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# Two-potential formulation in HHOB

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**Abstract:** The two-potential HHOB approximation is formulated parallel to the two-potential eikonal approximation. The theory developed for any target atom is applied to the special case of elastic $e^-$ – H atom scattering to calculate the differential scattering cross sections at the sample energy 200 eV. The results agree well with the recent measured and theoretical values. A significant improvement over the basic HHOB approximation is obtained.

## 1. Introduction

The High energy Higher Order Born (HHOB) approximation proposed by Yates (1979) is recently applied to various scattering problems (Rao and Desai 1981-83). It, being a computationally simple approximation, gives reasonably good results for the scattering parameters in the electron-Atom scattering processes. But as the scattering angle increases, the differential cross sections (DCS) deviate more and more from the corresponding experimental values. It is well-known that the Born approximation gives better results for weaker potentials. Keeping this in mind, we have made the present two-potential formulation, where the interaction potential $V$ treated in the Born approximation will be replaced by $V-V_1$, $V_1$ being an arbitrary potential. The formulation is done in the same line as the two-potential eikonal approximation (Ishihara and Chen 1975). The basic formula is derived for potential scattering and is generalized to the case of a target. In order to see the usefulness of this method, it is applied to elastic $e^-$ – H scattering at 200 eV. The improvement over simple HHOB approximation (Yates 1979) is quite appreciable.

## 2. Theory

Consider the scattering by a central field $V(r)$ an arbitrary potential $V_1$ is so chosen that $V_0 = V - V_1$ satisfies the semiclassical conditions.

Now

$$V(r) = V_0(r) + V_1(r).$$

We write the scattering amplitude in the two-potential form (Rodberg and Thaler 1967).

$$F(\theta)=\frac{1}{K_i}\sum_l(2l+1)T_lP_l(\cos\theta) \tag{1}$$

with

$$T_l=e^{i\delta_l(0)}\sin\delta_l^{(0)}+e^{2i\delta_l(0)}e^{i\delta_l(1)}\sin\delta_l^{(1)}$$

and

$$\delta_l^{(0)}=\delta_l-\delta_l^{(1)}$$

where $\delta_l$ and $\delta_l^{(1)}$ are the $l$th phase shifts for the potentials $V$ and $V_1$, $\theta$ is the scattering angle and $K_i$ is the incident momentum.

Hence

$$F(\theta)=\frac{1}{K_i}\sum_l(2l+1)e^{i\delta_l(0)}\sin\delta_l^{(0)}P_l(\cos\theta)$$

$$+\frac{1}{K_i}\sum_l(2l+1)e^{2i\delta_l(0)}e^{i\delta_l(1)}\sin\delta_l^{(1)}P_l(\cos\theta) \tag{2}$$

We now evaluate $\delta_l^{(0)}$ by Born approximation. The radial part of the Schroedinger equation for $V_0(r)$ is

$$\frac{d^2u_l^{(0)}}{dr^2}+\left\{K_i^2-\frac{l(l+1)}{r^2}-U_0(r)\right\}U_l^{(0)}=0$$

where

$$U_0(r)=\frac{2m}{\hbar^2}V_0(r) \tag{3}$$

The solution of this equation is

$$U_l^{(0)}(r)=F_l(K_ir)+\int_0^\infty dr'g_l(r,r')U_0(r')U_l^0(r') \tag{4}$$

where $g_l(r,r')$ is the Green's function.

