EIKONAL APPROXIMATION IN ELASTIC ATOMIC SCATTERING

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The eikonal approximation has been applied to investigate the $e\pm$—H and $e\pm$—He elastic scattering problems with the inclusion of the polarization effect. We have calculated the total and the differential cross section for all the systems and compared them with the available experimental results and other theoretical findings. The results in the first Born approximation including the polarization potential are also given. Our eikonal results as well as the polarized FBA results for the differential cross sections for electron scattering are in very satisfactory agreement with the experimental findings. The eikonal as well as the polarized FBA results which are very close to each other differ appreciably from the FBA results even at the energy as high as 1 keV. In the case of e^+—He scattering, our values for the total cross sections below the positronium threshold are in reasonably good agreement with the experimental findings and with those obtained by the refined calculations of Callaway *et al.* (1968) and Drachman (1966). The results for e^+–H scattering are similar in feature to those for e^+–He scattering.

INTRODUCTION

The application of the eikonal approximation and its various modifications, to atomic collision processes have drawn considerable attention in recent years (Glauber 1959; Mittleman 1970; Joachain and Vanderprooten 1971; Byron 1971; Joachain and Mittleman 1971; Chen *et al.* 1972). The eikonal approximation is suitable for intermediate and high incident energies and holds good for small angle scatterings (Mittleman 1970). The main advantage of this method is that it satisfies unitarity relation. Glauber's model (1959) for multiple scattering based on the eikonal approximation yields reliable results in the intermediate and high energy region for electron (proton) hydrogen scattering (Ghosh and Sil 1970, 1971; Ghosh and Bhadra 1971; and Tai *et al.* 1969, 1970). However, one has to encounter enormous complications when Glauber approximation is applied to complex atoms (Franco 1970). More- over, this mode predicts the same total and differential cross-sections for both $e\pm$—H scattering.

Here we are interested to apply the eikonal approximation which explicitly includes the polarization potential in addition to the static one, to investigate the elastic scattering of electrons and positrons by atoms. It is well known that the effect of polarization plays a vital role in the scattering theory at low and intermediate energies. Our approach is rather simple to apply to any complex atom and yields different results for electron and positron scattering. In this paper we have devoted ourselves to the investigations of the elastic scattering of electrons and positrons by hydrogen and helium atoms.

THEORY

The target proton is considered to be infinitely heavy and the position of the proton is taken as the origin of the co-ordinate system. Let $\vec{b}$ be the impact parameter vector relative to the origin. In the eikonal approximation the scattering amplitude is written as

$$F(\theta) = \frac{k}{i}\int_0^\infty J_0(qb)\left[exp\left(-i\chi(b)\right) -1\right] bdb, \qquad (1)$$

where $\vec{q} = \vec{k}-\vec{k}_1$; $\vec{k}$ and $\vec{k}_1$ being, respectively, the momenta of the incident and the scattered particle which is an electron or a positron as the case may be and J_0 is the zeroth order Bessel function.

The phase shift function $\chi(\vec{b})$ corresponding to the impact parameter may be written as

$$\chi(\vec{b}) = \frac{1}{\hbar v}\int_0^\infty V_{opt}(\vec{r})\, dz , \qquad (2)$$

where v is the velocity and $\vec{r}$ denotes the position vector of the incident particle and is given by $\vec{r} = \vec{b} + \hat{k}z$; $\hat{k}$, being the unit vector in the incident direction, and the optical potential $V_{opt}(\vec{r})$ (Goldberger and Watson 1964) can be written as

$$V_{opt}(\vec{r}) = V_{c1}(r) + V_{c2}(r) \qquad (3)$$

The first-order part of the optical potential takes the form

$$V_{c1}(r) = \langle o \mid V \mid o \rangle$$

which is simply the static potential of the atom $V_s(r)$. The second-order potential V_{c2} may be expressed as

$$V_{c2}(r) = \sum_{n\neq o} \frac{\langle o \mid V \mid n\rangle\langle n \mid V \mid o\rangle}{p^2 - T - (\omega_n - \omega_0) + i\epsilon}, \qquad (4)$$

where the summation runs over all the intermediate states of the target. Here ω_0 and ω_n represent the internal target energies, respectively, in the initial and the intermediate state $|n\rangle$ while $\epsilon \to 0^+$ as usual. 'p^2' is the energy of the incident electron and 'T' represents the kinetic-energy operator.

In the framework of adiabatic approximation the second-order optical potential (Goldberger and Watson 1964) asymptotically may be represented as

$$V_{c2}(r) \xrightarrow[r\to\infty]{} -\frac{\alpha}{2r^4}, \qquad (5)$$

where α is the polarizibility of the target atom.

For V_{c2} we have taken a polarization potential V_p which satisfies the correct asymptotic condition (*i.e.*, equation 5) and is free from singularity at the origin. We have taken the following polarization potentials due to Obedkov (1963) for H and He.

$$V_p(r) = -9\left[1-\left(1+2r+2r^2+\frac{4}{3}r^3+\frac{2}{3}r^4+\frac{4}{27}r^5\right)e^{-2r}\right]/4r^4$$

$$V_p(r) = -\left[9+\frac{4}{3}e^{-2\rho}\left(\rho^5+\frac{9}{2}\rho^4+9\rho^3+\frac{27}{2}\rho+\frac{27}{4}\right)\right]/2\rho^4,$$

with $\rho = \xi r$ where $\xi = 27/16$.

