

# ELASTIC SCATTERING OF ELECTRONS BY ATOMIC HYDROGEN

R. JHA AND N. C. SIL

DEPARTMENT OF THEORETICAL PHYSICS,  
INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE,  
JADAVPUR, CALCUTTA-32. INDIA

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**ABSTRACT.** Variational method of Hulthén (1944) has been used to calculate the  $S$ -wave phase-shifts in elastic scattering of electrons by atomic hydrogen in the energy range of 0 to 13.6 eV, by solving the integro-differential equation of Temkin and Lamkin (1961) in the adiabatic exchange approximation. Calculations have also been performed for the polarisation potential of Obédkov (1963).

## INTRODUCTION

We know that in the low energy collision of electron with hydrogen atom, both the exchange and polarisation effects have appreciable influence on the scattering process. The exchange effect arising out of the indistinguishability of the incident and bound electrons decreases with increase in energy. The polarisation effect which is due to the distortion of the atomic charge cloud under the influence of the incoming electron also falls with increase in energy but less rapidly compared to the exchange effect.

Variational calculations of the  $S$ -wave phase-shifts in elastic  $\bar{e}$ - $H$  scattering have been carried out by Massey and Moiseiwitsch (1951), and Staver (1951) and in the low energy limit by Seaton (1957), and by Borowitz and Greenberg (1957). All these calculations show that phase-shifts obtained in the exchange approximation differ markedly at low energies from those obtained in the central field approximation, which takes no account of the exchange effect. It may be mentioned that Massey and Moiseiwitsch (1951) took account of polarisation effect partially, by using the correlation term in the variational trial wave function. Bederson *et al.* (1958) have also carried out variational calculation of the problem taking into account exchange and polarisation. The polarisation potential has been taken from the works of Dalgarno and Lynn (1957). Malik and Trefftz (1960) have carried out numerical computation of the  $S$ ,  $P$  and  $D$  wave phase-shifts in low energy elastic scattering of electrons by atomic hydrogen, with the inclusion of exchange and polarisation effects, represented by the polarisation potential  $V_p(r) = \frac{-\alpha}{2(25+r^4)}$  where  $\alpha$  is the polarisability of hydrogen atom.

Temkin and Lamkin (1959, 1961) have introduced the polarised orbital method, similar in principle to perturbed stationary states method. In this method, Temkin and Lamkin (1961) have considered only the dipole polarisation potential, by making allowance for the dipole term in the first order perturbed hydrogen atom wave function derived by Dalgarno and Lewis (1955).

Here in the present work we have solved the integro-differential equation of Temkin and Lamkin (1961) by the variational method of Hulthén (1944) and have computed the  $S$ -wave phase-shifts in the low energy region. For comparison, we have further calculated the  $S$ -wave phase-shifts in the exchange approximation using another adiabatic dipole polarisation potential deduced by Ob'edkov (1963) the resulting integro-differential equation has been solved by the same variational method. For convenience, our calculations for the case of polarisation potentials of Temkin and Lamkin (1961) and those of Ob'edkov (1963) will be referred to as I and II respectively.

#### THEORY

The Schrödinger wave equation for the system of electron and hydrogen atom is

$$(H-E)\psi(r_1, r_2) = 0 \quad \dots (1)$$

$$H = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 - \frac{e^2}{r_1} - \frac{e^2}{r_2} + \frac{e^2}{r_{12}}, \text{ being the Hamiltonian of the}$$

system and  $E$ , the total energy of the system is  $\frac{\hbar^2 k^2}{2m} + E_0$ ,  $r_1$  and  $r_2$  are the distances of the electrons from the nucleus and other symbols have their usual meanings.

To take into account the exchange effect we approximate  $\psi$  as follow:

$$\psi^\pm(r_1, r_2) = \frac{1}{\sqrt{2}} [F(r_1) \psi_0(r_2) \pm F(r_2) \psi_0(r_1)] \quad \dots (2)$$

where  $\psi_0(r)$  is the wave function of the ground state of hydrogen atom,  $F(r)$  is the wave function of the scattered electron, and  $+v_s$  and  $-v_s$  signs refer to the singlet and triplet cases respectively, the scattered electron wave function  $F(r)$  have the asymptotic form

$$F(r) \rightarrow e^{ik \cdot r} + \frac{e^{ikr}}{r} f(\theta) \\ r \rightarrow \infty$$

$F(r)$  can be expanded as  $F(r) = \sum_{l=0}^{\infty} \frac{f_l(r)}{r} Y_l^0(\Omega)$ ,  $f_l(r)$  satisfying the boundary

condition

$$f_l(r) \rightarrow \sin \left( kr - \frac{l\pi}{2} + \eta_l \right);$$

$r \rightarrow \infty$

$f_s(r) \rightarrow 0$  where  $\eta_0$  being the phase-shift.  
 $r \rightarrow 0$