Now the exact phase shift is given by

$$\tan\delta_l^{(0)}=-\frac{1}{K_i}\int_0^\infty dr\,F_l(K_ir)U_0(r)U_l^{(0)}(r) \tag{5}$$

In second Born approximation

$$U_l^{(0)}=F_l(K_ir)+\int_0^\infty dr'\,g_l(r,r')U_0(r')F_l(K_ir') \tag{6}$$

Thus phase shift becomes

$$\tan\delta_l^{(0)}=-\frac{1}{K_i}\int_0^\infty dr\,F_l(K_ir)U_0(r)\Big\{F_l(K_ir)$$

$$+\int_0^\infty dr'\,g_l(r,r')U_0(r')F_l(K_ir')\Big\} \tag{7}$$

The first part of (2) is the amplitude factor for the potential $U_0$. When $\delta_l^{(0)}$ is small, we have

$$F_l^{(0)}=\frac{1}{K_i}\sum_l (2l+1)\,\delta_l^{(0)}\,P_l(\cos\theta) \tag{8}$$

Substituting for $\delta_l^{(0)}$ from (7),

$$F^{(0)}=\frac{1}{K_i}\sum_l (2l+1)\,P_l(\cos\theta)\left\{-\frac{1}{K_i}\int_0^\infty dr\,|\,F_l(K_i r)\,|^2\,U_0(r)\right\}$$

$$+\frac{1}{K_i}\sum_l (2l+1)\,P_l(\cos\theta)\left\{-\frac{1}{K_i}\int_0^\infty dr\,F_l(K_i r)\right.$$

$$\left. U_0(r)\int_0^\infty dr'g_l(r,r')U_0(r')F_l(K_i r')\right\}. \tag{9}$$

i.e. $\quad F_l^{(0)}=F_{l1}^{(0)}+F_{l2}^{(0)}$

The first part of (9) can be simplified as

$F_{l1}^{(0)}=-\frac{1}{4\pi}\int e^{i\,q\cdot r}U_0(r)dv$, which is the first Born amplitude. A similar procedure will give $F_{l2}^{(0)}$=second Born amplitude, a slight modification on which will give the corresponding expression in HHOB.

Thus

$$F(\theta)=F_l^{(0)}+\frac{1}{K_i}\sum_l (2l+1)P_l(\cos\theta)$$

$$e^{2i\delta_l^{(0)}}e^{i\delta_l^{(1)}}\sin\delta_l^{(1)}$$

Generalising this to the case of target,

$$F_{fi}(\theta)=\langle f\,|\,F_l^{(0)}\,|\,i\rangle+\frac{1}{K_i}\sum_l (2l+1)$$

$$P_l(\cos\theta)e^{i\delta_l^{(1)}}\sin\delta_l^{(1)}\,\langle f\,|\,e^{2i\delta_l^{(0)}}\,|\,i\rangle$$

i.e. $\quad F_{fi}(\theta)=f_{HHOB}+f_{PW} \quad (10)$

where

$$f_{HHOB}=f_{i\to f}^{(1)}+f_{i\to f}^{(2)}+\ldots$$

as given by Yates (1979) for the potential $V_0(r,r_1)$.

### 3. $e^{-}$–H elastic scattering

The interaction potential is given by

$$V(r,r_1)=-\frac{1}{r}+\frac{1}{|\,\boldsymbol{r}-\boldsymbol{r}_1\,|}$$

and

$$V_0(r,r_1)=V(r,r_1)-V_1(r) \tag{11}$$

We choose for the arbitrary potential $V_1(r)$, the static potential given by Bonham and Strand (1963) because of the simplicity in calculations and the ease with which it may be extended to other atoms. The summation of partial waves is done similar to Jhanwar *et al* (1978). Now the scattering amplitude given by (10) is easily evaluated from which DCS is calculated.

