\, \nabla_1 \Omega_i - \frac{1}{s_1}\,\Omega_i L_i\,. \tag{17}$$

This expression we can replace in (14).

For the final state wave function Ψ_f^- we shall use simply Φ_f (continuum distorted wave Born approximation). One can also replace Ψ_f^- by X_f^- defined in an analogous way as X_i^+ (full distorted wave approximation) but in reactions like (1) the distortion effect of this channel are not expected to be significant.

Therefore, the transition amplitude for reaction (1) is

$$b(\rho) = \mathrm{i} \int_{-\infty}^{+\infty} \mathrm{d}t \int \mathrm{d}\vec{r}_1 \, \mathrm{d}\vec{r}_2 \, \Phi_f^* \left\{ \frac{\mathrm{i}}{2} \Omega_i (\vec{v} \cdot \nabla_1) L_i + \nabla_1 L_i \nabla_1 \Omega_i + \right.$$
$$\left. + \frac{1}{s_2} \Omega_i L_i \right\}, \tag{18}$$

or more explicitly

$$b(\rho) = \mathrm{i} \int_{-\infty}^{+\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\Delta\varepsilon t} \int \mathrm{d}\vec{r}_1 \, \mathrm{d}\vec{r}_2 \, \mathrm{e}^{-\mathrm{i}\overrightarrow{v r_1}} [\varphi_{nl}(\vec{s}_1) \varphi_{n'l'}(\vec{x}_2)]^* \cdot$$
$$\cdot \left\{ \nabla_1 \varphi^-(\vec{x}_1, \vec{x}_2) \nabla_1 L_i(\vec{s}_1) + \frac{1}{s_2} \varphi^-(\vec{x}_1, \vec{x}_2) L_i(\vec{s}_1) \right\}; \quad \Delta\varepsilon = \varepsilon_{nl} + \varepsilon_{n'l'} - \varepsilon^- . \tag{19}$$

The last term in (19) is zero in the absence of the interaction between the electrons. It describes the capture reaction as arising from the interaction of incident proton with electron 2, which is correlated with the »active«

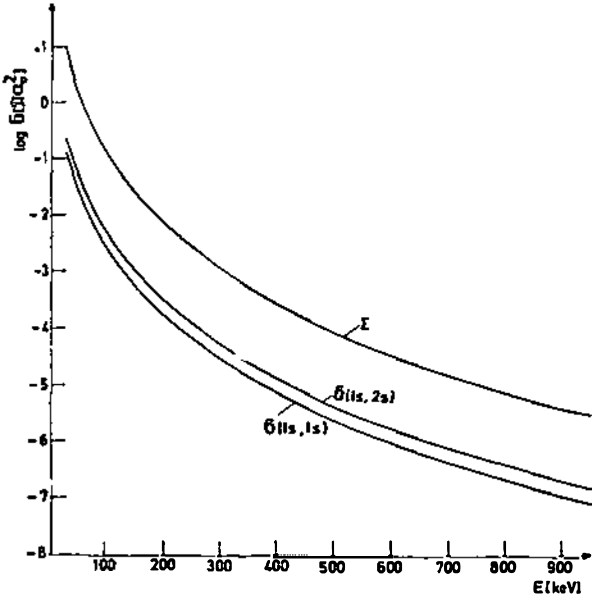

Fig. 1. Charge exchange cross sections in p+H$^-$ collisions. Σ is the total cross section given by formula (24).

electron 1 in the function φ^-. Therefore, we may assume that the contribution of this term in the transition amplitude is small and we shall neglect it. More support to this neglection follows also from the fact that at high energies the capture probability is mainly sensitive to the behaviour of the wave function of the captured electron close to the nucleus of the initial atom or ion.

