

# ELECTRON CAPTURE BY $\text{He}^+$ IONS PASSING THROUGH He ATOMS

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**ABSTRACT.** The expression for the cross section of the electron capture by  $\text{He}^+$  ions passing through normal He atoms has been derived by applying a variational method. The effect of exchange of the electrons and the influence of their transitory motion on the cross section have been taken into account.

## I N T R O D U C T I O N

The first theoretical investigation of charge exchange between  $\text{He}^+$  ions and He atoms has been done by Massey and Smith (1933) with the perturbed stationary states method which has been further applied by Dallaportea and Bonfiglioli (1943), Firsov (1951), Jackson (1954) and Moiseiwitsch (1956). The above authors have used a linear combination of the two lowest helium molecular ion states like  $\text{He}^+_{\Sigma}$ , viz, the ground state which is symmetric with respect to the exchange of the two nuclei and the antisymmetric state just above the ground state and have approximately solved the time dependent Schrodinger equation. In the above method the cross section depends mainly on the difference of the electronic binding energies of those two states for which Massey and Smith have used, with suitable extension, the electronic energy for  $\text{He}^+_{\Sigma}$  calculated by Pauling. The range of energies of the incident ion covered by Massey and Smith was from 500 ev. to 12 kev, whereas the same was further extended by Jackson from 200 ev. to 100 kev. Moiseiwitsch covered a still wider range of energies from 0.1 ev to 10 kev, further he used three sets of wave function to calculate the electronic binding energies. For the high energy region (100 kev. to 700 kev.) Schiff (1954) has given an estimate of the electron capture cross section for  $\text{He}^+$  ions passing through He atoms by applying Born approximation method; he has used complete interaction including the nucleus-nucleus interaction in the Hamiltonian and has assumed unit effective charge of the incident ionized helium atom. Snitzer (1953) has experimentally measured the capture cross section for  $\text{He}^+$  ions on He atoms for the energy region 100 kev. to 450 kev. further extension has been made recently by Everhart and his collaborators (1963) who covered a wide range of incident ion energy starting from 0.4 kev, to 25 kev. Everhart *et al* have further

observed that at a fixed scattering angle, the electron capture probability when plotted against the incident ion energy gives several resonant peaks and valleys

In the present paper we have derived the expression for electron capture by  $\text{He}^+$  ions passing through He atoms by applying a variational method which is valid for both moderately high and low velocities of the incident ions. In our formulation the momentum transfer term is included in the wave function and the effect of exchange of electrons is taken into account.

### THEORY

We consider the capture of an electron from the ground state of a helium atom  $A$  by the singly ionised helium ion  $B$ . We assume the nuclei  $B$  and  $A$  move with uniform velocities  $\frac{1}{2}\mathbf{v}$  and  $-\frac{1}{2}\mathbf{v}$  respectively, the effect of the nucleus-nucleus interaction is neglected. Initially at  $t = -\infty$  we have the two electrons attached to the nucleus  $A$  and one in nucleus  $B$ . We symmetrize the initial state wave functions by taking proper account of the effect of electron exchange.

The time rate of change of electron state wave function is given by the time-dependent Schrödinger equation

$$H\psi = i\hbar \frac{\partial\psi}{\partial t} \quad \dots (1)$$

where  $H$  is the Hamiltonian corresponding to the motion of the electrons in the coulomb field of the two nuclei

$$H = -\frac{\hbar^2}{2m} \sum_{i=1,2,3} \nabla_i^2 + V, \quad V = -\frac{2e^2}{r_{An}} + \frac{1}{r_{Bn}} + e^2 \sum_{i,j} \frac{1}{r_{ij}}$$

and  $\mathbf{r}_{An}$ ,  $\mathbf{r}_{Bn}$  are the position vectors of the  $n$ -th electron from the nucleus  $A$  and  $B$  respectively and  $r_{ij}$ 's are the inter electronic distances. The Schrödinger equation (1) is obtained by making stationary the following variation integral I.

$$I = \int \left( \frac{1}{2} \bar{\psi} H \psi - \frac{1}{2} \psi H \bar{\psi} + \frac{1}{2} i\hbar \bar{\psi} \frac{\partial\psi}{\partial t} - \frac{1}{2} i\hbar \psi \frac{\partial\bar{\psi}}{\partial t} \right) d\mathbf{v} dt \quad \dots (2)$$

with respect to small arbitrary variation of  $\psi$  and  $\bar{\psi}$  for a suitable approximation, we choose a trial wave function  $\psi_T$ .

$$\psi_T = A(t)\psi_i + B(t)\psi_f \quad \dots (3)$$

where  $\psi_i$  is the product of the two ground state wave functions, one for the helium atom with the nucleus  $A$  and the other for the ionised helium atom with the