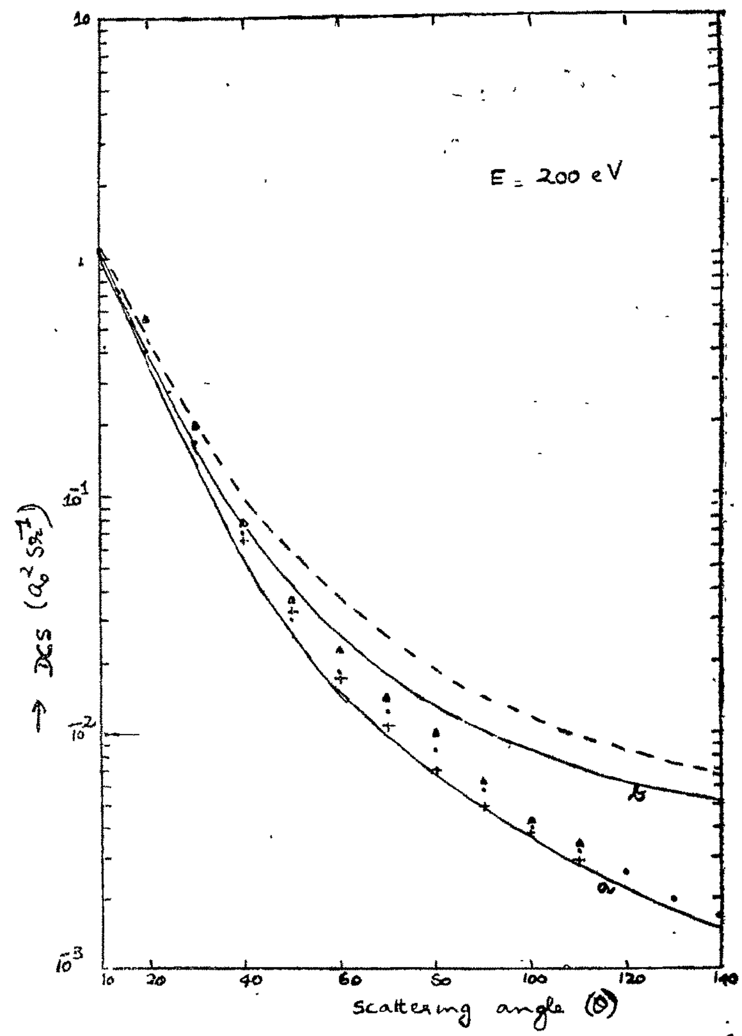


**Figure 1.** DCS for $e^-$—H atom elastic scattering at 200 eV.
Solid Curve a——present calculations, Solid Curve b——HHOB without third Born term, broken Curve——HHOB with third GES term ( Yates 1974 )
● ——experimental data (Williams 1975)
▲——experimental data (van Winger den *et al* 1977)
+ ——EBS results (Byron and Joachain 1977)

## 4. Results and discussion

The DCS for $e^{-}-\mathrm{H}$ elastic scattering at the sample energy 200 eV is shown in Figure 1. It is compared with other theoretical and experimental data. The agreement is nice, and as expected, the improvement over the basic HHOB approximation is quite appreciable. As in the case of simple HHOB approximation, better results may be expected at higher incident energies. It should be specially mentioned that the two-potential formulation gives better results than simple HHOB approximation even at large angles.

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# $e^-$–H(2S) elastic scattering in the two-potential eikonal approximation

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**Abstract.** The differential scattering cross-sections for $e^- - \mathrm{H}\,(2S)$ elastic scattering are calculated at intermediate energies by using the two-potential eikonal approximation. The results are compared with the recent theoretical data and the conventional Glauber cross-sections.

**Keywords.** Elastic scattering; electrons; hydrogen (2S state).

## 1. Introduction

The study of electron scattering from the excited states of atoms has important applications in various branches of physics, besides the intrinsic theoretical interest associated with it. Very little work has been reported on the electron scattering from the excited states of atoms as compared to the large amount of calculations involving the ground states. Motivated by the recent successful application of the two-potential eikonal approximation (Ishihara and Chen 1975) in various scattering phenomena (Tayal *et al* 1980), we have made a generalized application of the above approximation to study the electron scattering from any of the excited states of hydrogen atom. As a special case, we study the scattering from H(2S)—a fundamental process for which it is reasonable to expect that experimental data will become available in the near future.

The Glauber approximation is known to be in appreciable error at all angles when applied to the elastic electron-atom scattering at medium and lower energies. Ishihara and Chen (1975) have shown that this is mainly due to the inadequate semiclassical treatment of close-encounter collisions. The two-potential eikonal approximation provides an effective method to treat such collisions properly.

