CHAPTER – II

ELECTRON SCATTERING BY He, Ne, Ar ATOMS

2.1 INTRODUCTION :

The second chapter deals with some of the high-energy methods that find application in high-energy scattering. The reason for taking up this aspect here is two fold i.e. (i) in the present work we have dealt with high energy problems only, so that subject matter is independent and self consistent, (ii) the author himself started this work on the neutral targets and then switched over to the problems described later on. We begin with the out line of various theoretical methods after specifying high and low energy

The study of the electron collision with atoms, molecule or ion can not be done through a single theory that applies to any incident energy on any target. Specific quantum mechanical theories have been developed for specific domain of the energy of projectile electron. If the speed of incident electron is less than or nearly equal to the speed of target electrons then it is termed as low energy range. Thereafter the intermediate energy is near the excitation threshold of the target and extends up to a few times the ionization threshold. Then from a few times the ionization threshold upward is high energy region. This is up to very high energies where relativistic considerations become effective. This classification obviously depends very much on the target.

All the theories of collision physics in practice are quantum mechanical and developed from Schrodinger equation. The different methods are different approximate ways to solve Schrodinger equation. These are under two categories, (i) differential approach, (ii) integral approach. The approximate methods described here, applied in high-energy range are 1.Born Approximation, 2.Eikonal Approximation, 3.Eikonal-Born series 4.DAS technique, 5. Modified DAS technique and 6. Partial wave analysis. The high energy methods except partial wave analysis, arise from an integral equivalent of the Schrodinger equation i.e. Lippmann-Shrodinger equation. These theoretical methods of our interest are treated somewhat at length in the previous chapter. Here these methods are applied for actual targets i.e. He, Ne, and Ar atoms with different target potentials. The basic idea underlying different method is their applicability in high-energy range along with the way of obtaining higher accuracy in results.

2.2 APPLICATION OF BORN APPROXIMATION :

The zero order approximation i.e. $\psi_{k_i}^{+}(r) = \psi_0(r) = \phi_{k_i}(r)$ to the solution of Lippman-Schwinger equation gives the 1st Born approximation. The first Born scattering amplitude is given by

$$f_{B1} = -2\pi^2 \left\langle \phi_{k_f} \mid U \mid \psi_0 \right\rangle .$$

$$= -2\pi^2 \left\langle \phi_{k_f} \mid U \mid \phi_{k_i} \right\rangle \qquad (2.2.1)$$

The 2nd Born approximation is then obtained by considering second order perturbation and making corresponding approximation in the Lippman-Swinger equation i.e. $\psi_{k_i}^{+}(r) = \psi_1(r) = \phi_{k_i}(r) + \int G_0^{(+)}(r,r')U(r')\phi_{k_i}(r')dr'$, so the second Born scattering amplitude is obtained as

$$f_{B2} = -2\pi^2 \left\langle \phi_{k_f} \mid U \mid \psi_1 \right\rangle .$$

$$= -2\pi^2 \left\langle \phi_{k_f} \mid U + UGU \mid \psi_0 \right\rangle \qquad (2.2.2)$$

Thus the Born series is a perturbative expansion in powers of the potential $U(r)$. If the potential is weak enough, the expansion converges to a limit and at high energies it is valid only if $\frac{|U_0|a}{2k} << 1$, where a is range of potential, U_0 is strength of the potential and k is wave vector depending on the incident energy. These are the conditions for Born approximation.

First Born Approximation :

Let us analyze the first Born approximation. It is a function of scattering direction (θ,φ) and the momentum transfer q. For elastic scattering $q = |\underline{k}_i - \underline{k}_f| = 2kSin\theta/2$; where $\underline{k}_i, \underline{k}_f \rightarrow$ incident and scattered wave vector,

$|\underline{k}_i| = |\underline{k}_f| = k \rightarrow$ magnitude of wave vector.

The equation (2.2.1) is evaluated in the coordinate representation with $\phi_{k_i}(r) = (2\pi)^{-3/2} e^{ik_i \cdot r}$ and $\phi_{k_f}(r) = (2\pi)^{-3/2} e^{ik_f \cdot r}$ is given by

$$\therefore f_{B1} = -\frac{1}{4\pi} \int e^{i\underline{q}\cdot\underline{r}} U(\underline{r})\, d\underline{r} \;\; ; \quad U(r) = \frac{2m}{\hbar^2} V(r) \qquad (2.2.3)$$

Considering a target with internal structure and introducing initial and final state wave function of the target ψ_i, ψ_f;

$U(\underline{r}) = U_{fi}(\underline{r}) = \langle \psi_f \mid \text{Electro - static potential} \mid \psi_i \rangle$.

Different analytical forms of $U(r)$ are obtained for various potential fields.