Following Massey and Moisewitsch (1951) we arrive at the following integro-differential equation (using atomic units)

$$\left[ \frac{d^2}{dr_2^2} - \frac{l(l+1)}{r_2^2} + 2 \left( 1 + \frac{1}{r_2} \right) e^{-2r_2} + k^2 \right] f_s(r_2)$$

$$= \pm \left( \frac{4}{2l+1} \right) \frac{e^{-r_2}}{r_2} \left[ \frac{1}{r_2} \int_0^\infty f_s(r_1) \frac{2e^{-r_1}}{r_1} \times \frac{r_1^{l+1}}{r_2^{l+1}} dr_1 \right.$$

$$\left. - \left( \frac{k^2+1}{2} \right) \delta_{l,0} \int_0^\infty f_l(r_1) \frac{2e^{-r_1}}{r_1} dr_1 \right] \quad \dots (3)$$

In the above derivation, no allowance has been made for the polarisation effect. We should take into consideration the fact that the bound electron wave function will be perturbed by the scattered electron. The polarised atom acts as a dipole yielding an additional attraction for the scattered electron which can be represented by a polarisation potential  $V_p(r)$ . It appears as a potential term in the scattering equation, in addition to the already existing static potential part. Thus, in exchange-adiabatic approximation, we get

$$\left[ \frac{d^2}{dr_2^2} - \frac{l(l+1)}{r_2^2} + k^2 + 2 \left( 1 + \frac{1}{r_2} \right) e^{-2r_2} - 2V_p(r_2) \right] f_l(r_2)$$

$$= \pm \left( \frac{4}{2l+1} \right) \frac{e^{-r_2}}{r_2} \left[ \frac{1}{r_2} \int_0^\infty \frac{2e^{-r_1}}{r_1} f_l(r_1) \frac{r_1^{l+1}}{r_2^{l+1}} dr_1 \right.$$

$$\left. - \left( \frac{k^2+1}{2} \right) \delta_{l,0} \int_0^\infty \frac{2e^{-r_1}}{r_1} f_l(r_1) dr_1 \right] \quad \dots (4)$$

Ob'edkov (1963) has arrived at the following expression for  $V_p(r)$

$$V_p(r) = - \left( \frac{2}{3} \right)^6 \left[ \frac{64}{9r^2} - \left( 3r + 8 + \frac{32}{3r} + \frac{64}{9r^2} \right) e^{-1.5r} \right]^2 \quad \dots (5)$$

It has the asymptotic form  $\frac{-\alpha}{r^4}$  where  $\alpha$  is the polarisability of the atom.

The method of polarised orbitals of Temkin and Lamkin (1961) employs a trial wave function having the form

$$\psi_{\pm}(r_1, r_2) = F(r_1)[\psi_0(r_2) + \psi_{pol}(r_1, r_2)] \pm F(r_2)[\psi_0(r_1) + \psi_{pol}(r_2, r_1)]$$

where 
$$\psi_{pol}(r_1, r_2) = -\epsilon(r_1, r_2) \psi_0(r_2) \frac{1}{r_1^3} \left( \frac{r_2^3}{2} + r_2 \right) \cos \theta_{12}$$

and 
$$\begin{aligned} \epsilon(r_1, r_2) &= 1 \text{ for } r_1 > r_2 \\ &= 0 \text{ for } r_1 < r_2 \end{aligned}$$

According to Temkin and Lamkin

$$\iint Y_l^{0*}(\Omega_1) \psi_0^*(r_2) \left[ \nabla_1^2 + \nabla_2^2 + \frac{2}{r_1} + \frac{2}{r_2} - \frac{2}{r_{12}} + k^2 - 1 \right] \psi_{\pm}(r_1, r_2) dr_2 d\Omega_1 = 0$$

which they have regarded as consistent with the first order determination of the perturbed function. They have arrived at the following radial equation for *S*-wave scattering in polarised orbital approximation.

$$\begin{aligned} & \left[ -\frac{d^2}{dr_1^2} - 2e^{-2r_1} \left( 1 + \frac{1}{r_1} \right) - \frac{\alpha_1(r_1)}{r_1^4} - k^2 \right] u(r_1) \\ & \pm \left[ \begin{aligned} & 8r_1 e^{-r_1} \left\{ c_1 + \frac{1}{r_1} \int_0^{r_2} r_2 e^{-r_2} u(r_2) dr_2 - \int_0^{r_1} e^{-r_2} u(r_2) dr_2 \right\} \\ & - \frac{8}{3} r_1 e^{-r_1} \left( \frac{r_1^3}{2} + r_1^2 \right) \times \left\{ c_2 - \int_{\epsilon}^{r_2} \frac{e^{-r_2}}{r_2^3} u(r_2) dr_2 \right\} \end{aligned} \right] = 0 \quad \dots (6) \end{aligned}$$

where 
$$C_1 = \int_0^{\infty} \left\{ 1 - \left( \frac{1+k^2}{2} \right) r_2 \right\} e^{-r_2} u(r_2) dr_2$$

and 
$$C_2 = \int_{\epsilon}^{\infty} \frac{e^{-r_2}}{r_2^3} u(r_2) dr_2$$

The trial function  $u(r) = \sin kr + (a + be^{-r})(1 - e^{-r}) \cos kr$  and the polarisation potential  $V_p(r)$  is given by  $\frac{\alpha_1(r)}{2r^4}$

where

$$\alpha_1(r) = \frac{2}{3} - \frac{2}{3} e^{-2r} (r^5 + \frac{9}{2} r^4 + 9r^3 + \frac{27}{2} r^2 + \frac{27}{2} r + \frac{27}{4})$$