## 2. Theory

The basic idea underlying this approximation is to pull out an arbitrary potential $V_1$ from the interaction potential $V$ such that the rest of the interaction potential *i.e.* $V_0 = V - V_1$ satisfies the semiclassical conditions. $V_0$ is treated in the Glauber approximation and the contribution of $V_1$ is calculated quantum-mechanically by taking a few partial waves. For the scattering of an electron from a $Z$-electron atom, the interaction potential is given by

$$V(\bar{r}, \bar{r}_1, \ldots, \bar{r}_Z) = \frac{-Z}{r} + \sum_{j=1}^{Z} \frac{1}{|\mathbf{r} - \mathbf{r}_j|}, \tag{1}$$

where $\bar{r}, \bar{r}_1, \ldots, \bar{r}_Z$ are the incident and target electron co-ordinates. A short range central potential $V_{st}$, which is the static potential of the target atom, is chosen for $V_1$.

Now $$V_0(\bar{r}, \bar{r}_1, \ldots, \bar{r}_Z) = V(\bar{r}, \bar{r}_1, \ldots, \bar{r}_Z) - V_{st}(r). \tag{2}$$

In the two-potential eikonal approximation, the transition amplitude from the initial state $|i\rangle$ of the target to the final state $|f\rangle$ is given by (Ishihara and Chen 1975).

$$F_{fi}(\theta) = \frac{K_i}{2\pi i} \int d^2 b \exp(iq \cdot b) [\Gamma_{fi}(\bar{b}) - 1]$$

$$+ \frac{1}{K_i} \sum_l (2l+1) P_l(\cos\theta) \exp(i\delta_l^{(1)}) \sin \delta_l^{(1)} \int \frac{d\phi}{2\pi} \Gamma_{fi}(\bar{b}_l). \tag{3}$$

The notations are same as in Ishihara and Chen (1975).

Here, $$\Gamma_{fi}(b) = \langle f | \exp(i\chi) | i \rangle \tag{4}$$

where $\chi = \chi_0 + \Delta\chi$,

with $$\chi_0 = -\frac{1}{K_i} \int_{-\infty}^{\infty} dZ\, V_0. \tag{5}$$

The correction $\Delta X$ to the Glauber phase function contributes very little for energies greater than 100 eV and hence can be neglected.

To make use of (3) to study the electron-scattering from any of the excited states $(nlm)$ of hydrogen, it is necessary to have the $V_{st}$ and $\chi_0$ corresponding to those states. The general form of $V_{st}$ for elastic scattering is given by

$$V_{st}^{nlm} = \int d\,v_1\, \psi_{nlm}^* \psi_{nlm} (-1/r + 1/|\mathbf{r} - \mathbf{r}_1|), \tag{6}$$

where the standard form of the wavefunction is given by

$$\psi_{nlm} = 2/n^2 \{(n-l-1)!/[(n+l)!]^3\}^{1/2} (2r_1/n)^l \exp(-r_1/n)$$

$$L_{n-l-1}^{2l+1}(2r_1/n)\, Y_{lm}(\theta, \phi). \tag{7}$$

Using (6) and (7)

$$V_{st}^{nlm} = -\frac{1}{r} + \sum_{p=0}^{\infty} \sum_{m=0}^{n-l-1} \sum_{j=0}^{n-l-1} (-1)^{m+j} (4\pi/(2p+1))^{1/2}$$

$$\binom{n+l}{n-l-1-m} \binom{n+l}{n-l-1-j} \frac{(2/n)^{m+j+2l}}{m!\, j!} \times 4/n^4$$

$$(n-l-1)! / [(n+l)!] \times [(2l+1)^2 (2p+1)/4\pi]^{1/2}$$

$$\begin{pmatrix} l & p & l \\ o & o & o \end{pmatrix} \begin{pmatrix} l & p & l \\ m & o & m \end{pmatrix} \left\{ \frac{1}{r^{p+1}} \left[ S_1! / (2/n)^{s_1+1} \right.\right.$$