Let us first consider *Yukawa potential*, $U(r) = -U_0 \frac{e^{-\lambda r}}{r}$

$$\therefore f_{BI} = \frac{U_0}{4\pi} \int e^{i\underline{q}\cdot\underline{r}} \frac{e^{-\lambda r}}{r} d\underline{r} \; ;$$

$$= \frac{U_0}{4\pi} \int_0^{2\pi} d\varphi \int_0^{\infty} \int_0^{\pi} e^{iqr\,Cos\theta} Sin\theta \, d\theta \frac{e^{-\lambda r}}{r} r^2 dr$$

$$= \frac{U_0}{2} \int_0^{\infty} \frac{2Sin(qr)}{qr} e^{-\lambda r} r \, dr = \frac{U_0}{q} \int_0^{\infty} Sin(qr) e^{-\lambda r} dr$$

$$= \frac{U_0}{\lambda^2 + q^2} \qquad (2.2.4)$$

In the past, attempts have been made to determined potential field parameters. *Cox and Bonham* [54] reported parameters for a set of Yukawa potential terms, determined by least square fits of radial electron density function. The potential for neutral atoms with the expression of nuclear screening factor becomes

$$V(r) = -\frac{Ze^2}{r} \sum_i \gamma_i \exp(-\lambda_i r) . \qquad (2.2.5)$$

Now substituting $V(r)$ in equation (2.2.3) and performing angular integrations

$$f_{BI} = -\frac{2m}{\hbar^2 q} \int_0^{\infty} r \, Sin\, qr V(r) dr$$

$$= \frac{2Ze^2 m}{\hbar^2 q} \int_0^{\infty} \sum_i \gamma_i e^{-\lambda_i r} Sin\, qr \, dr$$

$$= \frac{2Z}{a_0 q} \sum_i \gamma_i \frac{q}{\lambda_i^2 + q^2} ; a_0 = \frac{\hbar^2}{me^2} = 1 \text{ atomic unit of length}$$

$$\therefore f_{BI} = 2Z \sum_i \frac{\gamma_i}{(\lambda_i^2 + q^2)} \quad \text{in atomic unit} \qquad (2.2.6)$$

Here magnitude of wave vector k is obtained in atomic unit as $\frac{2mE}{\hbar^2} = k^2$

$\Rightarrow \sqrt{2E_{au}} = k_{au}$; $\frac{e^2}{a_0} = 27.2\ eV = 1$ Hartree, atomic unit of energy and potential should be considered in atomic unit, so that f_{B1} evaluated in atomic unit. The scattering amplitude is also studied with the other analytical expression for *Thomas-Fermi-Direc* (TFD) [56] and *Hartree-Fock* (HF) [60] potential field for neutral atoms. These potentials have the following form

$$U^{TFD}(r) = -\frac{2Z}{ar}\sum_i \gamma_i e^{-\lambda_i r}\ ; \qquad a \rightarrow \text{Bohar radius.}$$

$$U^{HF}(r) = -\frac{2Z}{ar}\left[\sum_i \gamma_i e^{-\lambda_i r} + r\sum_i \gamma_i e^{-\lambda_i r}\right] \tag{2.2.7}$$

$$\therefore f_{B1}^{HF} = 2Z\left[\sum_i \frac{\gamma_i}{(\lambda_i^2 + q^2)} + \sum_i \gamma_i \frac{2\lambda_i}{(\lambda_i^2 + q^2)^2}\right] \tag{2.2.8}$$

The more reliable parameters in screening function are determined by analytical fitting procedure to Dirac-Hartree-fock-Slater (DHFS) self-consistent data are given by *F.Salvat* et al [38]. These analytical functions incorporating relativistic effects are used for the high energy range (**KeV**) of the present work. *Dirac Hartree Fock Slater screening potential* is the simple of superposition of three Yukawa potential given as

$$U^{DHFS}(r) = -\frac{2Z}{r}\sum_{i=1}^{3} \gamma_i e^{-\lambda_i r} \tag{2.2.9}$$

$$\therefore f_{B1} = 2Z\sum_i \frac{\gamma_i}{(\lambda_i^2 + q^2)} \tag{2.2.10}$$

<u>*Second Born Approximation*</u> :

The Major contribution in Born series after the first Born term is the second Born term. Let us now study the second Born approximation for the case of Yukawa potential. We have to evaluate the quantity $\overline{f}_{B2}$, which is written in momentum space as

$$\overline{f}_{B2} = 2\pi^2 \int d\mathrm{K} \langle k_f | U | \mathrm{K} \rangle \frac{1}{(\mathrm{K}^2 - k^2 - i\varepsilon)} \langle \mathrm{K} | U | k_i \rangle \tag{2.2.11}$$

The evaluation of the integral appearing on the right-hand side of eq. (2.2.11), is performed using the more general form of *Dalitz Integrals* [31,32]. In the case of single Yukawa potential $U(r) = -U_0 e^{-\alpha r}/r$ equation (2.2.11) becomes

$$\bar{f}_{B2} = (2\pi^2)^{-1} U_0^2 \int d\mathrm{K} \frac{1}{(\mathrm{K}^2 - k^2 - i\varepsilon)(\alpha^2 + |\mathrm{K} - k_f|^2)(\beta^2 + |\mathrm{K} - k_f|^2)}; \quad \alpha = \beta$$

$$= (2\pi^2)^{-1} U_0^2 I_{1,1}(\alpha, \alpha; k_i, k_f, k)$$

$$= (2\pi^2)^{-1} U_0^2 \int_0^1 L_2(k, \Gamma, \Lambda)\, dt \; ; \text{ where } L_2(k, \Gamma, \Lambda) = -\frac{\pi^2}{\Gamma(k^2 - \Gamma^2 - \Lambda^2 + 2ik\Gamma)}$$

$$\therefore \bar{f}_{B2} = -\frac{1}{2} U_0^2 \int_0^1 \frac{dt}{\Gamma(2ik\Gamma - \lambda^2)} \; ; \text{here } |k_i| = |k_f| = k \text{ and } \alpha = \beta = \lambda \tag{2.2.12}$$