Considering the helium ground state wave function (Mott and Massey 1965)

$$\Psi(r_1,r_2) = \frac{N^2}{\pi}\left[exp(-z_1r_1) + Cexp(-2z_1r_1)\right]\times\left[exp\,(-z_1r_2)+Cexp(-2z_1r_2)\right], \quad ..(6)$$

when N=1.484, Z_1=1.456 and C=0.6, the static potential $V_s(r)$ for helium atom was calculated.

Substituting $V_s(r)$ and $V_p(r)$ in equation (2) we obtain

$$\chi(\vec{b}) = (I_s + I_p)/v$$

$$\text{with} \quad I_s = \int_{-\infty}^{\infty} V_s(\vec{b}+\hat{k}z)dz\,, \qquad .. \quad .. \quad (7)$$

$$\text{and} \quad I_p = \int_{-\infty}^{\infty} V_p\,(\vec{b}+\hat{k}z)dz. \qquad .. \quad .. \quad (8)$$

The integration in expression (8) for I_p has been carried out numerically for both the systems. The expressions for I_s for Hydrogen and Helium atoms are obtained in close analytical forms which may be written as

$$I_s^H = -2[K_0(2b) + bK_1(2b)], \qquad .. \quad .. \quad (9)$$

$$\text{and } I_s^{He} = -5{\cdot}6\frac{N^4}{z_1^6}\Big[\Big\{K(2z_1b) + {\cdot}36\,K(1{\cdot}5z_1b) + {\cdot}045K(4z_1b)\Big\}$$
$$+z_1b\Big\{K_1(2z_1b)+ {\cdot}54(z_1b)K_1(1{\cdot}5z_1b)+{\cdot}04(z_1b)K_1\,(4z_1b)\Big\}\Big], \quad ..(10)$$

where K_0 and K_1 are the Bessel functions of the third kind. Now we are in a position to evaluate the scattering amplitude $F(\theta)$ by numerical integration over the impact parameter $\vec{b}$. For comparison we have also calculated the elastic scattering amplitudes $F(\theta)$ in the Born approximation by including the polarization potential (Polarized *FBA*). The final expression for the scattering amplitude for the e^-—H scattering is

$$F_B^H(\theta) = I_{BS}^H + I_{BP}^H$$

where $I_{BS}^H = 2(8+q^2)/\beta^2$,

and $I^{H}_{BP} = 4.5 \left[1+\frac{q}{2}\tan^{-1}\left(\frac{q}{2}\right)-\frac{\pi q}{4}\right]-6\left[\frac{2}{9}\frac{\lambda}{\beta^3}+\frac{2}{\beta^2}+\frac{1}{\beta}\right]$,

when $\beta = 4+q^2$ and $\lambda = 12-q^2$.

Here the subscripts S and P refer to the static and the polarization respectively. Similarly e^- —He scattering amplitude in the Born approximation may be expressed as

$$F^{He}_{B}(\theta)=I^{He}_{BS}+I^{He}_{BP}$$

where $I^{He}_{BS} = \frac{4N^2}{z_1^3}\left[\frac{X}{A}+\frac{16C}{27}\frac{Y}{B}+\frac{C^2}{8}\frac{W}{D}\right]$,

and $I^{He}_{BP} = \frac{4.5}{\xi^3}\left[\frac{9}{\xi}\tan^{-1}\left(\frac{q}{2\xi}\right)+2\right]-2\left[\frac{9\pi q}{8\xi^4}+\frac{4\xi}{3}\frac{G}{H^3}+\frac{12\xi}{H^2}+\frac{6}{\xi H}\right]$,

when $X = q^2+8z_1^2$, $Y = q^2+18z_1^2$, $W = q^2+32z_1^2$,

$A = (q^2+4z_1^2)^2$, $B = (q^2+9z_1^2)^2$, $D = (q^2+16z_1^2)^2$,

$G = 12\xi^2-q^2$ and $H = 4\xi^2+q^2$.

The differential and the total cross sections for the systems can be obtained by using the standard relations.

For the case of positron-hydrogen and positron-helium scattering the expressions for the static potentials $V_s(r)$ would have opposite signs.

Results and Discussion

The results of our numerical calculations for the elastic scattering cross sections of electrons and positrons by hydrogen and helium atom have been presented in figures 1 to 10. In our investigations we have neglected the non-adiabatic part of the polarization potential as well as the adiabatic quadrupole and the higher order interactions. The effects of quadrupole and the higher interactions are found to be negligibly small for electron-atom scattering because these fall of asymptotically as r^{-6} or faster (Temkin 1959, Obédkov 1963, Drachman 1966). So it has generally been argued (Callaway *et al* 1968) that it is reasonable to include only the dipole polarization potential to describe the distortion effect. It is not expected that the inclusion of the non-adiabatic parts is going to influence the nature of the results appreciably as it is apparent from the results due to Callaway *et al* (1968). Keeping these facts in mind we have chosen the dipole polarization potential of Obédkov (1963) for simplicity.