(c.f. Temkin and Lamkin 1961). In the exchange-adiabatic approximation, the last term on the right-hand side is neglected. Moreover, certain new non-local terms on the right hand side have been omitted by Temkin and Lamkin (1961), their importance for *p*-wave scattering has been pointed out by Sloan (1964). The coupled-integro differential equation (6) has been solved by the same variation method with the polarisation potential

$$V_p(r) = -\frac{\alpha_1(r)}{2r^4}$$

We have solved the above equation (4) in the exchange-adiabatic approximation, by Hulthén's variational method and have computed the *S*-wave phase shifts, by the trial function

$$f(r) = \frac{\sin kr}{kr} + (a + be^{-r})(1 - e^{-r}) \frac{\cos kr}{kr} \text{ with } V_p(r) \text{ as given by (5).}$$

Here *a* is the phase-parameter and *b* is the adjustable variational parameter.

RESULTS AND DISCUSSIONS

We have obtained the scattering lengths *A*± from our *S*-wave phase shifts (singlet and triplet) using modified effective range formula (O'Malley *et al*, 1962)

$$k \cot \eta_0(k^2) = -\frac{1}{A} + \frac{\pi\alpha k}{3} + \frac{4\alpha k^2}{3} \log(1.23\alpha^{\dagger}k) + \left( \frac{1}{2}r_0 + \frac{\pi\alpha^{\dagger}}{3} - \frac{\pi\alpha^{3/2}}{3A^2} - \frac{\pi^2\alpha^2}{9A^3} \right) k^2 + \dots$$

with the phase shift values  $\eta_0(.0001)$  and  $\eta_0(.000025)$ . We have obtained the scattering lengths

$$A^+(\text{singlet}) = 6.767, 5.136$$

$$A^-(\text{triplet}) = 1.965, 1.776$$

in units of *a*<sub>0</sub>, for cases I and II respectively. These may be compared with Temkin and Lamkin values *A*<sup>+</sup> = 5.6 *a*<sub>0</sub> and *A*<sup>-</sup> = 1.9*a*<sub>0</sub>. We have obtained the zero energy cross sections for the two cases (I and II) 57.37π*a*<sub>0</sub><sup>2</sup> and 35.841π*a*<sub>0</sub><sup>2</sup> respectively. In the adjoining table, we have given a list of our calculated *S*-wave phase-shift values and scattering lengths for the two cases along with those of Temkin and Lamkin (1961) for comparison.

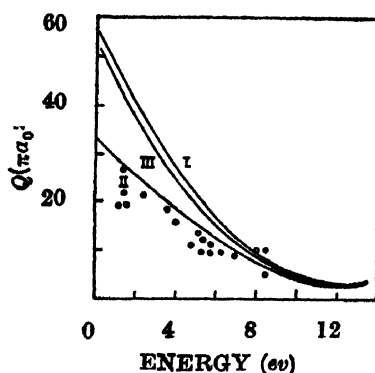
TABLE 1  
S-wave phase shifts in radians

K	I		II		III	
	Singlet ( $\cdot$ )	Triplet ( $-$ )	Singlet ( $\cdot$ )	Triplet ( $-$ )	Singlet ( $\cdot$ )	Triplet ( $-$ )
.01	3.077	3.123	3.074	3.125	3.086	3.136
.1	2.522	2.949	2.495	2.927	2.701	2.962
.2	2.025	2.737	1.999	2.738	2.131	2.814
.5	1.157	2.146	1.250	2.189	1.272	2.245
1	.666	1.480	.742	1.490	.753	1.702

TABLE 2

	A (Singlet)	A $^-$ (Triplet)
I	6.5	1.9
II	6.767	1.965
III	5.136	1.776

In the figure we have plotted our S-wave elastic cross sections against energy for the two cases and have compared the results of S-wave elastic cross section of Temkin and Lamkin (1961) and the experimental data of Brackman *et al.* (1958).



The S-wave cross section (in  $\pi a_0^2$ ) plotted against energy (in eV) of the incident electron.  
 Curve I—Present calculations with polarisation potential of Temkin and Lamkin (1961)  
 Curve II—Present calculations with polarisation potential of Obedkov (1963).  
 Curve III—S-wave elastic cross section (in adiabatic exchange approximation) by Temkin and Lamkin (1961)  
 Circle—Experimental points of Brackman *et al.* (1958).

We find that the agreement of Case II with experiment is better than with Case I. Again the results of our variational calculation in Case I is in close agreement with the corresponding results of numerical solution by Temkin and Lamkin (1961). Hence with a suitable choice of trial wave function it is possible to obtain results of comparable accuracy with those of numerical methods. The disagreement with experiment still left may be mainly due to the adiabatic assumption made in the polarisation potential and the neglect of higher order terms in it, especially the quadrupole one.

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