For superposition of Yukawa potential; $\alpha = \lambda_i, \beta = \lambda_j$

$$\therefore \bar{f}_{B2} = -\frac{1}{2} U_0^2 \sum_{i,j} \gamma_i \gamma_j \int_0^1 \frac{dt}{\Gamma[2ik\Gamma - \lambda_i^2 t - \lambda_j^2 (1-t)]} \; . \tag{2.2.13}$$

Let $A = \Gamma(\lambda_i^2 t + \lambda_j^2 (1-t))$ and $B = 2k\Gamma^2$

$$\therefore \int_0^1 \frac{dt}{\Gamma[2ik\Gamma - \lambda_i^2 t - \lambda_j^2 (1-t)]} = \int_0^1 \frac{dt}{iB - A} = \int_0^1 -\frac{A + iB}{A^2 + B^2} dt$$

Let $\frac{A + iB}{A^2 + B^2} = f(\lambda_i, \lambda_j, t)$

$$\therefore \bar{f}_{B2} = \frac{1}{2} U_0^2 \sum_{i,j} \gamma_i \gamma_j \int_0^1 f(\lambda_i, \lambda_j, t)\, dt$$

$$\therefore \mathrm{Re}\, \bar{f}_{B2} = \frac{1}{2} U_0^2 \sum_{i,j} \gamma_i \gamma_j \int_0^1 \frac{A}{A^2 + B^2} dt \quad \text{and}$$

$$\mathrm{Im}\, \bar{f}_{B2} = \frac{1}{2} U_0^2 \sum_{i,j} \gamma_i \gamma_j \int_0^1 \frac{B}{A^2 + B^2} dt \tag{2.2.14}$$

Using Numerical integration

we have $\int_0^1 f(t)\, dt = \sum_{i=1}^{n} w_i f(t_i)$; $t_i \rightarrow$ Gaussian points.

$w_i \rightarrow$ Gaussian weight factors.

In the case of HF potential of the form, $\gamma_1 \frac{e^{-\lambda_1 r}}{r} + \gamma_2 (\frac{\partial}{\partial \lambda_2}) \frac{e^{-\lambda_2 r}}{r}$; $\alpha = \lambda_1, \beta = \lambda_2$

$$\bar{f}_{B2} = \frac{1}{2}U_0^2\left[\gamma_1^2 + 2\gamma_1\gamma_2(-\frac{\partial}{\partial\lambda_2}) + \gamma_2^2(\frac{\partial^2}{\partial\lambda_2^2})\right]\int_0^1 f(t)\,dt\,. \qquad (2.2.15)$$

2.3 EIKONAL BORN SERIES APPROACH :

Semi-classical methods are useful approximation technique when de Broglie wave length of the incident particle is sufficiently short compared to the range of the potential '***a***' (i.e. energy of incident particle is high, so that $ka >> 1$). The eikonal scattering wave function is derived from the Lippmann-Schwinger equation as discussed in section 1.3. In this section eikonal approximation is applied to the simple problem of non-relativistic potential scattering. Comparison of higher order terms of eikonal and Born series leads to the eikonal Born series approach [8]. The theoretical approach to such process based on a detail study of Born and Eikonal multiple scattering series is given by Bayron, Joachain and Mund [6].

Eikonal scattering amplitude (1.4.1) and Born scattering amplitude (1.2.18) is defined by the Born series and Eikonal multiple scattering expansion as

$$f_{ex} = \sum_{n=1}^{\infty}\bar{f}_{Bn} = \bar{f}_{B1} + \bar{f}_{B2} + \bar{f}_{B3} + \cdots \;;\; \text{and}$$

$$f_E = \sum_{n=1}^{\infty}\bar{f}_{En} = \bar{f}_{E1} + \bar{f}_{E2} + \bar{f}_{E3} + \cdots \qquad (2.3.1)$$

The sum of the first n terms

$$f_{Bn} = \sum_{j=1}^{n}\bar{f}_{Bj} \quad \Rightarrow f_{B1} = \bar{f}_{B1} \text{ and } \Rightarrow f_{B1} = \bar{f}_{B1}$$

$$\Rightarrow f_{B2} = \bar{f}_{B1} + \bar{f}_{B2}\,, \text{ similarly}$$

$$f_{En} = \sum_{j=1}^{n}\bar{f}_{Ej}\,, \text{ where } \bar{f}_{En} = -\frac{ik}{n!}i^n\int_0^{\infty}J_0(\Delta b)[\chi(b)]^n b\,db \quad \Rightarrow \mathrm{Re}\,\bar{f}_{E2} \equiv 0 \text{ and}$$

$$\bar{f}_{Bn} = -2\pi^2 < \phi_{kf}\,|\,U\,|\,\phi_{ki} > \;\Rightarrow \mathrm{Re}\,\bar{f}_{B2} \neq 0 \qquad (2.3.2)$$