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nucleus  $B$ ,  $\psi_f$  is the product with  $A$  and  $B$  interchanged. Here we have restricted our calculations to two electron states. The  $\psi_i$  and  $\psi_f$  can be written as

$$\psi_i = \frac{1}{\sqrt{3}} (\psi_{r_1} + \psi_{r_2} + \psi_{r_3}) - (4a), \quad \psi_f = \frac{1}{\sqrt{3}} (\psi_{r_1}' + \psi_{r_2}' + \psi_{r_3}') \quad (4b)$$

$$\text{where } \psi_1 = u_{A(2,3)} v_{B^+(1)} \left\{ \frac{\alpha(2)\beta(3) - \alpha(3)\beta(2)}{\sqrt{2}} \right\} \alpha(1)$$

$$\psi_2 = u_{A(3,1)} v_{B^+(2)} \left\{ \frac{\alpha(3)\beta(1) - \alpha(1)\beta(3)}{\sqrt{2}} \right\} \alpha(2)$$

$$\psi_3 = u_{A(1,2)} v_{B^+(3)} \left\{ \frac{\alpha(1)\beta(2) - \alpha(2)\beta(1)}{\sqrt{2}} \right\} \alpha(3)$$

$$\psi_1' = v_{B(2,3)} u_{A^+(1)} \left\{ \frac{\alpha(2)\beta(3) - \alpha(3)\beta(2)}{\sqrt{2}} \right\} \alpha(1)$$

$$\psi_2' = v_{B(3,1)} u_{A^+(2)} \left\{ \frac{\alpha(3)\beta(1) - \alpha(1)\beta(3)}{\sqrt{2}} \right\} \alpha(2)$$

$$\psi_3' = v_{B(1,2)} u_{A^+(3)} \left\{ \frac{\alpha(1)\beta(2) - \alpha(2)\beta(1)}{\sqrt{2}} \right\} \alpha(3)$$

$\psi_1, \psi_2, \dots$  etc are each normalised, the factor  $1/\sqrt{3}$  in equations (4a) and (4b) is included so as to normalise  $\psi_i$  and  $\psi_f$  for infinite separation between  $A$  and  $B$ . Here  $u_{A(1,2)}$  denotes the normalised ground state wave function of the helium atom with electrons 1 and 2 around the nucleus  $A$ ; this wave function consists of two parts—one due to the orbital motion of the electrons around the nucleus  $A$  and the other due to the translatory motion of the electrons.  $u_{A^+(3)}$  is the normalised ground state wave function of helium ion with the electron 3 around the nucleus  $A$  and consists of two parts—one orbital and the other translatory. Similarly,  $v_B$  and  $v_{B^+}$  denote ground state normalised wave functions of He atom and  $He^+$  ion respectively with  $B$  as the nucleus.  $\alpha$  and  $\beta$  are the spin wave functions. In our calculation we shall use Hylleraas type wave function for the

orbital part of  $u_A$  with effective charge  $\lambda = \frac{27}{16}$ .

$$u_{A(1,2)} = \frac{\lambda^3}{\pi} \exp \left\{ -\lambda(r_{A1} + r_{A2}) + \frac{i}{\hbar} Et \right\} \exp \left[ \frac{-im}{\hbar} \left\{ \frac{1}{2} \mathbf{v} \cdot (\mathbf{r}_1 + \mathbf{r}_2) + \frac{1}{4} v^2 t \right\} \right]$$

$$v_{B^+(3)} = \sqrt{\frac{8}{\pi}} \exp \left\{ -2r_{B3} + \frac{i}{\hbar} ct \right\} \exp \left[ \frac{im}{\hbar} \left( \frac{1}{2} \mathbf{v} \cdot \mathbf{r}_3 - \frac{1}{8} v^2 t \right) \right]$$

$$v_B(1, 2) = \frac{\lambda^3}{\pi} \exp \left\{ -\lambda(r_{B_1} + r_{B_2}) + \frac{i}{\hbar} Et \right\} \exp \left[ \frac{im}{\hbar} \left\{ \frac{1}{2} \mathbf{v} \cdot (\mathbf{r}_1 + \mathbf{r}_2) - \frac{1}{4} v^2 t \right\} \right]$$

$$u_{A^+}(3) = \sqrt{\frac{8}{\pi}} \exp \left\{ \left( -2r_{A_1} + \frac{i}{\hbar} \epsilon t \right) \right\} \exp \left[ \frac{-im}{\hbar} \left( \frac{1}{2} \mathbf{v} \cdot \mathbf{r}_3 + \frac{1}{8} v^2 t \right) \right]$$

$\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$  are the respective position vectors of the three electrons with respect to the centre of mass  $C$  (at rest) of  $A$  and  $B$ .  $E$  and  $\epsilon$  are the binding energies of normal He atom and ground state  $\text{He}^+$  atom respectively

