

VARIATIONAL METHOD AND THE ELASTIC SCATTERING OF SLOW ELECTRONS BY HYDROGEN ATOM

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ABSTRACT. The collision of electron and hydrogen atom has been investigated by the variational method of Hult en in the energy range below the threshold for the excitation of second quantum level (10.2 eV) of atomic hydrogen. The influence of the polarisation has been taken in the wave function which includes a term indicating virtual excitation to $2s$ and $2p_0$ levels, here this choice leads to the occurrence of pronounced resonance at 9.74 eV energy which agrees with the theoretical results of Burke and Seely (1962) in their $1s$ - $2s$ - $2p$ close coupling approximation. Recently Schulz (1964) has experimentally found a resonance peak at 9.7 eV energy.

INTRODUCTION

The scattering of electrons by hydrogen atom is theoretically the simplest of all electron-atom collision problems, hence it has been the subject of detailed theoretical investigation. This has many important applications in astrophysics, controlled thermonuclear devices and other processes.

A number of experiments have been carried out on slow electron scattering by atomic hydrogen by Neynaber (1961), Brackmann, Fite *et al.*, (1958). Recently Schulz (1964) has reported an experimental evidence for a resonance in the elastic scattering of electrons by atomic hydrogen, below the onset of excitation of the electronic states of hydrogen atom.

The scattering at low energy involves the effect of exchange because of the indistinguishability of the incident electron from atomic electron. There is a great probability of the incident electron being captured and the atomic electron being ejected in the process of slow collision. Moreover, due to the influence of the incoming electron, there is a polarisation effect arising out of the distortion of the spherically symmetrical charge distribution of $1s$ -electron cloud in the neutral atomic hydrogen.

Massey and Moiseiwitsch (1951) have used variational method to calculate the S -wave phase shift due to scattering of electrons by atomic hydrogen, taking the exchange effect and the partial distortion of the atomic cloud. They have treated this distortion by introducing explicitly in the trial wave function a term which depends on the electron-electron correlation distance r_{12} . In some of the

more recent works (cf. Burke and Schey (1962) with the use of modern computing machines, sets of coupled equations resulting from the retention of only a few selected excited states of the hydrogen atom in the wave function, have been solved numerically. Burke and Schey (1962) have utilised a close-coupling approximation in which the total wave function has been expanded in hydrogen eigen states and only terms corresponding to the 1s, 2s and 2p states are retained. In their investigations, they have found that except for the very low energy region below .68 ev the short-range distortion effect dominates over the long-range one and the 2s-state gives a larger contribution to the phase-shift than 2p state. Moreover, once all states corresponding to second quantum level have been incorporated in the formulation of the problem, all other remaining states have negligible effects. Recently, Temkin and Pohlé (1963) have calculated the singlet S-wave phase shift in electron hydrogen atom collisions below the inelastic threshold, they have obtained two resonances, the first one centred at 9.4 ev is broader than the second one occurring at 10.1 ev.

In the present paper, we have investigated the the S-wave phase-shift values in electron-hydrogen atom collisions. Since the proton is very massive compared to the electron the wavefunction for the electron-hydrogen system will depend only upon the coordinates of the bound and free electrons. Here we assume that the distortion of the initial 1s-state is in the form of a superposition of higher excited states induced temporarily when the incident electron is close to the target; but when the colliding electron is far away, the original 1s-state of the bound electron is restored. Our formulation is in conformity with the remark of Burke and Schey (1962). For simplicity of calculations, we have considered the virtual excitation to 2s and $2p_0$ states only, the polar axis being taken along the target nucleus. We have used Hulthén's variational method to calculate the S-wave phase-shift as a function of energy and we have neglected the effect of exchange. By making use of Breit-Wigner formula we obtain a resonance at an energy 9.74 ev which agrees favourably with the most recent experimental findings by Schulz (1964).

It is worth mentioning that previous calculations with the variational method by Massey and Moisewitsch (1951) and Geltman (1960) have failed to show the occurrence of resonance, whereas our suitable choice of the wavefunction brings out the resonance with the same variational method.

THEORY

The wave function $\psi(\mathbf{r}_1, \mathbf{r}_2)$ of the system of two electrons moving in the field of a proton satisfies the wave equation

$$(H-E)\psi(\mathbf{r}_1, \mathbf{r}_2) = 0 \quad \dots (1)$$

with
$$H = \left[-\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} \right]$$

in atomic units (i.e. $e = m = \hbar = 1 = a_0$); here \mathbf{r}_1 and \mathbf{r}_2 are the co-ordinate of the atomic electron and impinging electron, respectively, relative to the proton and r_{12} is the distance between the electrons.