We have chosen as negative hydrogen ion wave function that of Silverman et al.[6]

$$\varphi^-(\vec{x}_1,\vec{x}_2) = N\{\exp(-a x_1 - b x_2) + (1 \longleftrightarrow 2)\},$$

$$a = 1.039, \quad b = 0.283, \quad \varepsilon^- = -0{,}5133. \tag{20}$$

4. *Results and discussion*

The calculations of the cross section $\sigma(nl, n'l')$ for reaction (1) are made using the Fourier transform method[3]. The cross section is given by

$$\sigma(nl, n'l') = 2\pi \int_0^\infty \eta \, d\eta \, |R(\vec{\eta})|^2, \tag{21}$$

$$R(\vec{\eta}) = \frac{1}{2\pi} \int d\vec{\rho} \, e^{i\vec{\eta}\vec{\rho}} \, b(\rho), \tag{22}$$

where $\vec{\eta}$ is a vector in the $\vec{\rho}$ plane. With $b(\rho)$ from (19) the above integral can be easily calculated. From the expression (22) one immediately sees that $R(\vec{\eta})$ will be zero unless $l' = 0$. A non-zero contribution for $l' \neq 0$ would be obtained by introducing angular correlations in φ^-. Such a wave function is also given by Silverman et al.[6] but the non spherical term in this function is very small. In the energy region we are interested in, the main contribution to the cross section comes from $n' = 1$ and $n' = 2$. This is a consequence of the small overlap of the function $\varphi_{n'0}(\vec{x}_2)$ with term $\exp(-a x_2)$ in (20), and has been confirmed by the calculations. Therefore we have only plotted on Fig. 1 the cross sections $\sigma(1s, 1s)$ and $\sigma(1s, 2s)$. We have investigated the variation of $\sigma(nl, n'l')$ with nl (for $nl = 1s, 2s, 2p$) and found that for high energies ($E > 50$ KeV) the Oppenheimer's n^{-3} rule holds.

Table

E (KeV)	$\sigma(2s,1s)/\sigma(1s,1s)$	$\sigma(2s,2s)/\sigma(1s,2s)$	$\sigma(2p,1s)/\sigma(1s,1s)$
5	1.55	0.34	12.7
25	0.437	0.318	0.976
50	0.277	0.169	0.405
75	0.207	0.177	0.275
100	0.216	0.211	0.222
500	0.131	0.131	0.051
1000	0.121	0.121	0.031

For small energies ($E < 50$ KeV), the influence of the parameter $\Delta\varepsilon$ on the ratio $\sigma(2\,l,\ n'\,l')/\sigma(1\,s,\ n'\,l')$ becomes important and the Oppenheimer's rule is violated (see the Table). But in this energy range, the continuum distorted wave approximation is not supposed to be valid. Therefore for the cross section Σ for all transitions

$$\Sigma = \sum_{nl}\sum_{n'l'} \sigma(n\,l,\ n'\,l'), \tag{23}$$

in view of the preceding discussion, we have

$$\begin{aligned}\Sigma \cong & \sum_{nl} \{\sigma(n\,l,\ 1\,s) + \sigma(n\,l,\ 2\,s)\} = \\ & = \sigma(1\,s,\ 1\,s) + 1.616\,\{\sigma(2\,s,\ 1\,s) + \sigma(2\,p,\ 1\,s)\} + \\ & + \sigma(1\,s,\ 2\,s) + 1.616\,\{\sigma(2\,s,\ 2\,s) + \sigma(2\,p,\ 2\,s)\}.\end{aligned} \tag{24}$$

The result for Σ is plotted in Fig. 1.

We note that our previous considerations of the reaction (1) can be easily extended to arbitrary negative ions.

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ПРЕМИН НА ЕЛЕКТРОНОТ ОД НЕГАТИВНИТЕ ВОДОРОДНИ ЈОНИ КОН БРЗИТЕ ПРОТОНИ

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Содржина

Извршено е обопштуване на методата на деформираните континуумски бранови кои случај от кога взаимодејствуват еден позитивен и еден негативен јон. Битен момент во овоа обопштуване претставува фактот што во почетното состојание експлицитно се јавува долго-дометната Кулонова интеракција која мора да се земе во предвид. Во крајното состојание интеракцијата меѓу неутралните атоми опаѓа многу побрзо со растојанието. Присуствието на два активна електрона во системот исто така доведува до определени математички проблеми кои во досега проучуваните реакции од овој вид (едно-електронски системи) не се појавувале.

Без никакви ограниченија на општоста на методата, таа е изложена на примерот на реакцијата

$$p + H^- \to H(n\,l) + H(n'\,l')$$

чиј пресек е пресметнат за разни спецификации на квантните броеви $n\,l$ и $n'\,l'$, како и вкупниот пресек за истата.