Performing the space integration, we may write

$$I = \int L dt \quad \dots \quad (5)$$

where  $L = \frac{1}{2} [2(\dot{A}\dot{A} + \dot{B}\dot{B})F_1 + 4(\dot{A}\dot{A} + \dot{B}\dot{B})F_2 + 2(\dot{A}\dot{B} + \dot{B}\dot{A})F_3 + 4(\dot{B}\dot{A} + \dot{A}\dot{B})F_4]$

$$+ i\hbar \{ (\dot{A}\dot{A} - \dot{A}\dot{A} + \dot{B}\dot{B} - \dot{B}\dot{B})f_1 + 2(\dot{A}\dot{A} + \dot{A}\dot{A} + \dot{B}\dot{B} - \dot{B}\dot{B})f_2$$

$$+ (\dot{A}\dot{B} + \dot{B}\dot{A} + \dot{B}\dot{A} - \dot{A}\dot{B})f_3 + 2(\dot{B}\dot{A} - \dot{A}\dot{B} + \dot{A}\dot{B} - \dot{B}\dot{A})f_4 \}$$

where

$$F_1 = -\int \tilde{\psi}_1 V_1 \psi_1 dV, \quad V_1 = -e^2 \left( \frac{2}{r_{B_1}} + \frac{2}{r_{B_2}} + \frac{2}{r_{A_1}} - \frac{1}{r_{13}} - \frac{1}{r_{23}} \right)$$

$$F_2 = -\int \tilde{\psi}_1 V_2 \psi'_1 dV, \quad V_2 = -e^2 \left( \frac{2}{r_{A_1}} + \frac{2}{r_{A_2}} + \frac{2}{r_{B_1}} - \frac{1}{r_{13}} - \frac{1}{r_{23}} \right)$$

$$F_3 = -\int \tilde{\psi}_2 V_3 \psi'_3 dV, \quad V_3 = -e^2 \left( \frac{2}{r_{B_1}} + \frac{2}{r_{B_2}} + \frac{2}{r_{A_2}} - \frac{1}{r_{12}} - \frac{1}{r_{23}} \right)$$

$$F_4 = -\int \tilde{\psi}_3 V_3 \psi_2 dV$$

$$f_1 = \int \tilde{\psi}_1 \dot{\psi}_1 dV, \quad f_2 = \int \tilde{\psi}_1 \dot{\psi}'_1 dV, \quad f_3 = \int \tilde{\psi}_2 \dot{\psi}'_3 dV, \quad f_4 = \int \tilde{\psi}_3 \dot{\psi}_2 dV$$

where dots denote differentiation with respect to time.

Finally from the variational principle, by making  $I$  stationary with respect to the small arbitrary variations of  $A$  and  $B$ , we get the following differential equations

$$2(F_1 + 2F_4)\dot{A} + 2(F_2 + 2F_3)\dot{B} + i\hbar \{ 2(f_1 + 2f_4)\dot{A} + 2(f_2 + 2f_3)\dot{B} \\ + (\dot{f}_1 + 2\dot{f}_4)A + (\dot{f}_2 + 2\dot{f}_3)B \} = 0 \quad \dots \quad (6)$$

$$2(F_2 + 2F_3)\dot{A} + 2(F_1 + 2F_4)\dot{B} + i\hbar \{ 2(f_1 + 2f_3)\dot{A} + 2(f_2 + 2f_4)\dot{B} \\ + (\dot{f}_2 + 2\dot{f}_3)A + (\dot{f}_1 + 2\dot{f}_4)B \} = 0 \quad \dots \quad (7)$$

From the above two equations we obtain

$$(F_1 + F_2 + 2F_3 + 2F_4)(A + B) + i\hbar \{ (f_1 + f_2 + 2f_3 + 2f_4)(\dot{A} + \dot{B}) \\ + \frac{1}{2}(\dot{f}_1 + \dot{f}_2 + 2\dot{f}_3 + 2\dot{f}_4)(A + B) \} = 0 \quad \dots \quad (8)$$

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$$(F_1 + 2F_4 - F_2 - 2F_3)(A - B) + i\hbar\{f_1 + 2f_3 - f_2 - 2f_3\}(\dot{A} - \dot{B}) \\ + \frac{1}{2}(f_1 + 2f_4 - f_2 - 2f_3)(\dot{A} - \dot{B}) = 0 \quad \dots (9)$$

Applying the initial conditions i.e. at  $t = -\infty$ ,  $A = 1$ ,  $B = 0$  we finally get by solving the above two equations the capture probability as

$$|B_{f, \nu}|^2 = \sin^2 \phi_2$$

where 
$$\phi_2 = \frac{1}{\hbar} \int_{-\infty}^{\infty} (F_2 + 2F_3)(1 + 2f_3) - \frac{(F_1 + 2F_4)(f_2 + 2f_3)}{(1 + 2f_4)^2 (f_2 + 2f_3)^2} dt$$

For the case of very low relative velocity of the incident ion with respect to the helium atom we may evaluate  $F$ 's and  $f$ 's after neglecting the translatory part of the electron wave functions. We expect, from the expression for the capture probability resonance structure with changes of energy. The details of calculations for the capture cross-section will be published soon.

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