$$\left. - \exp(-2r/n) \sum_{k=0}^{S_1} \frac{s_1!}{k!} \frac{r^k}{(2/n)^{s_1-k+1}} \right] + r^p \exp(-2r/n)$$

$$\left. \sum_{k=0}^{S_2} \frac{S_2!}{k!} \frac{r^k}{(2/n)^{s_2-k+1}} \right\}, \tag{8}$$

where $S_1 = p + 2 + m + j + 2l$ and

$S_2 = 1 + m + j + 2l - p$

$\begin{pmatrix} l & p & l \\ o & o & o \end{pmatrix}$ are the usual Wigner notations.

The general form of $\chi_0^{nlm}$

is $$\chi_0^{nlm} = \frac{-1}{k_i} \int_{-\infty}^{\infty} V \, dz + \frac{1}{k_i} \int_{-\infty}^{\infty} V_{st}^{nlm} \, dz. \tag{9}$$

For all states of $H$, the interaction potential

$V(b, z, b_1, z_1) = -(1/r) + (1/|\mathbf{r} - \mathbf{r}_1|)$, so that

$$-\frac{1}{k_i} \int_{-\infty}^{\infty} V \, dz = \frac{2}{k_i} \ln \frac{|b - b_1|}{b}. \tag{10}$$

Now $\int_{-\infty}^{\infty} V_{st}^{nlm}\, dz$ may be calculated from (8) using standard integration techniques. Since this is a very lengthy expression, we take up the $(ns)$ states.

$$\int_{-\infty}^{\infty} V_{st}^{ns}\, dz = \frac{8}{n^4}\,\frac{(n-1)!}{(n!)}\sum_{m=0}^{n-1}\sum_{j=0}^{n-1}(-1)^{m+j}$$

$$\binom{n}{n-1-m}\binom{n}{n-1-j}(2/n)^{m+j}\,\frac{1}{m!\,j!}\left\{\sum_{k=0}^{S_3}\right.$$

$$\frac{S_3!}{k!\,(2/n)^{S_3-k+1}}(-1)^{k+1}\left(\frac{\partial^{k+1}}{\partial\lambda^{k+1}}\right)K_0(b\lambda)$$

$$\left.-\sum_{k=0}^{S_3+1}\frac{(S_3+1)!}{k!\,(2/n)^{S_3+2-k}}(-1)^k\frac{\partial^k}{\partial\lambda^k}K_0(b\lambda)\right\}, \tag{11}$$

where $S_3 = m + j + 1$ and $\lambda = 2/n$. Using (10) and (11) we can find the general expression for $\chi_0^{ns}$ for any $(ns)$ state.

As a special case, we find $\Psi$, $V_{st}$ and $\chi_0$ for $H\,(2S)$ from (7), (8) and (10)

$$\Psi_{2s} = \frac{1}{4\sqrt{2\pi}}(2 - r_1)\exp(-r_1/2) \tag{12}$$

$$V_{st} = -\left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{8}\right)e^{-r} \tag{13}$$

and $$\chi_0 = +\frac{2}{k_i}\ln|\mathbf{b} - \mathbf{b}_1/b| - \frac{2}{k_i}\left[1 - \frac{3}{4}\frac{\partial}{\partial\lambda} + \frac{1}{4}\frac{\partial^2}{\partial\lambda^2} - \frac{1}{8}\frac{\partial^3}{\partial\lambda^3}\right]K_0(\lambda b), \tag{14}$$

where $\lambda = 1$.

$\Gamma(b)$ given by (4) may be easily evaluated now.

The summation of partial waves is done similar to the procedure adopted by Jhanwar *et al* (1978). The exact and Born phase shifts are calculated for the potential $V_{st}$ and the $l$ value is so chosen that beyond this $l$ value, the phase shifts differ by less than 3%. The rest of the partial wave contribution is taken as described by Jhanwar *et al* (1978). Now the scattering amplitude and hence the DCS may be evaluated using (3).