Expanding the total wave function ψ in terms of the eigen states of the target Hamiltonian, we have

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = (\sum_n + \int) \psi_n(\mathbf{r}_1) F_n(\mathbf{r}_2) \quad \dots (2)$$

where the summation and integration signs have their usual meanings. Here $\psi_n(\mathbf{r}_1)$ represents the wave function for the n -th state of the hydrogen atom and satisfies the eigen-value equation $(\nabla_1^2 - \frac{2}{r_1} - 2E_n) \psi_n(\mathbf{r}_1) = 0$ where E_n represents the eigen-energy of the n -th state of the atom. If the kinetic energy of the incident electron is $\frac{K_0^2}{2}$, the functions F_n must have the asymptotic forms

$$F_0 \sim e^{i\mathbf{K}_0 \cdot \mathbf{r}_2} + \frac{e^{iK_0 r_2}}{r_2} f(\theta_2, \phi_2)$$

and
$$F_n \sim \frac{e^{iK_n r_2}}{r_2} f_n(\theta_2, \phi_2) \quad \dots (3)$$

where
$$E = \frac{K_0^2}{2} + E_0 = \frac{K_n^2}{2} + E_n$$

Here E_0 and E_n represent the energies of the ground state and the n -th state of the atom respectively and \mathbf{K}_0 and \mathbf{K}_n represent respectively the momenta of the incident electron and scattered electron after excitation of the n -th state of the atom.

To solve equation (1) under the prescribed boundary conditions in (2), we shall apply the variational method of Hulthén (1944). We make a choice of the following trial wave function

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \chi(\mathbf{r}_1, \mathbf{r}_2) F(\mathbf{r}_2)$$

where
$$\chi(\mathbf{r}_1, \mathbf{r}_2) = \psi_{1s}(r_1) \left(1 - \frac{\alpha^2 + \beta^2}{2} e^{-2r_2} \right) + \alpha \psi_{2s}(r_1) e^{-r_2} + \beta \psi_{2p_0}(r_1, r_2) e^{-r_2}$$

$$F(\mathbf{r}_2) = \left\{ e^{i\mathbf{K}_0 \cdot \mathbf{r}_2} + (a + b e^{-r_2})(1 - e^{-r_2}) \frac{\cos K_0 r_2}{K_0 r_2} \right\},$$

here we have taken only the S-wave part of the scattered wave and $\chi(\mathbf{r}_1, \mathbf{r}_2)$ satisfies the normalisation condition $\int \chi^* \chi d\mathbf{r}_1 = 1$, correct to terms of the order of α^2 and β^2 . The wave function $F(\mathbf{r}_2)$ having adjustable parameters a and b has the asymptotic form $\{e^{i\mathbf{k}_0 \cdot \mathbf{r}_2} + a \cos K_0 r_2 / K_0 r_2\}$ and is finite at the origin. The S-wave phase-shift η_0 is given by $\eta_0 = \tan^{-1} a$.

We substitute the trial wave function $\psi(\mathbf{r}_1, \mathbf{r}_2)$ in the variational integral $L = \int \psi (H - E)\psi^* d\mathbf{r}_1 d\mathbf{r}_2$... (4)

and evaluate it. The value of the phase-parameter 'a' is obtained from the following set of simultaneous equations

$$L(\alpha, \beta, b; a) = 0$$

$$\frac{\partial L}{\partial \alpha} = 0$$

$$\frac{\partial L}{\partial \beta} = 0$$

$$\frac{\partial L}{\partial b} = 0$$

It is to be noted that cubes and higher powers of α and β in L have been neglected.

The elastic S-wave cross-section Q_0 is $\frac{4\pi}{K_0^2} \sin^2 \eta_0$

In discussing the resonance effect, we decompose the total phase shift into two parts as $\eta_{total} = \eta_{potential} + \eta_{resonance}$ where $\eta_{potential}$ is the slowly varying potential part of the phase-shift and $\eta_{resonance}$ is the phase shift due to the resonance effect. Following Burke and Schey, we write

$$Q_{total} = \frac{\pi}{K_0^2} |A_{res} + A_{pot}|^2$$

where $A_{res} = e^{2i\eta_{pot}} [e^{2i\eta_{res}} - 1]$

and $A_{pot} = [e^{2i\eta_{pot}} - 1]$

The S-wave resonant part of the cross section is written as

$$Q_{res} = \frac{\pi}{K_0^2} |A_{res}|^2 = \frac{4\pi}{K_0^2} \sin^2 \eta_{res}$$

Hence we get Q_{res} as a function of K_0^2 .

