ELASTIC SCATTERING OF ELECTRONS BY HYDROGEN ATOM

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ABSTRACT. The total cross sections of elastic scattering of electrons by hydrogen atom at the incident energies of 13.6 ev, 54.4 ev, 122.4 ev. 217.6 ev have been calculated in the Born-Oppenheimer (B.O.) approximation with the neglect of the core interaction term and taking into account the distortion of the plane incident wave in the field of the torget atom.

INTRODUCTION

The cross sections of elastic scattering of electrons by atoms are easily calculated with the Born approximation which, however, is valid only at high incident energies; if we include exchange effect in the above, we get the Born Oppenheimer formula which leads generally to poor results at low energies for exchange scattering amplitudes. As the derivation of the B.O. formula is not logically perfect, a number of modifications of the B.O. approximation have been proposed (Feenberg 1932, Mittleman 1962, Bell and Moiseiwitsch 1963, Ochkur 1964). Ochkur suggests that as the first order Born approximation has been derived according to the first order perturbation theory, the first order B.O. formula for exchange scattering amplitude should not contain terms which are not within the frame work of the first order approximation. So he retains only the first term in the expansion of the B.O. formula in the powers of k_0^{-2}(k_0 = wave number of the incident electron). As a result the effect of the core potential term is neglected. Kang and Sucher (1966) have justified this omission by proving that in the exchange amplitude for electron-atom collision, the core interaction term vanishes identically when the core (proton) is infinitely heavy.

Again in the first Born and B.O. formulae the wave function for the colliding electron is approximated by the incident plane wave on the supposition that the incident energy is high. At low energies, the distortion of the plane waves should be considered. This is generally done by having recourse to higher order approximations. In his investigation of the elastic scattering of electrons by helium and hydrogen atoms, Sachl (1958) has given a formulation for taking into account

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the distortion of the s-wave part of the incident wave. The present paper is an extension of Sachl's work in that here we consider the distortion of higher waves. However Sachl's distorted wave is singular at the origin, while our function is free from this singularity. We have omitted the core interaction term from the B.O. formula as suggested by Kang and Sucher (1966). With the neglect of this term, the elastic cross section for collision becomes very large compared to the theoretical results obtained by the close coupling method of Burke, Schey and Smith (1963) and by the first order exchange approximation of Bell and Moiseiwitsch (1963). The inclusion of the effect of distortion of the incident waves considerably improves the result except at $k_0 = 1$ where the validity of the Born or B.O. approximation is questionable and where distortion and polarization of the atom play an important role.

DIRECT AND EXCHANGE SCATTERING AMPLITUDES

The wave equation for the scattering of an electron by a H atom (in atomic units) is

$$\left(-\tfrac{1}{2}\Delta_1^2-\tfrac{1}{2}\Delta_2^2-\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{r_{12}}-E\right)\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = 0 \qquad \ldots \quad (1)$$

where $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ and E are respectively the wave function and the total energy of the system. The boundary conditions on $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ are

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)) \sim \exp i\boldsymbol{k}_0 \cdot \boldsymbol{r}_1 \psi_0(\boldsymbol{r}_2) + \sum_n \frac{\exp ik_n r_1}{r_1} f_n(\theta_1, \phi_1)\psi_n(\boldsymbol{r}_2) \quad \text{as } r_1 \to \infty \qquad \ldots \quad (2)$$

$$\sim \sum_n \frac{\exp ik_n r_2}{r_2} g_n(\theta_2, \phi_2)\psi_n(\boldsymbol{r}_1) \qquad \text{as } r_2 \to \infty \qquad \ldots \quad (3)$$

Here $\psi_n(\boldsymbol{r})$ is the wave function of the n-th state of the H atom with eigen energy E_n; $\boldsymbol{k}_0$ and $\boldsymbol{k}_n$ are the momenta of the incident and scattered electrons.

