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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^- – 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 $\Delta\chi$ 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 χ_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 χ_0^{nlm}

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

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

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

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 χ_0^{ns} for any (*ns*) state.

As a special case, we find Ψ, V_{st} and χ_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.

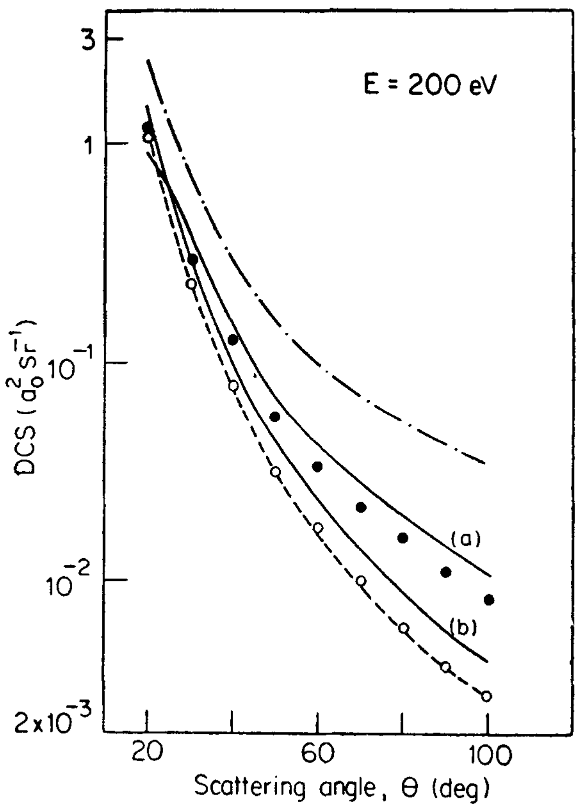

Figure 1. Differential scattering cross-sections for the elastic scattering of electrons from H(2S) at 200 eV.
Solid curve a.—present calculations, broken curve—present calculation in the Glauber approximation. Solid curve b—data of Pundir *et al* (1982). dash—dot curve HHOB results (Rao and Desai 1983).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

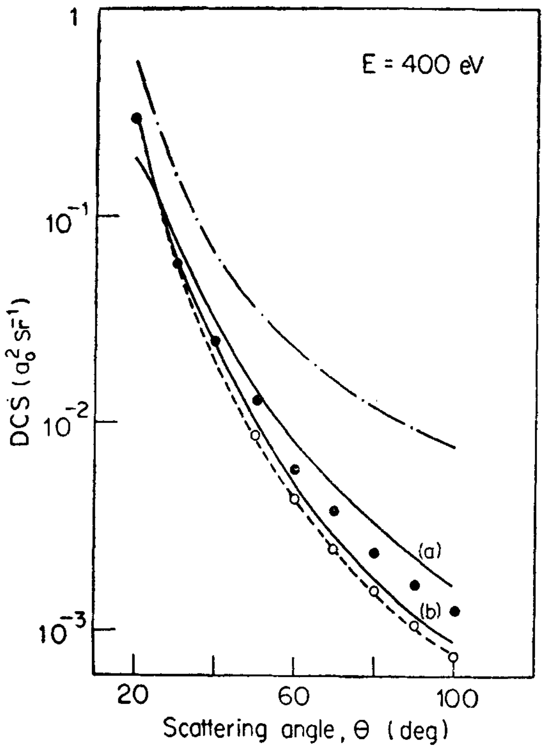

Figure 2. Differential scattering cross-sections for the elastic scattering of electrons from H(2S) at 400 eV. References are same as in figure 1.

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

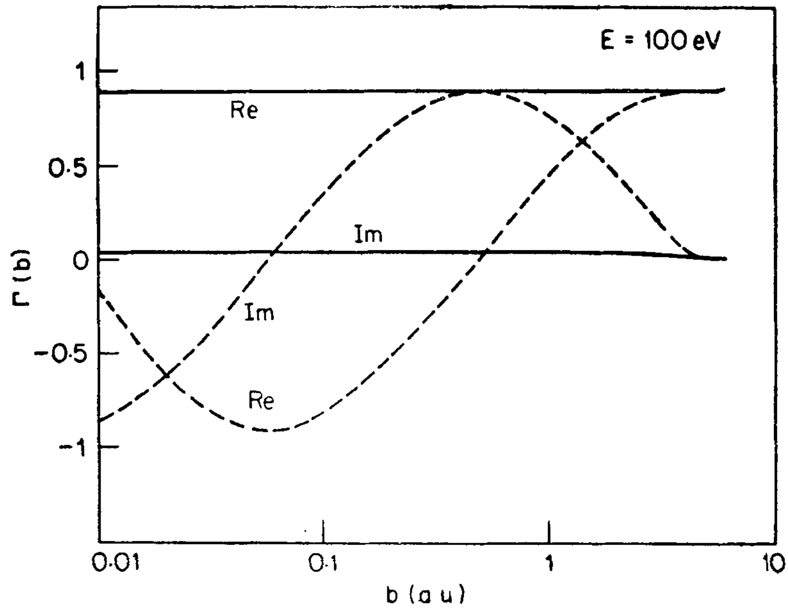

Figure 3. Real and imaginary parts of $\Gamma(b)$ for the potential V_0 (solid curve) and for the total interaction V (dashed curve) for elastic $\bar{e}$–H(2S) scattering at 100 eV.

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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