Now writing each term in the form of Δ and k; $\mathrm{Im}\,\bar{f}_{B2}(k,\Delta) = A_{B2}(\Delta)/k + \ldots$ and $\mathrm{Im}\,\bar{f}_{E2}(k,\Delta) = A_{E2}(\Delta)/k + \ldots.$ Byron and Joachain [37] have shown that for Yukawa-type potential equation (2.3.2) reads as

$$\bar{f}_{Bn}(k,\Delta) = \frac{A_{Bn}}{k^{n-1}} + O(k^{-n}) \text{ and } \bar{f}_{En}(k,\Delta) = \frac{A_{En}}{k^{n-1}} + O(k^{-n}) \qquad (2.3.3)$$

for all n and all values of the momentum transfer. For large enough k the relations imply that $\overline{f}_{En}(k,\Delta) = \mathrm{Re}\,\overline{f}_{Bn}(k,\Delta)$ n odd

$$\mathrm{Im}\,\overline{f}_{En}(k,\Delta) = \mathrm{Im}\,\overline{f}_{Bn}(k,\Delta) \quad n \text{ even.} \tag{2.3.4}$$

From the analysis of first few terms (up to $n=4$) the equivalence of the higher orders terms of Born and eikonal series also holds for an arbitrary super position of Yukawa potentials suggested by BJM.The agreement is good for all momentum transfer for large k. *i.e.* For superposition of Yukawa potential and large value of incident wave number each term of eikonal multiple scattering series gives the value of corresponding term in the Born series. [7]

Restricting to the weak coupling case such that $|U_0|a/2k << 1$, where the Born series converges and imposing the condition of validity of the eikonal approximation i.e. $ka >> 1$ and $|U_0|/k^2 << 1$ asymptotic form of the exact scattering amplitude for fixed Δ and large k can be written as [57]

$$f_{ex}(k,\Delta) = f_{B1}(\Delta) + \left[\frac{A(\Delta)}{k^2} + i\frac{B(\Delta)}{k}\right] + \frac{C(\Delta)}{k^2} + O(k^{-3}). \tag{2.3.5}$$

$$= f_{B1}(\Delta) + \overline{f}_{B2} + \overline{f}_{B3} + \ldots.$$

On the other hand the relation $f_{E1} = f_{B1}$, (2.3.3) and (2.3.4) imply that the eikonal scattering amplitude is given by

$$f_E(k,\Delta) = f_{B1}(\Delta) + i\frac{B(\Delta)}{k} + \frac{C(\Delta)}{k^2} + O(k^{-3}). \tag{2.3.6}$$

$$= f_{B1}(\Delta) + \overline{f}_{E2} + \overline{f}_{E3} + \ldots..$$

Upon comparison of equations (2.3.5) and (2.3.6) it is clear that neither $f_{B2} = f_{B1} + \overline{f}_{B2}$ nor f_E are correct to order k_i^{-2}. Indeed f_{B2} lacks the real term of order k^{-2} i.e. $\frac{C(\Delta)}{k^2}$ and similarly the real term $\frac{A(\Delta)}{k^2}$ is missing in f_E. It is obvious from above expression the term is present in f_{ex} $\frac{A(\Delta)}{k^2} = \mathrm{Re}\,\overline{f}_{B2}$

Thus Born amplitude can be improved as $f = f_{B1} + \overline{f}_{B2} + f_{E3}$ or eikonal amplitude can be improved by $f = f_E + \mathrm{Re}\,\overline{f}_{B2}$. We found that it is better to consider later correction, which includes more terms of higher order in $(1/k)$ than the previous one. In the other way, since $A(\Delta) \propto U_0^2$ and $C(\Delta) \propto U_0^3$

(i) U_0 is sufficiently small (i.e.<1) second Born amplitude f_{B2} is more accurate than f_E

(ii) U_0 is not sufficiently small $\mathrm{Re}\,\overline{f}_{B2} + f_E$ is better approximation.

In the present work on light (He) as well as heavy atoms (Ne, Ar), the second case exist.

Now by adding the important missing term $\mathrm{Re}\,\overline{f}_{B2}$ to the eikonal amplitude f_E excellent improvement is seen. Therefore DCS is also improved. This is a much better approximation than f_{B1} for calculation of DCS, since the terms involving $A(\Delta), B(\Delta)$ and $C(\Delta)$ in equation (2.3.5) contribute equally in correcting the first Born differential cross section. Thus the eikonal Born series amplitude which gives consistent picture of the scattering amplitude through order k_i^{-2} is given by

$$f_{EBS} = f_E + \mathrm{Re}\,\overline{f}_{B2} \tag{2.3.7}$$

Eikonal amplitude :