It is usual to expand the wave function $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ in the form

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = (\sum_n + \int)\psi_n(\boldsymbol{r}_2)F_n(\boldsymbol{r}_1) \qquad \ldots \quad (4)$$

where $\sum_n$ is the summation over discrete states and $\int$ denotes integration over functions of continuous spectrum. The function $F_n(\boldsymbol{r})$ in (4) satisfies the integral equation

$$F_n(\boldsymbol{r}) = e^{i\boldsymbol{k}_n \cdot \boldsymbol{r}}\delta_{0n} - \frac{1}{2\pi}\int\int \frac{e^{ik_n|\boldsymbol{r}-\boldsymbol{r}_1|}}{|\boldsymbol{r}-\boldsymbol{r}_1|} \cdot \left(\frac{1}{r_{12}} - \frac{1}{r_1}\right)$$

$$\times \psi(\boldsymbol{r}_1, \boldsymbol{r}_2)\psi_n^*(\boldsymbol{r}_1)\, d^3r_1 d^3r_2 \qquad \ldots \quad (5)$$

Then comparing the asymptotic form of $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ in the equation (4) with the right hand side of the equation (2) one easily obtains for the direct scattering amplitude for elastic scattering

$$f_0(\theta, \phi) = -\frac{1}{2\pi}\int\int e^{-i\boldsymbol{k}.\boldsymbol{r}_1}\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)\psi_0^*(\boldsymbol{r}_1)d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 \quad \ldots \quad (6)$$

where $\boldsymbol{k}$ is the momentum of the scattered electron.

In an analogous manner, we derive the formula for exchange amplitude $g_0(\theta, \phi)$ for elastic scattering in the form

$$g_0(\theta, \phi) = -\frac{1}{2\pi}\int\int e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_2}\left(\frac{1}{r_{12}}-\frac{1}{r_2}\right)\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)\psi_0^*(\boldsymbol{r}_2)d^3\boldsymbol{r}_1\, d^3\boldsymbol{r}_2 \quad \ldots \quad (7)$$

Therefore the total elastic scattering cross section for e^-H collision is

$$\sigma = 2\pi\int_0^\pi \{\tfrac{1}{4}|f_0+g_0|^2+\tfrac{3}{4}|f_0-g_0|^2\}\sin\theta d\theta \quad \ldots \quad (8)$$

In the usual Born approximation one substitutes

$$F_0(\boldsymbol{r}) = e^{i\boldsymbol{k}_0\cdot\boldsymbol{r}} \quad \ldots \quad (9)$$

and

$$F_n(\boldsymbol{r}) = 0,\ n \neq 0 \quad \ldots \quad (10)$$

This approximation called the zero order approximation is justified when $k_0 >> 1$

The second term on the right hand side of (5) when $n = 0$ measures the distortion of the incident plane wave in the presence of the atom. One gets series expansions for $f_0(\theta, \phi)$ and $g_0(\theta, \phi)$ by iteration using (5). The convergence of these series is very poor at low energies. Moreover the higher order terms of f_0 and g_0 cannot be evaluated without great computational efforts.

We shall, however, take for $F_0(\boldsymbol{r})$ an approximate solution of the following equation derived from the equations (1), (4) and (10).

$$(\Delta_1^2+k_0^2)F_0(\boldsymbol{r}_1) = 2V_{00}(r_1)F_0(\boldsymbol{r}_1) \quad \ldots \quad (11)$$

where

$$V_{00}(r_1) = \int\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\psi_0^*(\boldsymbol{r}_2)\psi_0(\boldsymbol{r}_2)d^3\boldsymbol{r}_2$$

$$= -e^{-2r_1}\left(1+\frac{1}{r_1}\right) \quad \ldots \quad (12)$$

DERIVATION OF AN APPROXIMATE EXPRESSION FOR $F_0(\boldsymbol{r})$

Let us expand $F_0(\boldsymbol{r})$:

$$F_0(\boldsymbol{r}) = \sum_{l=0}^{\infty} r^{-1}f_l(r)P_l(\cos\theta)$$

where $P_l(\cos\theta)$ is the Legendre polynomial of the order l. Then $f_l(r_1)$ satisfies the equation

$$\frac{d^2f_l}{dr_1^2}+\left[k_0^2-2V_{00}(r_1)-\frac{l(l+1)}{r_1^2}\right]f_l(r_1)=0$$

and
$$f_l(r_1)\underset{r_1\to\infty}{\longrightarrow}\frac{e^{-i\eta_l}}{k_0}\sin\left(k_0r-\frac{l\pi}{2}+\eta_l\right),$$

the scattering phaseshift η_l of the l-th order partial wave being assumed to be known from the formula (Mott and Massey 1965, p. 464)

$$\eta_l=-\pi\int_0^\infty J^2_{l+\frac{1}{2}}(k_0r)V_{00}(r)rdr \quad \ldots \quad (13)$$