Moreover, in the e^- —He scattering we have taken an approximate wave function of the helium atom represented by the expression (6) (Mott and Massey 1965). We have calculated the FBA results for the total cross sections by using this static potential. Kennedy (1968) has also obtained the FBA values with an accurate wave function with 52 parameters. It has been seen that our values for the total cross sections (FBA) are very close to those obtained by Kennedy. Therefore, it can be concluded that our static potential for the helium atom is reasonably good.

A. *Electron–Helium Scattering*—In order to test the present eikonal approximation it is better to study first the e^-—He scattering for there are some recent accurate absolute measurements (Vriens *et al.* 1968) renormalised by Chamberlain *et al.* (1970) and Bromberg (1969) for the differential cross section at different scattering angles

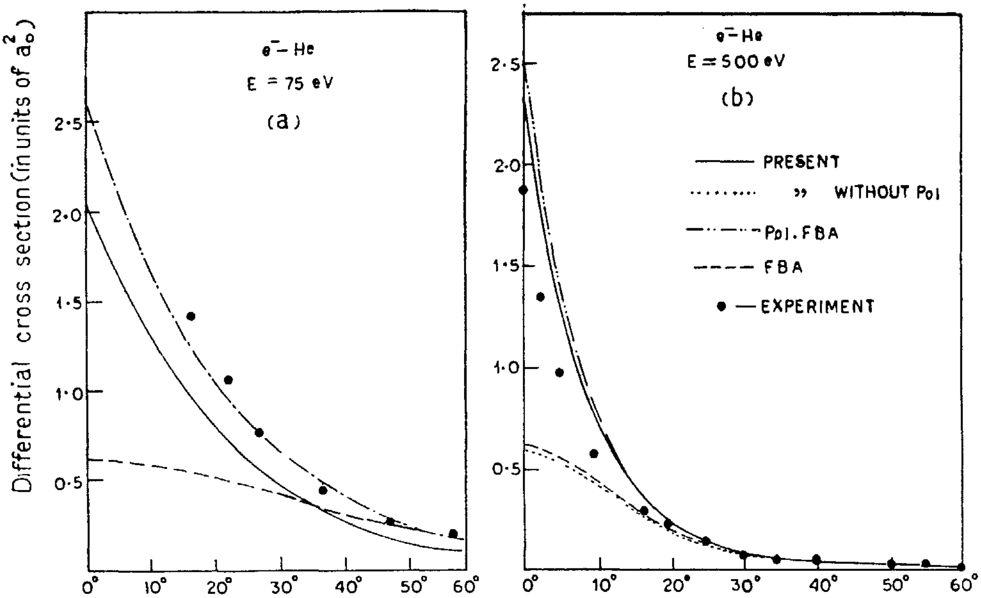

FIG. 1. The differential cross section for the Electron-helium scattering at (a) 75 eV and (b) 500 eV.

in the high and intermediate energies. In Fig. 1, we have shown our results for the differential cross sections for electron-helium scattering at (a) 75 eV and (b) at 500 eV along with the corresponding polarized FBA and FBA results and compared them with the corresponding experimental measurements by Huges *et al.* (1932) as normalized by Bromberg (1969) at 75 eV, and by Vriens *et al.* (1968) renormalised by Bromberg (1969) at 500 eV. We have also calculated the differential cross sections for different incident energies* in between 75 eV and 500 eV and compared them with the available experimental as well as theoretical results. Some of these results (at 100, 200 and 300 eV) have been displayed in an earlier communication (Saha *et al.* 1973). From all these results of the differential cross sections it is apparent that the agreement between the present values obtained by the eikonal approximation and the recent experimental findings at the incident energy 150 eV and above are highly satisfactory. For the incident energy 100 eV and below our values are slightly less than the experimental results but the shapes of the present differential cross section curves reproduce the shapes of the corresponding experimental curves quite well. The results obtained by the polarized FBA give somewhat better agreement below 200 eV with the experimental findings than those obtained by using the eikonal method. From $E \geqslant 200$ eV the polarized Born curves slightly overestimate the differential cross sections. Of course at 500 eV both the curves—the eikonal and the polarized FBA—nearly coincide as

*The curves for the differential cross section for different energies will be available from the authors on request.

expected. The effect of polarization can easily be estimated from the curves at 500 eV where we have plotted the results with and without the inclusion of the polarization effect for both the approximations. Moreover, it may be pointed out that our curves for the eikonal approximation at the incident energy 200 eV and above are almost indistinguishable from those obtained by LaBahn and Callaway (1969) who have performed sophisticated partial wave calculations including the effects of the static potential, electron exchange and both the adiabatic and the non-adiabatic polarizations of the target atom. Their values at 100 eV like ours, also lie below the experimental observations for small angle scattering. The results of Khare and Shobha (1971) have got more or less the same type of agreement with experiments as those of LaBahn and Callaway (1969) and ours. Khare and Shobha have taken in their calculations the effects of the static and the polarization potentials and have included the exchange effect through Ochkur approximation (1964).