**3. Results and discussion**

The e$^-$–H (2S) elastic differential cross-sections are calculated at 200 eV and 400 eV when data are available for comparison (figures 1 and 2). The results are compared with eikonal-Born series (EBS), optical model (OM) and the Glauber (G) results along with the most recently reported two-potential results (Pundir *et al* 1982) and high energy higher order Born (HHOB) results (Rao and Desai 1983). In the absence of any experimental data at present, it is rather difficult to comment on the accuracy of the various approaches. In the study of electron-scattering from H, He and Li, two-potential eikonal approximation is in good agreement with the experimental data and the other sophisticated theories. The HHOB results are always overestimating, especially in the large angle region (Rao and Desai 1981, 1983). Glauber approximation is well-known for its shortcomings—appreciable under estimation of the cross-section except at small angles where it logarithmically diverges. The present results lie between the above two results and nearer the EBS results and are in good agreement with experiments in other scattering processes.

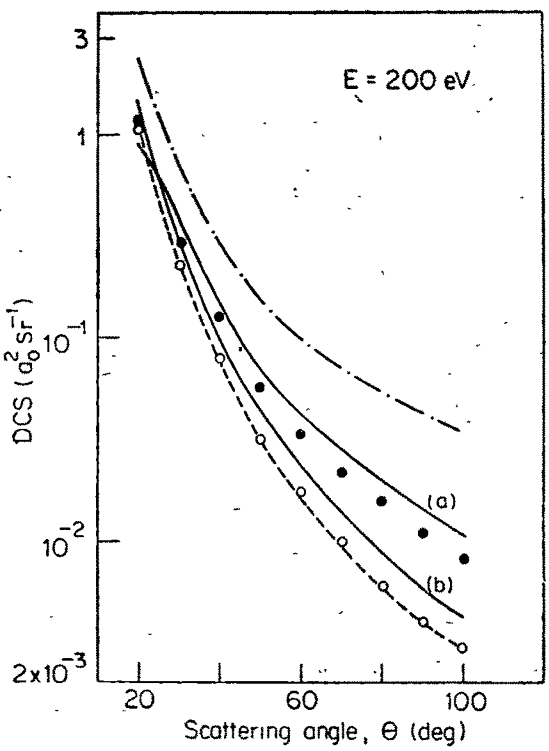


**Figure 1.** Differential scattering cross-sections for the elastic scattering of electrons from H(2S) at 200 eV.
Solid curve a.—present calculations, broken curve—present calculation in the Glauber approximation. Solid curve b—data of Pundir *et al* (1982). dash—dot curve HHOB results (Rao and Desai 1983). + — EBS results (Joachain *et al* 1977). . — OM results (Joachain and Winters 1980).

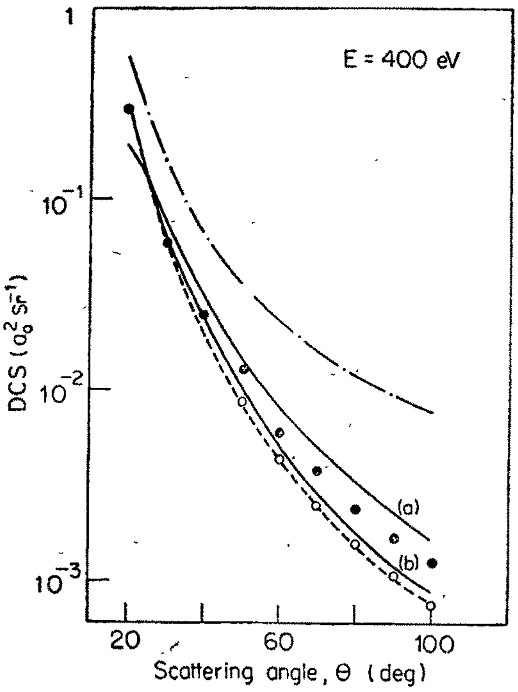


**Figure 2.** Differential scattering cross-sections for the elastic scattering of electrons from H(2S) at 400 eV. References are same as in figure 1.