Calculation of L

The variation integral L in (4) can be written in the form :

$$L = L_1 + L_2$$

where

$$L_1 = \int A^* P d\mathbf{r}_2 + \int B^* Q d\mathbf{r}_2 + \iint C^* R \psi_{2p_0}^*(\mathbf{r}, \mathbf{r}_2) \psi_{2p_0}(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2$$

and
$$L_2 = \int \int \left(\frac{2}{r_2} - \frac{2}{r_{12}} \right) [A^* \psi_{1s}^*(r_1) + B^* \psi_{2s}^*(r_1) + C^* \psi_{2p_0}^*(\mathbf{r}_1, \mathbf{r}_2)]$$

$$\times [A \psi_{1s}(r_1) + B \psi_{2s}(r_1) + C \psi_{2p_0}(\mathbf{r}_1, \mathbf{r}_2)] d\mathbf{r}_1 d\mathbf{r}_2$$

in which

$$A = \left(1 - \frac{\alpha^2 + \beta^2}{2} e^{-2r_2} \right) F(\mathbf{r}_2)$$

$$B = \alpha e^{-r_2} F(\mathbf{r}_2)$$

$$C = \beta e^{-r_2} F(\mathbf{r}_2)$$

$$P = \nabla_2^2 \{F(\mathbf{r}_2)\} - \left(\frac{\alpha^2 + \beta^2}{2} \right) \nabla_2^2 \{e^{-2r_2} F(\mathbf{r}_2)\} + K_0^2 F(\mathbf{r}_2) - K_0^2 \left(\frac{\alpha^2 + \beta^2}{2} \right) e^{-2r_2} F(\mathbf{r}_2)$$

$$Q = \nabla_2^2 \{e^{-r_2} F(\mathbf{r}_2)\} + K_0^2 e^{-r_2} F(\mathbf{r}_2) + 2(\epsilon_1 - \epsilon_2) e^{-r_2} F(\mathbf{r}_2)$$

$$R = \frac{1}{\cos \theta_{12}} \nabla_2^2 \{e^{-r_2} F(\mathbf{r}_2) \cos \theta_{12}\} + K_0^2 e^{-r_2} F(\mathbf{r}_2) + 2(\epsilon_1 - \epsilon_2) e^{-r_2} F(\mathbf{r}_2)$$

A^* , B^* and C^* are the complex conjugates of A , B and C respectively, and ϵ_1 and ϵ_2 are the binding energies of the ground state (1s) and 2s (also 2p) states of the atom respectively.

On carrying out the integrations over $d\mathbf{r}_1$ and over the angular co-ordinates θ_2 , ϕ_2 of $d\mathbf{r}_2$ -space, we get

$$\begin{aligned} L_1 &= \frac{2\pi}{K_0^2} \int_0^\infty [ps(1 + \cos 2K_0 r_2) + s \sin 2K_0 r_2] dr_2 \\ &- \frac{4\pi}{K_0^2} \int_0^\infty [q(1 - \cos 2K_0 r_2) + pq \sin 2K_0 r_2] dr_2 \\ &- \frac{\pi\alpha^2}{2K_0^2} \int_0^\infty [7p^2(1 + \cos 2K_0 r_2) + 14p \sin 2K_0 r_2] e^{-2r_2} dr_2 \\ &- \pi\alpha^2 \int_0^\infty [7r_2^2] e^{-2r_2} dr_2 \\ &- \frac{\pi\beta^2}{2K_0^2} \int_0^\infty [7p^2(1 + \cos 2K_0 r_2) + 14p \sin 2K_0 r_2] e^{-2r_2} dr_2 \\ &- \frac{\pi\beta^2}{K_0^2} \int_0^\infty [4p^2(1 + \cos 2K_0 r_2) + 8p \sin 2K_0 r_2] \frac{e^{-2r_2}}{r_2^2} dr_2 \\ &- \pi\beta^2 \int_0^\infty [7r_2^2 + 8] e^{-2r_2} dr_2 \end{aligned}$$

where

$$\begin{aligned} p &= (a+be-r_2)(1-e-r_2) \\ q &= ae^{-r_2}+b(2e-2r_2-e-r_2) \\ s &= -ae^{-r_2}+b(e-r_2-4e-2r_2) \end{aligned}$$