B. *Electron–Hydrogen Scattering*—Figs. 2 and 3 contain our results of differential cross sections for e^- —H scattering at 50 and 200 eV respectively along with the corresponding values of the polarized *FBA* and *FBA*. Experimental measurements on the angular dependence of the differential (e^- —H) elastic cross sections are available (Teubner *et al.* as quoted by Tai *et al.* 1969) in relative magnitude for these incident energies. To compare with our results the experimental findings are normalised to our eikonal results at 60° for each energy. The eikonal curves give very satisfactory agreement with experiments. It should be mentioned that the polarized FBA curves given in the figures are quite close to the eikonal curves for all these

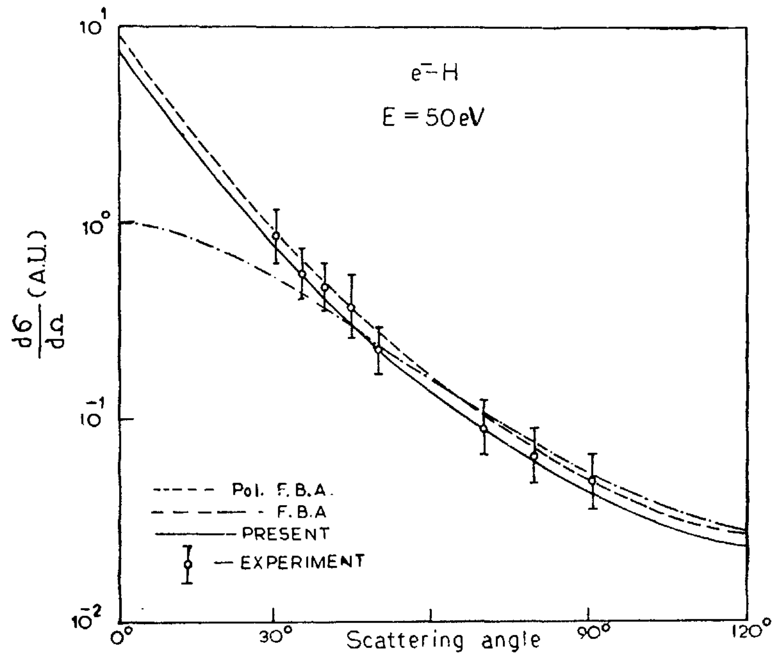

FIG. 2. The differential cross section for the Electron-hydrogen scattering at 50 eV.

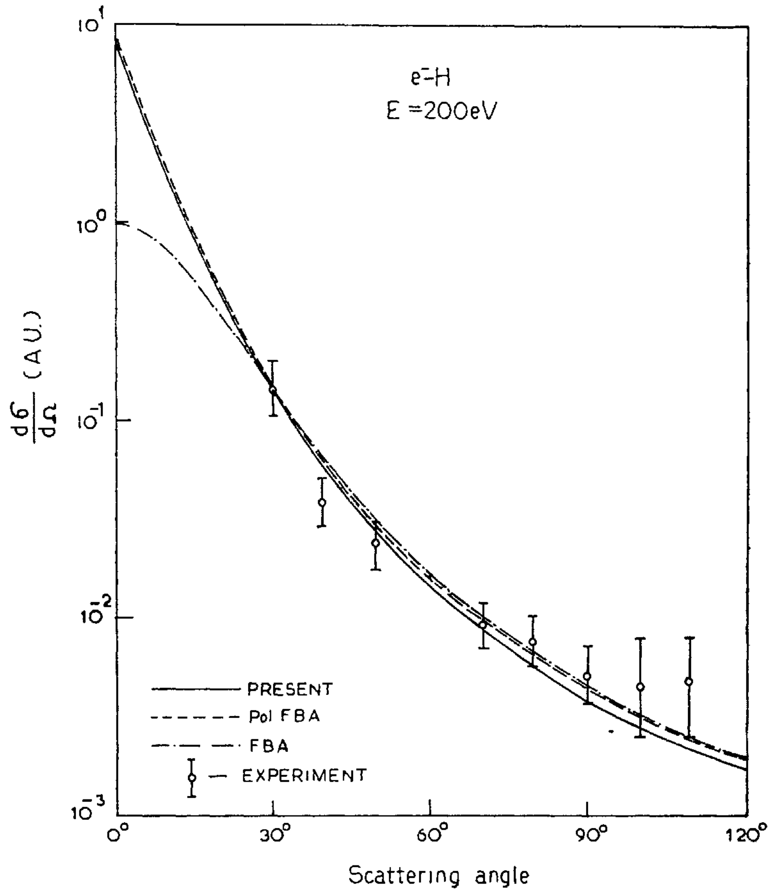

FIG. 3. The differential cross section for the Electron hydrogen scattering at 200 eV.

energies. Similar type of agreement have been obtained by the Glauber approximation (Tai *et al.* 1969) and by the first order multiple scattering approximation (Sinfailam and Chen 1972). But the magnitudes of the cross sections calculated by the different approximations (including ours) are however different.