Consider eikonal amplitude equation (1.3.8) in cylindrical polar coordinates and integrating over the z variable, the scattering amplitude is given by

$$f_E = \frac{k}{2\pi i}\int d^2b\, e^{i\underline{\Delta}\cdot\underline{b}}(e^{i\chi(b)} - 1) \qquad \text{Surface integral } ds = d^2b = bdb\,d\varphi \tag{2.3.8}$$

$$\text{where } \chi = -\frac{1}{2k}\int_{-\infty}^{\infty} U(\underline{b}, z)\, dz\,;\; U(b,z) = \frac{2m}{\hbar^2}V(\underline{r}) \tag{2.3.9}$$

$$= -\frac{1}{k}\int_0^{\infty} U(\underline{b}, z)\, dz \text{ is called eikonal phase shift function.}$$

The cylindrical coordinate system has been chosen with $r = b + z\hat{n}$, where $\hat{n}$ is perpendicular to the wave vector transfer $\Delta = k_i - k_f$. For radial field which possess cylindrical symmetry equation (2.3.7) reduces to

$$f_E = \frac{k}{i}\int_0^{\infty} bdb\, J_0(\Delta b)(e^{i\chi(b,k)} - 1)\;;\quad \Delta = 2k\sin\theta/2 \tag{2.3.10}$$

where $J_0(\Delta b) = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\; e^{i\underline{\Delta}\cdot\underline{b}}$ is the Bessel function of integer order.

Now $e^{i\chi(b,k)} = Cos\chi + i\, Sin\chi$

$\therefore \mathrm{Re}\, f_E = k\int_0^{\infty} db\, b\, J_0(\Delta b)\, Sin\{\chi(b,k)\}$ and

$$\therefore \operatorname{Im} f_E = k\int_0^{\infty} db\, b\, J_0(\Delta b)[Cos\{\chi(b,k)\}-1], \qquad (2.3.11)$$

where –ve sign out side the last integral is neglected.

For $U = -U_0 \dfrac{e^{-\alpha r}}{r}$,

$$\chi(k,b) = \frac{U_0}{k} K_0(\alpha b); \quad \text{where } K_0 \rightarrow \text{modified Bessel function of order zero.} \qquad (2.3.12)$$

In the case of superposition of Yukawa type potential $U = -U_0 \sum_{i=1}^{2} \gamma_i \dfrac{e^{-\lambda_i r}}{r}$

$$\chi(b,k) = \frac{U_0}{k} \sum_{i=1}^{2} \gamma_i K_0(\lambda_i b) \qquad (2.3.13)$$

Equations in (2.3.11) are evaluated numerically, where presence of Bessel function J_0 makes the evaluation typical. We must take care about zeros of the Bessel function. So the definite integral with limit 0 to ∞ is performed block wise according to the positions of Bessel's zeroes. Thus block-wise integration

$\int_0^{\infty} = \int_0^{a} + \int_a^{b} + \int_b^{c} + \cdots n$ terms; $a, b, c \cdots$ are x-coordinates where $J(x) = 0$.

$= a_0 - a_1 + a_2 - a_3 \cdots\cdots$

$= \sum_{k=0}^{\infty} (-1)^k \, a_k$ is a convergent series.

The sum of the series is given by the Euler's transform [A.Witz]

$s = \sum_{k=0}^{\infty} \dfrac{(-1)^k \Delta^k}{2^{k+1}}$, where Δ^k is obtained from the difference table.

Numerical integration of each block is done by the Gaussian integration $\int_0^1 f(x)dx \cong \sum_{i=1}^{8} w_i f(x_i)$. The limit is changed $\int_a^b f(y)dy \rightarrow \int_0^1 f(x)dx$ by choosing the new variable $x = \dfrac{y-a}{b-a}$. Initial integration up to 8-blocks are added then Euler's transform is done using next 4-blocks, which gives sum of the remainder series. Finally resultant eikonal amplitude is obtained using equation (2.3.11) as

$$f_E = \mid \operatorname{Re} f_E^2 + \operatorname{Im} f_E^2 \mid^{1/2} \qquad (2.3.14)$$

And the differential cross-section is obtained from (2.2.14) and (2.3.11) as

$$\frac{d\sigma}{d\Omega} = |f_{EBS}|^2 = \left|\mathrm{Re}\, f_E + \mathrm{Re}\,\overline{f}_{B2}\right|^2 + |\mathrm{Im}\, f_E|^2 \qquad (2.3.15)$$

Calculation of $\overline{f}_{E3}$:

Analytical evaluation of the term f_{E3} i.e. $\mathrm{Re}\,\overline{f}_{B3}, \mathrm{Re}\,\overline{f}_{E3}$ is difficult so $\overline{f}_{E3}$ is obtained by numerical evaluation of equation (2.3.2). By expanding the quantity $e^{i\chi}$ in the eikonal amplitude equation (2.3.10) in powers of χ, the eikonal multiple scattering series is defined as

$$f_E = \sum_{n=1}^{\infty} \overline{f}_{En} \ ,$$

where $\overline{f}_{En} = \frac{k}{2\pi i}\frac{i^n}{n!}\int d^2b \exp(i\Delta \cdot b)[\chi(k,b)]^n$.

$$= -\frac{i^{n+1}k}{n!}\int_0^{\infty} J_0(\Delta b)[\chi(k,b)]^n \quad \text{for central real potential} \qquad (2.3.16)$$

$$\therefore \overline{f}_{E3} = -\frac{k}{6}\int_0^{\infty} J_0(\Delta b)[\chi(k,b)]^3 b\, db \qquad (2.3.17)$$