As in $\bar{e}$–H(1S) elastic scattering (Ishihara and Chen 1975), here also the two-potential eikonal approximation should improve the conventional Glauber results because of two reasons: (*i*) The singularity in interaction $V_{st}$ is properly taken care of by partial wave analysis (ii) The semi-classical condition necessary for the Glauber approximation is better for the interaction $V_0$ than for $V$. This aspect is clearly brought out by the comparison of the eikonal phase function $\Gamma(b)$ for the potentials $V$ and $V_0$ (figure 3). $\Gamma(b)$ for $V_0$ is a smooth function of $b$ while that for $V$ oscillates for small $b$ values. The first term of (14) is the usual Glauber phase for the scattering process considered here. The singularity of this term at $b = 0$ is cancelled by the second term. Hence, in contrast to Glauber approximation, $\Gamma(b)$ varies smoothly in the two-potential formulation. Similar behaviour is observed in electron scattering from H(1S), He and Li (Ishihara and Chen 1975; Tayal *et al* 1980). It may be noted that as in $\bar{e}$–H(1S) scattering, here also Re $[\Gamma(b)] \gg$ Im $[\Gamma(b)]$ everywhere. Hence $\Gamma(b)$ contains almost no scattering, but mostly absorption.

The $\bar{e}$–H(2S) scattering cross-section at 100 eV (not shown here) is compared with corresponding $\bar{e}$–H(1S) cross-section and are found to approach each other for larger angles where the interaction between the incident electron and the target nucleus progressively dominates the scattering. Similar type of behaviour was observed in the EBS (Joachain *et al* 1977) and two-potential (Pundir *et al* 1982) calculations. The present approximation is good for lower energies also whereas others like HHOB are good for $E > 200$ eV only. In view of the simplicity of the

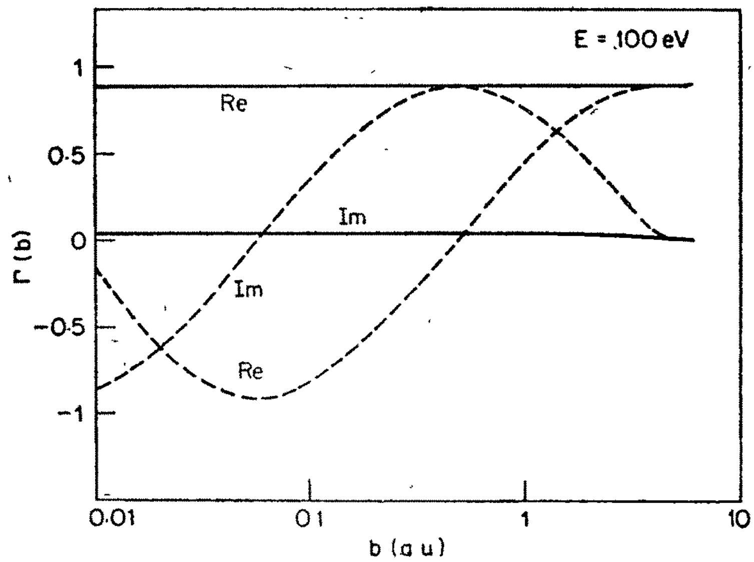


**Figure 3.** Real and imaginary parts of $\Gamma(b)$ for the potential $V_0$ (solid curve) and for the total interaction $V$ (dashed curve) for elastic $\bar{e}$–H(2S) scattering at 100 eV.

present approach, we expect that it would provide reasonable description of the scattering process from the excited metastable states of hydrogen atom.

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# e$^-$-He Elastic Scattering in the Two-Potential HHOB Approximation

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The two-potential formulation in the high energy higher order Born approximation (HHOB) is applied to the case of elastic scattering of electrons by helium atom, at intermediate energies. The calculated scattering parameters are found to be in good agreement with other theoretical and experimental data.