Similarly, we get

$$\begin{aligned} L_2 &= \frac{4\pi}{K_0^2} \int_0^\infty \left[\left(1 + \frac{1}{r_2} \right) e^{-2r_2} \right] t dr_2 \\ &+ 8\pi \int_0^\infty [(r_2^2+r_2)e^{-2r_2}] dr_2 \\ &+ \frac{\pi\alpha^2}{2K_0^2} \int_0^\infty \left[\left(r_2^2+2r_2+6 + \frac{8}{r_2} \right) e^{-3r_2} - 8 \left(1 + \frac{1}{r_2} \right) e^{-4r_2} \right] t dr_2 \\ &+ \pi\alpha^2 \int_0^\infty [(r_2^4+2r_2^3+6r_2^2+8r_2)e^{-3r_2} - 8(r_2^2+r_2)e^{-4r_2}] dr_2 \\ &+ \frac{\pi\beta^2}{2K_0^2} \int_0^\infty \left[\left(-\frac{96}{r_2^3} \right) e^{-2r_2} + \left(r_2^2+6r_2+22 + \frac{56}{r_2} + \frac{96}{r_2^3} + \frac{96}{r_2^3} \right) e^{-3r_2} \right. \\ &\quad \left. - 8 \left(1 + \frac{1}{r_2} \right) e^{-4r_2} \right] t dr_2 \\ &+ \pi\beta^2 \int_0^\infty \left[\left(-\frac{96}{r_2} \right) e^{-2r_2} + \left(r_2^4+6r_2^3+22r_2^2+56r_2+96 + \frac{96}{r_2} \right) e^{-3r_2} \right. \\ &\quad \left. - 8(r_2^2+r_2) e^{-4r_2} \right] dr_2 \\ &+ \frac{\pi\alpha\beta}{2K_0^2} \int_0^\infty \left[\left(\frac{48}{r_2^3} \right) e^{-2r_2} - \left(2r_2^2+8r_2+24 + \frac{48}{r_2} + \frac{48}{r_2^2} \right) e^{-3r_2} \right] t dr_2 \\ &+ \pi\alpha\beta \int_0^\infty \left[(48)e^{-2r_2} - (2r_2^4+8r_2^3+24r_2^2+48r_2+48)e^{-3r_2} \right] dr_2 \end{aligned}$$

$$\begin{aligned}
 & - \frac{32 \times 2^4}{27} \times \frac{\pi \alpha}{2K_0^2} \int_0^\infty \left[(3r_2 + 2) e^{-5/2r_2} \right] t dr_2 \\
 & - \frac{32 \times 2^4}{27} \times \pi \alpha \int_0^\infty \left[(3r_2^3 + 2r_2^2) e^{-5/2r_2} \right] dr_2 \\
 & + \frac{32 \times 2^4}{243} \cdot \frac{\pi \beta}{2K_0^2} \int_0^\infty \left[\left(27r_2 + 72 + \frac{96}{r_2} + \frac{64}{r_2^2} \right) e^{-5/2r_2} - \frac{64}{r_2^2} e^{-r_2} \right] t dr_2 \\
 & + \frac{32 \times 2^4}{243} \times \pi \beta \int_0^\infty \left[(27r_2^3 + 72r_2^2 + 96r_2 + 64) e^{-5/2r_2} - 64e^{-r_2} \right] dr_2
 \end{aligned}$$

where $t = p^2(1 + \cos 2K_0 r_2) + 2p \sin 2K_0 r_2$

There is no further difficulty in carrying out the integrations appearing in L_1 and L_2 , although the calculations become very tedious due to the occurrence of a large number of terms. For simplicity in calculations, we have taken $b = 0$.

In the low energy region we first find the solutions of the quadratic equation $L = 0$ obtained by putting $\alpha = \beta = 0$. One of the solutions agrees with the results of Massey and Moisewitsch (1951). Now to find the required solution of the sixth degree equation at low energy we search the root in the neighbourhood of the particular solution mentioned above; a root is obtained differing only slightly