where $J_{l+\frac{1}{2}}(k_0r)$ is an ordinary Bessel function. The equation (11) is the scattering wave equation in the static field approximation. Then an approximate solution of the equation (11) has the asymptotic form

$$F_0(\boldsymbol{r})\sim e^{i\boldsymbol{k}_0\cdot\boldsymbol{r}}+f(\theta)r^{-1}e^{ik_0r}.$$

where $f(\theta)$ is the corresponding scattering amplitude defined by

$$f(\theta)=(2ik_0)^{-1}\sum_{l=0}^{\infty}(2l+1)(e^{2i\eta_l}-1)P_l(\cos\theta) \quad \ldots \quad (15)$$

Using the expansion

$$e^{i\boldsymbol{k}_0\cdot\boldsymbol{r}}=\sum_l(2l+1)i^lj_l(k_0r)P_l(\cos\theta)$$

and identifying the equation (14) with the asymptotic solution of the equation (11) in terms of the spherical Bessel and Neumann functions, $j_l(k_0r)$ and $n_l(k_0r)$, one easily proves that

$$F_0(\boldsymbol{r})\sim e^{i\boldsymbol{k}_0\cdot\boldsymbol{r}}+\sum_{l=0}^{\infty}(2l+1)i^{l+1}e^{i\eta_l}\sin\eta_l[j_l(k_0r)+in_l(k_0r)] \quad \ldots \quad (16)$$

In order that we may use the expression (16) for the complete wave function $F_0(\boldsymbol{r})$ valid for all r, we remove the singularity at $r=0$ by multiplying the Neumann function n_l by the correction factor $(1-e^{-\alpha r})^{2l+1}$ where α is a quantity dependent on l and k_0. We however have taken $\alpha=1$. This value of α should however be obtained variationally using

$$F_0(\boldsymbol{r})=e^{i\boldsymbol{k}_0\cdot\boldsymbol{r}}+\sum_{l=0}^{\infty}(2l+1)i^{l+1}(\tfrac{1}{2}\sin 2\eta_l+i\sin^2\eta_l)$$
$$\times[j_l(k_0r)+i(1-e^{-\alpha r})^{2l+1}n_l(k_0r)] \quad \ldots \quad (17)$$

as the trial wave function of the equation (15) with η_l given by the equation (13). Since we use the approximate values of the phase shifts η_l given by the equation (13), we obtain an approximation for $F_0(\boldsymbol{r})$ which takes some account of the distortion of the plane waves. We now calculate $f_0(\theta, \phi)$ and $g_0(\theta, \phi)$ from the integral equation (6) and (7) using the above value of $F_0(\boldsymbol{r})$

CALCULATION OF SCATTERING AMPLITUDES

4.1. *Direct scattering amplitude*

Substituting the approximate wave function $F_0(\boldsymbol{r})$ given by (17) in (6) we obtain

$$f_0(\theta, \phi) = f_0^{(1)} + f_0^{(2)} + f_0^{(3)}$$

where $$f_0^{(1)} = -\frac{1}{2\pi} \int e^{i\,\boldsymbol{q}\cdot\boldsymbol{r}_1} V_{00}(r_1) d^3\boldsymbol{r}_1 \quad \text{with } \boldsymbol{q} = \boldsymbol{k}_0 - \boldsymbol{k}, \qquad \dots (18)$$

$$f_0^{(2)} = -\frac{1}{2\pi} \sum_{l=0}^{\infty} (\tfrac{1}{2} \sin 2\eta_1 + i \sin^2 \eta_l) i^{\,l+1}$$

$$\times \int e^{-i\mathbf{k}\cdot\boldsymbol{r}_1} V_{00}(r_1) j_l(k_0 r_1) P_l(\cos\theta_1) d^3\boldsymbol{r}_1 \qquad \dots (19)$$

and $$f_0^{(3)} = -\frac{1}{2\pi} \sum_{l=0}^{\infty} (\tfrac{1}{2} \sin 2\eta_l + i \sin^2 \eta_1) i^{l+2}$$

$$\times \int e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_1} V_{00}(r_1)(1-e^{-r_1})^{2l+1} n_l(k_0 r_1) P_l(\cos\theta_1) d^3\boldsymbol{r}_1 \qquad \dots (20)$$