In Fig. 4 we have plotted our eikonal and the polarized FBA values for the total cross sections along with the corresponding FBA results and compared them with the Glauber results (Franco 1968) and the experimental findings (Neynaber 1961). The curve due to the eikonal approximation is better than the FBA curve when compared to the experimental data at the low energy region (below 12 eV). The Glauber curve is, however, superior to our curve in the said region. The polarized FBA results give rather better agreement with the experimental data than the eikonal results in the low energy regions.

In the high energies the present two curves, the eikonal and the polarized FBA, which agree amongst themselves very closely differ appreciably from the Glauber and the FBA curves. FBA is supposed to be accurate at 200 eV for the electron-hydrogen system. But this has been questioned by Sinfailam and Chen (1972),

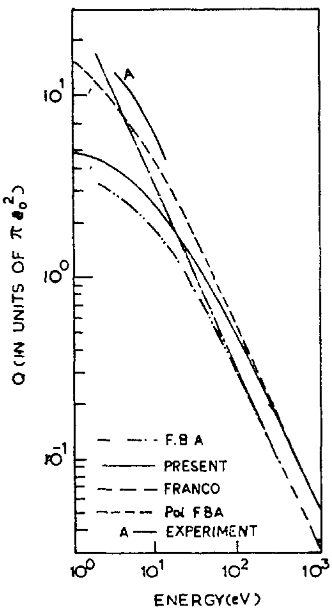

FIG. 4. The total cross section for the Electron hydrogen scattering.

Sil and Ghosh (1972) and also by Banerji *et al.* (1973). Sinfailam and Chen have reported appreciable differences between their results and FBA values even in the keV region.

For both the processes discussed above we have seen that our results for electron-atom scattering differ appreciably from the experimental results in the low energy region. This discrepancy may be attributed to the fact that we have neglected the exchange effect.

C. *Positron-Helium Scattering*—Very recently Costello *et al.* (1972) have measured the total cross section for e^+—*He* elastic scattering from 1 to 4 eV and 17 to 26 eV. In Fig. 5 we have shown the curve (in linear scale) for the total cross section in the eikonal approximation from 1 to 30 eV along with the corresponding polarized FBA curve and compared them with other theoretical results (Drachman 1966, Callaway *et al.* 1968) as well as with the experimental findings of Costello *et al.* (1972). In the same Figure we have inserted our results obtained by the eikonal approximation and the polarized FBA from 30 to 1000 eV (shown in semi-log scale). Our results from 1 to 4 eV are in very close agreement with experiments and the theoretical results of Drachman (1966) who has applied a modified adiabatic method including the second order polarization potential of Dalgarno and Lynn (1957). It may be mentioned that the results of Drachman (1966) are identical with the experimental findings in the region 1 to 4 eV. From 5 eV to the positronium formation threshold energy, our values are some what greater than those obtained by Drachman (1956), as shown in Figure 5. In this energy region our values given reasonably good agreement with the experimental findings and the theoretical results of Callaway *et al.* (1968) based on their extended polarization

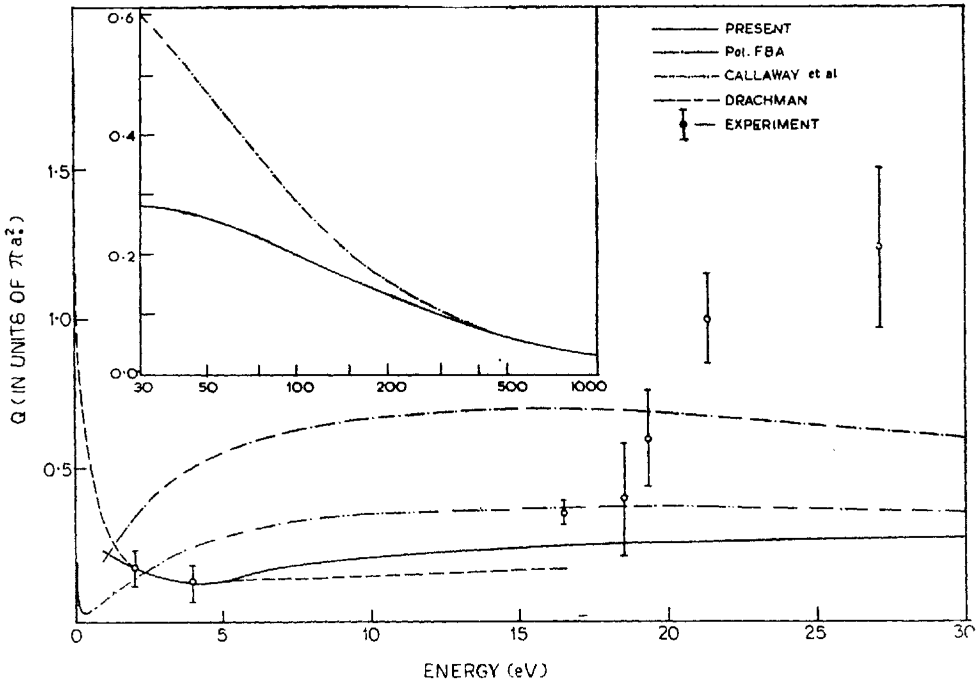

FIG. 5. The total cross section for the Positron helium scattering.