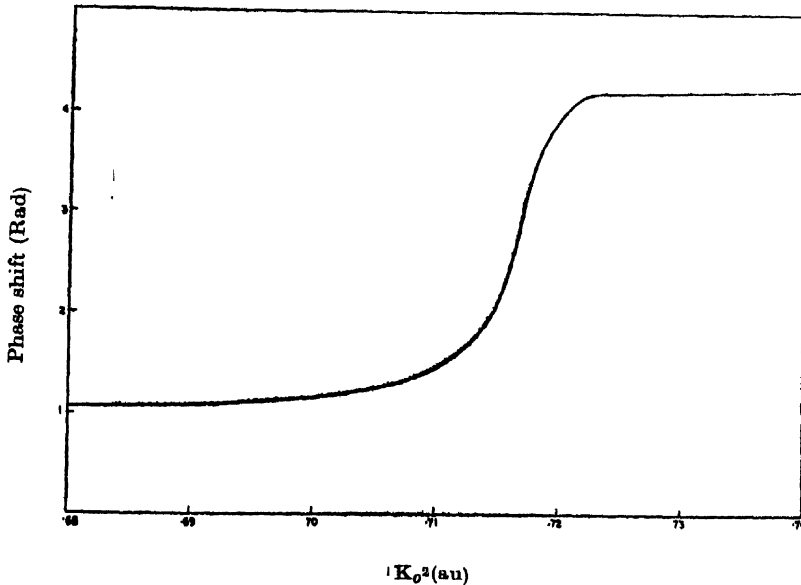


Fig. 1. The S-wave phase shift is plotted as a function of K_0^2 in the neighbourhood of resonance.

from the particular solution chosen of the quadratic equation. Once the root has been fixed for a particular low energy, the phase-shifts for higher energies have been obtained by solving the sixth degree equation and using the continuity property of the phase-shift.

RESULTS AND DISCUSSIONS

We have evaluated the S-wave phase-shift values for the case $b = 0$ in the trial function $F(\mathbf{r}_2)$, for energies ranging from 3.4 eV to 9.85 eV by using only the coupling of 1s, and the virtually excited 2s and 2p₀ states.

We give a plot of S-wave phase shift values η_0 versus K_0^2 in Fig. 1. In the present calculation the 2s state gives a large correction to the S-wave phase shift than the 2p₀ state at the energy range under consideration. This fact has been corroborated by the results obtained by Bruke and Sehey (1962).

The most notable characteristic part of our result is the sharp increase in phase shift values above $K_0^2 = .70$. The curve has a pronounced resonating behaviour, with a definite flattening out before the threshold is reached.

In the Fig. (2), we have plotted Q_{res} as a function of K_0^2 Using Breit-Wigner cross section formula

$$Q_{res} = \frac{4\pi}{K_0^2} \frac{\Gamma^2/4}{(E - E_{res})^2 + \frac{\Gamma^2}{4}}$$

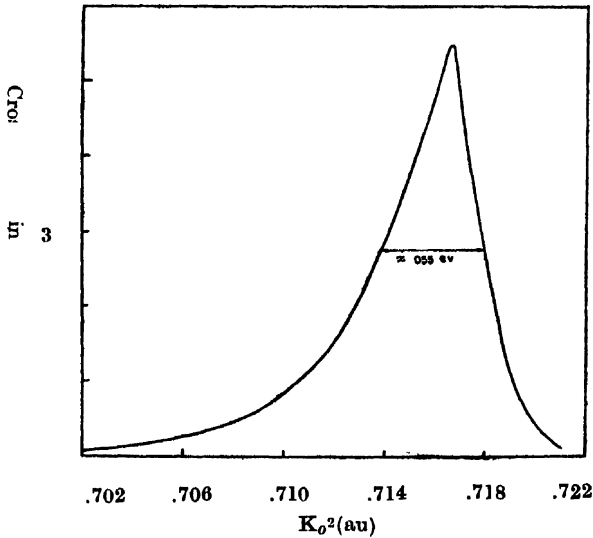


Fig. 2. The resonant part of S-wave cross-section is plotted as a function of K_0^2 .

we obtain $E_{res} = (.7158 \text{ a.u.}) 9.735 \text{ eV}$, which agrees very favourably with experimental findings by Schulz (1964). The value of our resonance cross section comes out to be $5.203\pi a_0^2$ and the calculated value of the width Γ of the resonance state is found to be about .055 eV.

In experiments by Schulz (1964) it has been observed that the width of resonance in atomic hydrogen is approximately double that of helium, which could not be resolved due to limited energy resolution (~ 3 ev) and the drop in the elastic scattering cross section, indicative of resonance is centred in the vicinity of 9.7 + .15 ev. Hence the position of hydrogen resonance in our case is in very good agreement with the experimental findings by Schulz (1964). Also our total S-wave cross section Q_0 , for the energy 3.4 ev comes out to be equal to 12.32 in units of πa_0^2 whereas the experimental value of the total cross section from the curve of Neynaber (1961) is about 11.18 πa_0^2 . Hence our result for total S-wave cross section without exchange in the low energy region agrees reasonable well with experiment.

Recently, several theoretical papers have appeared showing the existence of of resonance level below the threshold for excitation of the second quantum level. Thus, Burke and Sehey (1962) have obtained a resonance at 9.61 ev, with a width of .109 ev in 3S state and the corresponding resonance cross section being 5.66 πa_0^2 . Numerical calculations taking the effect of exchange into account are in progress and will be published soon.

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