Utilizing the identities (Magnus and Oberhettinger 1954, p. 77) :

$$\int_0^{2\pi} e^{ik_0 r_1 \sin\phi \sin\theta_1 \cos\phi_1} . d\phi_1 = 2\pi J_0(k_0\, r_1 \sin\phi \sin\theta_1) \qquad \dots (21)$$

$$\int_0^{\pi} e^{ik_0 r_1 \cos\phi \cos\theta_1} . J_0(k_0 r_1 \sin\phi \sin\theta_1) P_l(\cos\theta_1) \sin\theta_1\, d\theta_1$$

$$= \left(\frac{2\pi}{k_0 r_1}\right)^{\frac{1}{2}} i^l P_l(\cos\phi)\, J_{l+\frac{1}{2}}(k_0 r) \qquad \dots (22)$$

and the equation (13),
we obtain

$$f_0^{(2)} = -\frac{1}{k_0} \sum_{l=0}^{\infty} (2l+1)(\sin^2\eta_l - i\tfrac{1}{2} \sin 2\eta_l)\eta_l P_l(\cos\theta) \qquad \dots (23)$$

In order to obtain the expansion of $f_0^{(3)}$ we use the relations (21) and (22) and

(Magnus and Oberhettinger 1954, p. 37)

$$\int^{\infty} e^{-2at}\, J_{l+\frac{1}{2}}(k_0 r) J_{-l-\frac{1}{2}}(k_0 r) dr$$

$$= \frac{1}{\pi} \int_0^{\pi/2} \frac{\cos(2l+1)\phi}{(a^2+k_0^2\cos^2\phi)^{\frac{1}{2}}}\, d\phi \quad \ldots \quad (24)$$

EXCHANGE SCATTERING AMPLITUDES

Kang and Sucher (1966) have shown that in the exchange amplitude for electron-atom collision, the core potential term vanishes identically when the proton is heavy. Accordingly we have omitted this term from the B.O. formula (7).

On substitution of the approximate wave function $F_0(\boldsymbol{r})$ defined in (17) in the B.O. formula thus modified, we get

$$g_0(\theta, \phi) = g_0^{(1)} + g_0^{(2)} + g_0^{(3)} \quad \ldots \quad (25)$$

where $$g_0^{(1)} = -\frac{1}{2\pi}\int\int \frac{1}{r_{12}}\, e^{i(\boldsymbol{k}_0 \cdot \boldsymbol{r}_1 - \boldsymbol{k} \cdot \boldsymbol{r}_2}\, (\psi_0^*(\boldsymbol{r}_1)\psi_0(\boldsymbol{r}_2) d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2. \quad \ldots \quad (26)$$

$$g_0^{(2)} = -\frac{1}{2\pi}\sum_{l=0}^{\infty} i^{l+1}(2l+1)(\tfrac{1}{2}\sin 2\eta_l + i\sin^2\eta_l) \times$$

$$\times \int\int \frac{1}{r_{12}}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_2}\psi_0^*(\boldsymbol{r}_1) j_l(k_0 r_1)\, \psi_0(\boldsymbol{r}_2)\, P_l(\cos\theta_1) d^3\boldsymbol{r}_1\, d^3\boldsymbol{r}_2 \quad \ldots \quad (27)$$

and $$g_0^{(3)} = -\frac{1}{2\pi}\, \Sigma i^{l+2}(2l+1)(\tfrac{1}{2}\sin 2\eta_l + i\sin^2\eta_l)$$

$$\times \int\int \frac{1}{r_{12}}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_2}\psi_0^*(\boldsymbol{r}_1)(1-e^{-r_1})^{2l+1} n_l(k_0 r_1)\, \psi_0(\boldsymbol{r}_2)\, P_l(\cos\theta_1) d^3\boldsymbol{r}_1$$

$$\times d^3\boldsymbol{r}_2 \quad \ldots \quad (28)$$

$g_0^{(1)}$ is the contribution to $g_0(\theta, \phi)$ from the unperturbed incident wave function $e^{i\boldsymbol{k}_0\cdot\boldsymbol{r}}$ and is given in the following closed analytical form (Corinaldesi and Trainor 1952, Kang 1966) :

$$g_0^{(1)} = -\frac{8(4k_0^2+q^2)}{q^3(1+k_0^2)^3}\sin^{-1}\frac{q}{(q^2+4)^{\frac{1}{2}}} - \frac{16}{(1+k_0^2)^2(q^2+4)}$$