Now in the case of super position of Yukawa potential $U(b,z) = -U_0 \sum \gamma_i \frac{e^{-\lambda_i}}{r}$

$$\chi = -\frac{1}{2k}\int_{-\infty}^{\infty} U(b,z)dz = \frac{U_0}{k}\sum_{i=1}^{2}\gamma_i K_0(\lambda_i b) \qquad (2.3.18)$$

$$\therefore \chi^3 = \frac{U_0^3}{k^3}\left[\sum_{i=1}^{2}\gamma_i K_0(\lambda_i b)\right]^3 \qquad (2.3.19)$$

Substitute equation (2.3.19) in equation (2.3.17)

$$\overline{f}_{E3} = -\frac{U_0^3}{6k^2}\int_0^{\infty} J_0(\Delta b)\left[\sum_{i=1}^{2}\gamma_i K_0(\lambda_i b)\right]^3 b\, db$$

Let $y = \Delta b$

$$\therefore b = \frac{y}{\Delta} \text{ and } db = \frac{dy}{\Delta}$$

$$\therefore \overline{f}_{E3} = -\frac{U_0^3}{6k^2}\int_0^{\infty}\frac{y}{\Delta^2}J_0(y)\left[\sum_{i=1}^{2}\gamma_i K_0(\lambda_i\frac{y}{\Delta})\right]^3 dy \qquad (2.3.20)$$

Integral in R.H.S. is evaluated by block wise integration, where limits are Bessel's zeroes for each block.

Let $I_E = \int_0^{\infty}\frac{y}{\Delta^2}J_0(y)\left[\sum_{i=1}^{2}\gamma_i K_0(\lambda_i\frac{y}{\Delta})\right]^3 dy = \int_0^{\infty} f(y)\,dy$

$$I_E = \int_0^{24} f(y)\,dy + \int_{24}^{552} f(y)\,dy + \ldots\ldots + \int_{369}^{\infty} f(y)\,dy$$

$$= \int_{x_0=0}^{x_1} f(y)\,dy + \int_{x_1}^{x_2} f(y)\,dy + \ldots\ldots + \int_{x_{12}}^{\infty} f(y)\,dy \text{ ; where } x_0, x_1, \ldots \text{ are Bessel's zeroes.}$$

$$= \sum_{i=0}^{11}\int_{x_i}^{x_{i+1}} f(y)\,dy + \int_{x_{12}}^{\infty} f(y)\,dy$$

$$= \sum_{i=0}^{7}\int_{x_i}^{x_{i+1}} f(y)\,dy + \left[\sum_{i=8}^{11}\int_{x_i}^{x_{i+1}} f(y)\,dy + \cdots\right]$$

= Sum of initial 8-blocks + Euler's transform.

Now integral in the above equation

$\int_{x_i}^{x_{i+1}} f(y)\,dy = \int_a^b f(y)\,dy$ is evaluated by Gaussian integration.

Let $x = \frac{y-a}{b-a} \quad \Rightarrow y = x(b-a)+a$ and $dy = (b-a)\,dx$

$$\Rightarrow \int_{x_i}^{x_{i+1}} f(y)\,dy = \int_0^1 f(x)\,dx = \sum_{i=1}^{8} f(x_i)w_i ,$$

where $x_i \rightarrow$ Gaussian points,

$w_i \rightarrow$ Weight factor.

$$f(x) = \frac{(b-a)}{\Delta^2}[x(b-a)+a]J_0(x(b-a)+a)\left[\sum_i \gamma_i K_0(\lambda_i\frac{x(b-a)+a}{\Delta})\right]^3 \qquad (2.3.21)$$

Program discription :

Energy 35 KeV; k in Hartree a.u.

Potential : DHFS;

Method : EBS

Program : He13.c

Calculation : $f_{EBS} = f_E + \mathrm{Re}\,\overline{f}_{B2}$

EBS given by equation (2.3.15) is evaluated for the He atom target. Where Euler's transform has an important roll.

Program structure :

Header file for calculation of J_0, K_0.