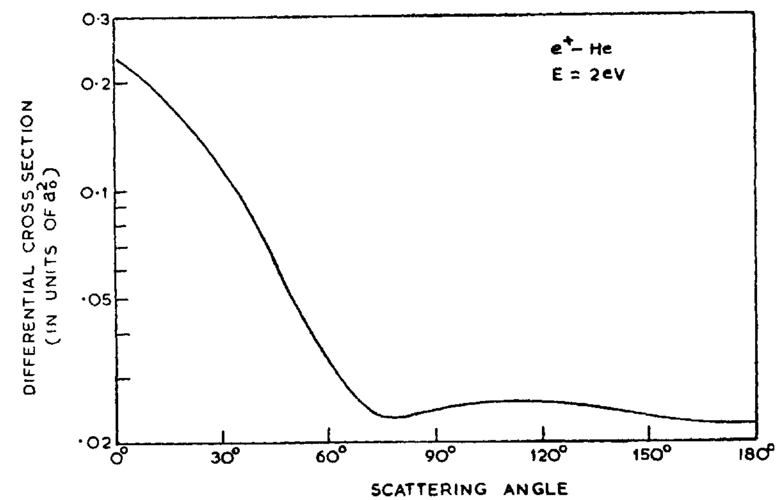

FIG. 6. The differential cross section for the Positron helium scattering at 2 eV.

potential approximation. It may be pointed out that the results obtained by Kraiday (1967) who has taken the effect of the polarization and the virtual positronium formation are in very close agreement with those of Callaway *et al.* (1968) below the

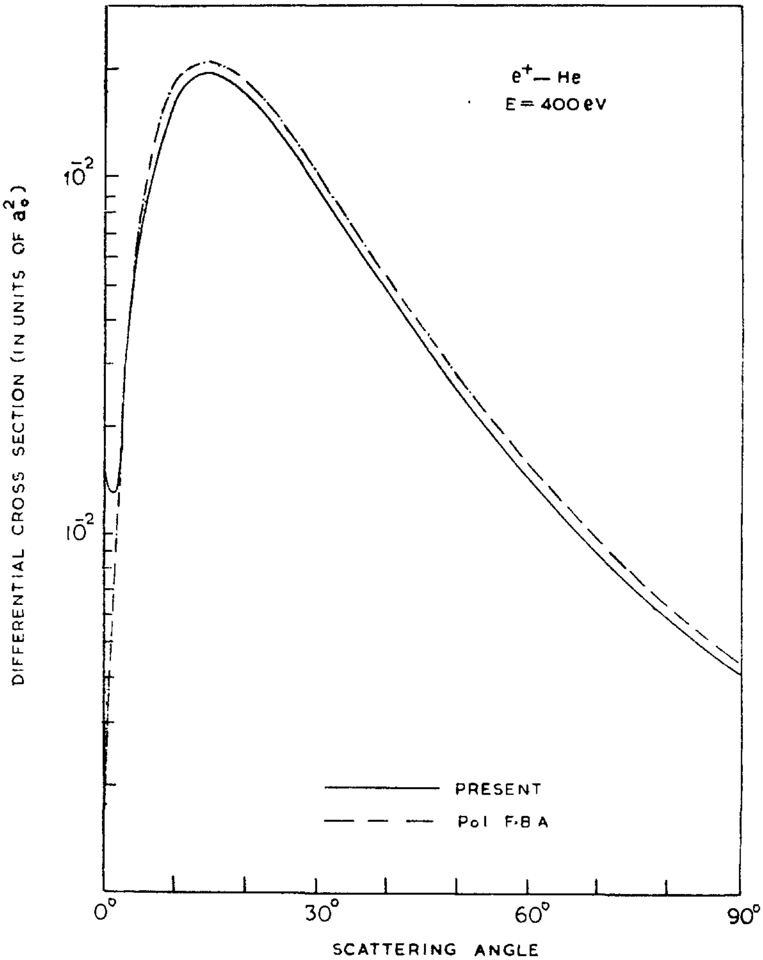

FIG. 7. The differential cross section for the Positron helium scattering at 400 eV.

positronium formation threshold. Above this threshold our values as well as those of Callaway *et al.* (1968) differ appreciably from the experiments. The effect of positronium formation may reduce this differences but we would not expect large changes to occur in the low energy region. The curve due to the polarized FBA fails to reproduce the trend of the experiment in the low energy region (up to 30 eV). In the inserted figure where we have shown the eikonal curve and the polarized FBA curve from 30 to 1000 eV, it is apparent that at about 350 eV the curves coincide as expected.