$$+\frac{16k_0^2}{(1+k_0^2)^3 q^2} - \frac{32}{(1+k_0^2)(q^2+4)^2} \quad \ldots \quad (29)$$

where $$q = 2k_0 \sin\theta/2.$$

Using the expansion

$$\frac{1}{r_{12}} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \frac{(n-|m|)!}{(n+|m|)!}\, \delta_n(r_1, r_2)\, P_n^{|m|}(\cos\theta_1)\, P_n^{|m|}(\cos\theta_2)\cos m(\phi_1-\phi_2)$$

where $\delta_n(r_1, r_2) = r_1^n/r_2^{n+1}$ or r_2^n/r_1^{n+1} according as $r_1 < r_2$ or $r_1 > r_2$,

and integrating over the angular coordinates with the help of the relations (21) and (22) we easily show that

$$g_0^{(2)} = 8 \sum_{l=0}^{\infty} (\sin^2\eta_l - i\, \tfrac{1}{2} \sin 2\eta_l)\, P_l(\cos\theta) \int_0^{\infty} r_1^2 e^{-r_1} j_l(k_0 r_1) \times \left[\int_0^{\infty} \delta_l(r_1, r_2) r_2^2 e^{-r_2} j_l(k_0 r_2) dr_2 \right] dr_1 \quad \ldots (30)$$

and $$g_0^{(3)} = 8 \sum_{l=0}^{\infty} (\tfrac{1}{2} \sin 2\eta_l + i \sin^2 \eta_l) P_l(\cos\theta). \int_0^{\infty} r_1^2 e^{-r_1} (1 - e^{-r_1}) \times n_l(k_0 r_1) \left[\int_0^{\infty} \delta_l(r_1, r_2) r_2^2 e^{-r_2} j_l(k_0 r_2) dr_2 \right] dr_1 \quad (31)$$

To obtain analytical expressions for $g_0^{(2)}$ and $g_0^{(3)}$ we substitute the values of j_l and n_l and integrate (30) and (31) over r_2 and r_1.

RESULTS AND DISCUSSION

The calculations of the integrals involving j_l and n_l in $f_0^{(2)}$, $g_0^{(2)}$ and $g_0^{(3)}$are straightforward but become tedious as the value of l increases. Fortunately the contribution to the direct and exchange scattering amplitudes $f_0(\theta, \phi)$ and $g_0(\theta, \phi)$ from these integrals for $l \geqslant 2$ are negligibly small when $k_0 \geqslant 2$. So in our work we have considered the $s-$, $p-$ and $d-$wave distortions of the incident wave. When the core interaction term is omitted from the B.O. formula, the total cross section becomes very large compared to those obtained by Wu (1960) with the usual B.O. formula. However when we use the distorted wave function $F_0(r)$ in the modified B.O. formula, the values of the scattering cross sections drop considerably. As there are no experimental data on the elastic scattering of electrons by H atoms at high energies in the table below we compare our results with some

TABLE

Total cross-sections of *e-H* elastic collisions

(in units of)

Incident energy wave numbers k_0 (in a_0^{-1})	B.O. approximation (Wu (1960)]	Close coupling approx. [Burke *et al.* (1963)]	First Order approx. [Bell and Moiseiwitsch (1963)]	Present Without distortion	Calculation with distortion
1	2.105	4.748	2.710	14.78	12.46
2	.680	.795	.797	.99	.81
3	.290	—	.300	.40	.35
4	.157	—	.158	.29	.27

recent theoretical findings of others. At $k_0 = 2$ there is some agreement between our result with the distortion of the plane incident wave taken into account and that of Burke *et al.* (1963) or of Bell and Moiseiwitsch (1963). The cross sections at other energies deviate substantially from those of Wu (1960) or Bell and Moiseiwitsch (1963), mainly due to our neglect of core interaction term. The very large cross section at $k_0 = 1$ may be due to the failure of our approximation method at this energy. Moreover at such a low energy the polarization potential due to the distortion of the atom plays an important role. With Ochkur's modification which retains only the leading term in the expansion of the formula for the exchange scattering amplitude in powers of k_0^{-2} and virtually neglects the effect of the core potential terms in the formula, Jha *et al.* (1967) have obtained total cross section for e-H elastic collision at $k_0 = 1$ in close agreement with that of Burke *et al.* (1963). This suggests further examination of the derivation of the B.O. formula.

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