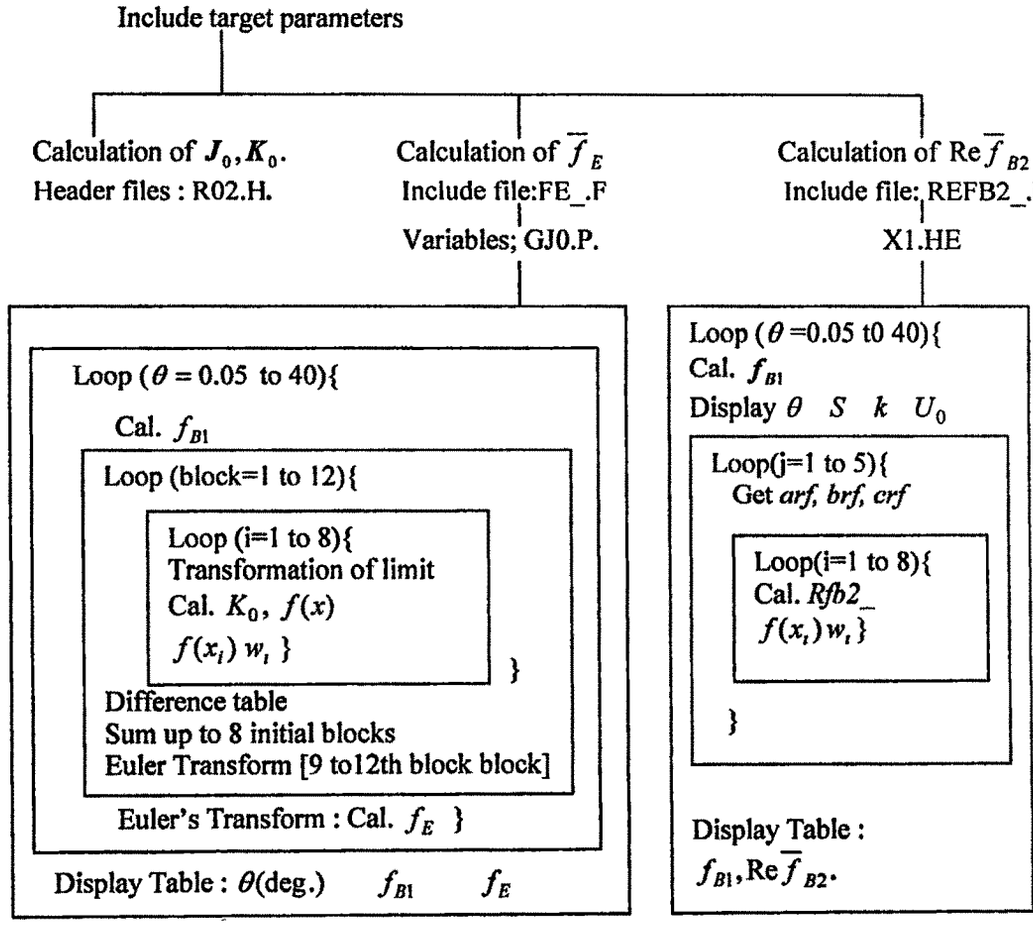
Global declaration of variables & array.

Include files for different function programs.

Function *main() {*

Declaration of variables

Include target parameters



Calculation of f_{EBS}

Display Table :

θ, f_{B1}, $\mathrm{Re}\overline{f}_{B2}$, f_E, f_{EBS}, *DCS (a.u.)*

} End of *main ()*.