In Fig. 6 we have shown the differential cross section for e^+—*He* scattering in the eikonal approximation at 2 eV. Fig. 7 represents the eikonal differential cross section curve for 400 eV along with the polarized FBA results. At high energies the nature of the polarized FBA curve is some what similar to that of the eikonal curve. The effect of the polarization is to increase the differential cross sections in the forward directions for the electron atom scattering. In the case of the positron-atom scattering the static potential is repulsive and the polarization potential is attractive. The net effect of the polarization potential is to make the potential seen by the positron less repulsive or possibly even attractive depending on the energy of the incident positron. At 2 eV the eikonal values of the differential cross section for e^{+}—*He* scattering in the small angles are approximately three times less than the corresponding value for e^{-}—*He* scattering. For the positron case another peak has been obtained around 110° scattering angle whereas there is no peak except in the forward direction for the electron case. With the increase in energy the position of the second peak is shifted towards the 0° scattering angle and the second peak becomes more prominent with respect to the first peak in the forward direction. Up to 25 eV, the first peak value is greater than the second peak value. After this the second peak value is greater than that of the first*. Therefore, we think that the nature of the curves is not unphysical. It may be mentioned that at 2 eV the polarized FBA curve which is not shown here after giving a minimum at about 7° steadily rises up to 180°, the value at 180° is greater than that at 0°.

D. *Positron–Hydrogen Scattering*—Still now the experimental results for the elastic scattering of positrons by hydrogen atoms are not available, we, therefore, have to depend mainly on the theoretical results. In Fig. 8 we have plotted our total cross section values of the eikonal and the polarized FBA approximations and compared them with those of Burke *et al.* (1963), Garibotti and Massaro (1971) and Wakid and LaBahn (1971). We have inserted the eikonal curve and the curve due to Callaway *et al.* (1968) for the total cross section against the wave number '*K*' ranging from 0.1 to 1.0 in the same figure' Callaway *et al.* (1968) who have used the extended polarization approximation have obtained a minimum at K=0.2 whereas our minimum lies at K=0.6. This feature has also been noticed in the case of e^{+} *He* scattering, in which case our values rather coincide with experiments. From K=0.6 to 1.0 our results are less than those of Callaway *et al.* (1966) just as in the case of e^{+} —*He* scattering. The eikonal curve lies slightly below the curve due to Burke *et al.* (1963) who have applied the close-coupling approximation taking the effect of couplings to 1s, 2s and 2p states. Garibotti and Massaro (1971) who have applied the Padé approximants method have obtained values which are very close to the present eikonal results. After 50 eV the polarized FBA curve is very close to the curve due to Garibotti and Massaro (1971) and the eikonal curve. The curve obtained by Wakid and LaBahn (1971) who have used the polarized close coupling approximation lies well below our eikonal curve. It should be mentioned that the effect of positronium formation has not been taken into account in any of these works. More refined calculation in this region may be necessary to ascertain the exact behaviour of the cross section.

In Fig. 9 we have shown the eikonal differential cross section values for 2 eV. Fig. 10 represents the eikonal and the polarized FBA values for the differential

*Tables for the differential cross sections at different energies will be available from the authors on request

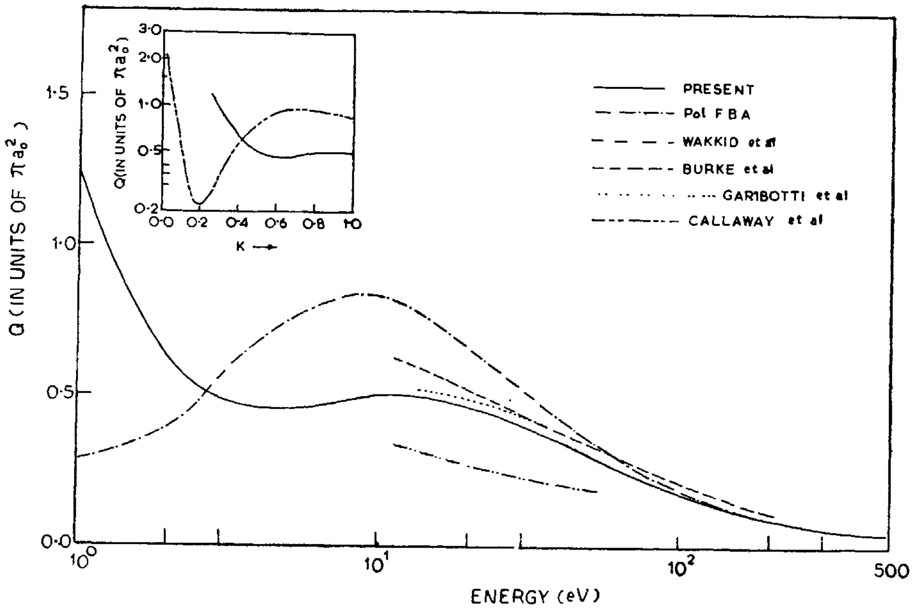

FIG. 8. The total cross section for the Positron hydrogen scattering.