The two-potential formulation in HHOB[1] is developed along the same lines as the two-potential eikonal approximation[2]. The basic idea in this formulation is to pull out from the interaction potential $V$ an arbitrary potential $V_1$ such that the rest of the interaction $V_0 = V - V_1$ satisfies semiclassical conditions. For the scattering of an electron from the helium atom, the interaction potential is given by

$$V(r_0, r_1, r_2) = \frac{-2}{r_0} + \sum_{j=1}^{2} \frac{1}{|r_0 - r_j|}$$

where $r_0$, $r_1$, and $r_2$ are the position vectors of the incident and target electrons. For $V_1$, we have chosen the static potential $V_{st}$ given by Bonham and Strand[3]. Hence $V_0 = V - V_{st}$ is slowly varying and $|V_0| \ll E$ for all $r_0$.

Now the contribution of $V_0$ to the scattering amplitude can be obtained in the HHOB approximation and that of $V_{st}$ by partial wave analysis (PWA). The transition amplitude from the target state $|i>$ to be state $|f>$ is given as

$$F_{fi}(\theta) = F_{HHOB} + F_{PW}$$

where $F_{HHOB} = f^{(1)}_{i \to f} + f^{(2)}_{i \to f} + \ldots$

as given by Yates for the potential $V_0 = V - V_{st}$ and $F_{PW}$ is the scattering amplitude in the PWA.

For the ground state of helium, we have used the Hartree-Fock orbitals $\varphi_{1s}$ of Byron and Joachain[4]. The first and second Born amplitudes in HHOB are obtained in the closed form[1,5]. Similarly $F_{HHOB}$ is calculated for the potential $V_0$. The procedure for the summation of the partial waves is similar to that given by Jhanwar *et al.*[6] Knowing the scattering amplitudes, the differential cross-section (DCS) can be obtained through $O(1/k_i^2)$.

The total cross-section is calculated using the formula

$$\sigma^{\text{total}} = \frac{4\pi}{k_i} \operatorname{Im} F(\theta = 0)$$

The DCS curve obtained in the present analysis at 200 eV is shown in Fig. 1. As expected, the present results agree well with other available data: both experimental[7-9] and theoretical[5,10,11]. It may be noted that the two-potential formulation in HHOB approximation yields better results than the simple HHOB approximation, especially at large angles. The total cross-section (TCS) results shown in Table 1 are also encouraging.

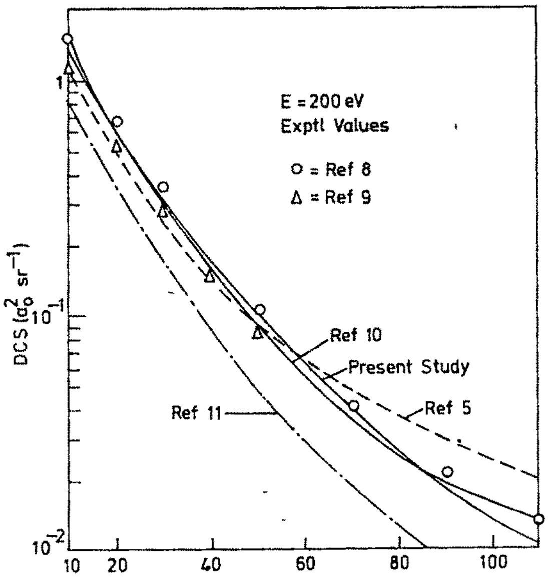


Fig. 1—DCS for electron-helium elastic scattering at 200 eV

Table 1—Comparison of the Total Cross-sections (in units of $a_0^2$) for e$^-$-He Scattering from Different Sources

| Energy eV | Present study | Ref. 5 (HHOB) | Ref 10: Winters *et al.* | Ref 10: Byron & Joachain | EBS |
|---|---|---|---|---|---|
| 200 | 3.58 | 2.93 | 3.55 | 3.37 | 2.92 |
| 400 | 2.08 | 1.69 | 2.00 | 1.86 | 1 71 |

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