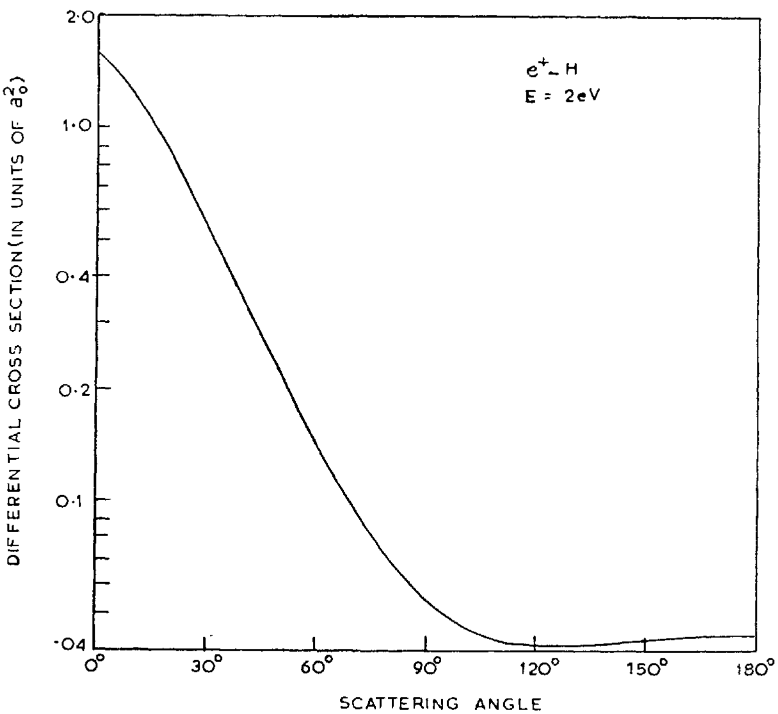

FIG. 9. The differential cross section for the Positron hydrogen scattering at 2 eV.

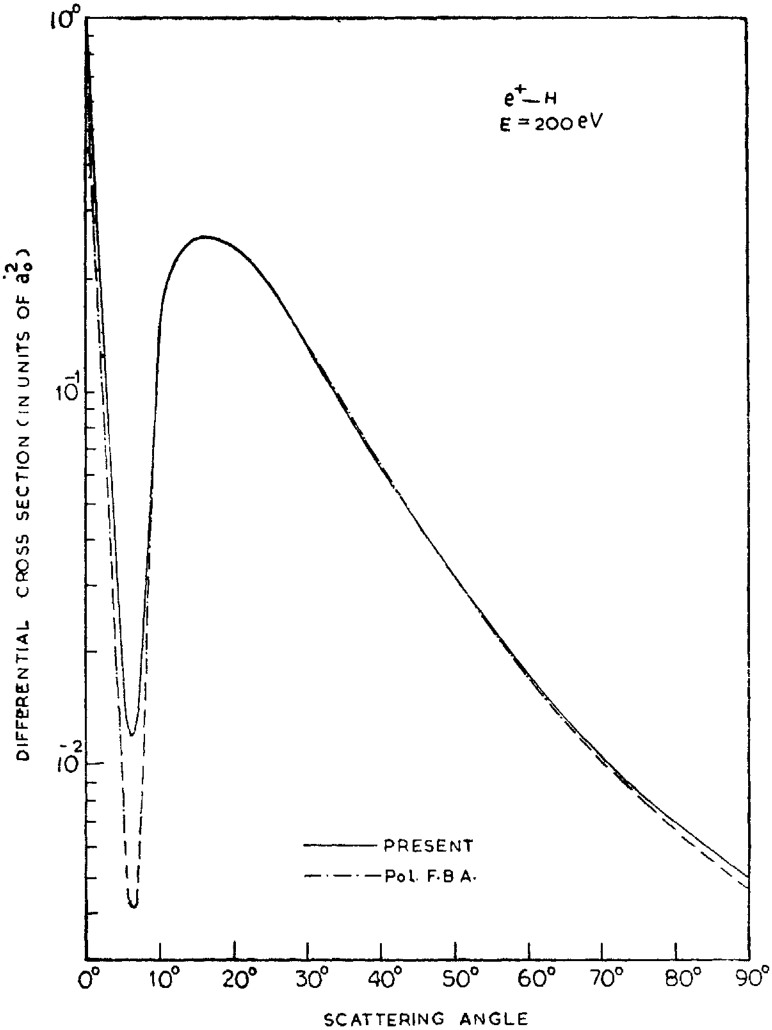

FIG. 10. The differential cross section for the e^+—H scattering at 200 eV.

cross section at 200 eV upto 90° scattering angle. The nature of the differential curves in this case is somewhat similar to that in the case of e^+ —*He* scattering except that here the second peak value is always less than the first peak value. This difference may be due to the fact that the effect of the polarization is more in the case of hydrogen than in the case of helium atom.

CONCLUSION

The object of this paper is to justify the suitability of the application of the eikonal approximation to the elastic atomic collision processes, the effect of the polarization of the target atom being taken into consideration. On the basis of this work, we can conclude that the eikonal method has qualitatively very satisfactory behaviour. The present approach is very simple to apply in atomic scattering problems and reproduces without much labour the results obtained by much more sophisticated and refined calculations. Moreover, this method may be applied to more complex atoms (Sarkar *et al.* 1973) without increasing the complication of the numerical calculations. The effect of the polarization plays a key role in atomic collision problems. Here in this method, however, we have not been able to take into account to the effect of the rearrangement channel.

The polarized FBA method is still simpler and in the case of the electron scattering it gives quite satisfactory results but for the positron scattering the polarized FBA fails to reproduce reliable results.

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