Program : He13.c

```
/* EBS Method :  fE  +  RefB2_ ,DCS for He DHFS potential
   35 KeV   k in Hartree A.U.                          he13.c */

/* Calculation   of   fEBS = fE  +   RefB2_  */

#define PI 3.142
#define Ao .529
#include <math.h>
#include "r01.h"

/* Globle declaration of array & variables */
int i,j;
static float       iv =.1,            ic =.1/2;
static float SAo=0,lp1=.0595636,lp2=1,lp3=.0595636/2; /*theta */
float  h,t;
double k,del,d1,d2;
double r,bt,v,l0,ar,u0,z;
static double l[20],a1[10],b1[10];
double x0,w0,x[10],w[10];
static double fb1[50],rfb2_[50],rfe[50],ife[50],fe[50];

/* Different function programs are included  */
#include "fe.f "
#include "Refb2_.f"

main(){

/* Declaretion of variables */
double ifEBS[50],rfEBS[50],fEBS[50];
clrscr();

/* Input data  */
z=2.0;                      /*  He Atom      */
u0=2* z;
k=sqrt(2* 35000/(2* 13.6));/*  Hartree A.U. */
for(i=0;i<=10;++i)a1[i]=b1[i]=0;
#include "pmt.He"

/* Calculation of fE  for  SAo .1  to  1    */

Fe();
```

```
/* Calculation of RefB2_ for SAo .1 to  1   */

Refb2_();

/*  Out put Table heading  */
printf("\nS(Ao-1)  fb1(Ao)    ReFB2_ (Ao)  Fe(Ao)    RefEBS(Ao)
ImfEBS(Ao)  DCS(Ao^2)");
printf("\n_____________________________________________________\n\n");

/*  Calculation  of  fEBS    */

SAo=(float)0;i=1;
for(t=lp1;SAo<lp2;t +=lp3,++i){h=t;
    h=h* PI/180;
    del=2* k* sin(h/2);SAo=del* 96.18/50.73;
    rfEBS[i]=rfb2_[i]+rfe[i];
    ifEBS[i]=ife[i];
     fEBS[i]=sqrt(pow(rfEBS[i],2)+pow(ifEBS[i],2));
    printf("%.2f  %.4f   %e  %.4f  %.4e  %.4f  %.4f \n",SAo,
    fb1[i]* Ao,rfb2_[i]* Ao,fe[i]* Ao,rfEBS[i]* Ao,ifEBS[i]* Ao,
                                  (float)pow(fEBS[i]* Ao,2.0));
}
getch();
}□

/* Calculation of eikonal amplitude fe.f  */

void Fe()
{
int i0,i1,j0,j1,n,b0,c0,c1,c2,c3;
double f,a,b,m,y;
double fi,s0,s0i,s,si,k0;
double s1,s1i,s2,s2i,t0,t0i,t1,t1i,p;
double f0[20][20],f0i[20][20];

#include "GJ0.P"
i0=1;i=0;
for(t=lp1;SAo<lp2;t +=lp3,++i0){h=t;
    h=h* PI/180;
    del=2* k* sin(h/2);d1=del;d2=d1* d1;
    SAo=del* 96.18/50.73;
    f=(double)0;                                    /* First Born */
    fb1[i0]=(double)0;
    for(i=1;i<=2;++i)
    f=f+a1[i]/(b1[i]* b1[i]+d2);f=u0* f;fb1[i0]=f;
    printf("\n\n@ = %.4f  SAo = %.2f k = %.2f u0 = %.2f",(float)t
                                                ,SAo,(float)k,u0);
    printf("\nfb1  = %.4f (a.u.) ",fb1[i0]);

    b0=11;
    for(j=0;j<=b0;++j){
     a=l[j];b=l[j+1];
     m=b-a;
     s0=s0i=(double)0;
     for(i=1;i<=8;++i){
```

```
        x0=x[i];w0=w[i];
         y=x0* (b-a)+a;                /* Transformation */
        k0= a1[1]* K0(b1[1]* y/d1)+a1[2]* K0(b1[2]* y/d1);
        f = m* y* J0(y)* sin((u0* k0)/k);f =k* f/d2;
        fi=m* y* J0(y)* (cos((u0* k0)/k)-1);fi=k* fi/d2;
        s0 = s0+f* w0;
        s0i= s0i+fi* w0;}
    if(s0<0)s0=-s0;f0[j][0]=s0;
    if(s0i<0)s0i=-s0i;f0i[j][0]=s0i;}          /* 0th column */

    n=8;c0=b0-n;
    for(j=1;j<=c0;++j)                        /* Initialization */
    for(i=0;i<=b0;++i) f0[i][j]=f0i[i][j]=(double)0;
    for(i=n;i<=b0-1;++i){
        f0[i][1]=f0[i+1][0]-f0[i][0];     /* 1st column */
        f0i[i][1]=f0i[i+1][0]-f0i[i][0];}
    for(j=1;j<=c0;++j){ c1=b0-j-1;        /* 2nd & 3rd column */
      for(i=n;i<=c1;++i){f0[i][j+1]=f0[i+1][j]-f0[i][j];
                  f0i[i][j+1]=f0i[i+1][j]-f0i[i][j];}}

    s1=s1i=(double)0; /* addition of initial blocks */
    for(i=0;i<n;++i) {p=pow(-1,i);s1 =s1+p* f0[i][0];
                                  s1i=s1i+p* f0i[i][0];}

/*  Euler transform to remaining series  */
    s2=s2i=(double)0;c3=b0-n;
    for(j=0;j<=c3;++j) { p=pow(-1,j);
      t0 =f0[n][j]/pow(2,j+1); t1 =p* t0;
      t0i=f0i[n][j]/pow(2,j+1);t1i=p* t0i;
      s2 =s2+t1;
      s2i=s2i+t1i;
        }
rfe[i0]=(s1+s2);ife[i0]=(s1i+s2i);fe[i0]=sqrt(pow(rfe[i0],2)
                                          +pow(ife[i0],2));
 printf("\a\nRefE = %7.4e ImfE = %7.4e \nfE = %7.4e",rfe[i0],
                                           ife[i0],fe[i0]);
}
/* Table  */
  printf("\n\nS(Ao-1)  fb1      Fe        ");
  printf("\n_____________________________\n\n");

  for(i=1,t=iv;t<=lp2;++i,t+=ic)
  printf("%1.2f  %7.4f  %e \n",(float)t,fb1[i],fe[i]);

getch();
}
```

/* Calculation of real part of 2nd Born term RefB2_.f */

```
void Refb2_()
{
int i0;
float ar1,br1;
static float arf[20],brf[20],crf[20];
double x1,w1,r0,r1,r2,f,s,S;
#include "x1.He"

i0=1;SAo=(float)0;
for(t=lp1;SAo<lp2;t +=lp3,++i0){h=t;
    h=h* PI/180;
    del=2* k* sin(h/2);d1=del;d2=d1* d1;
    SAo=del* 96.18/50.73;
    f=(double)0;                                    /* First Born */
    fb1[i0]=(double)0;
    for(i=1;i<=2;++i)
    f=f+a1[i]/(b1[i]* b1[i]+d2);f=u0* f;fb1[i0]=f;
    printf("\n\n@ = %.4f  SAo = %.2f k = %.2f u0 = %.2f ",
                                    (float)t,SAo,(float)k,u0);
    printf("\nfb1   = %.4f (a.u.) ",fb1[i0]);
    S=(double)0;
    for(j=1;j<=4;++j){ ar1=arf[j];br1=brf[j];
      s=(double)0;
      for(i=1;i<=8;++i){
         x1=x[i];w1=w[i];
         r0=ar1* ar1* x1+(br1* br1* (1-x1));
         r2=r0+(x1* (1-x1)* del* del);
         r1=sqrt(r2);
          f=r0/(r1* (r0* r0+4* k* k* r2));
          s=s+w1* f;}
      S=S+s* u0* u0* crf[j]/2;
        } rfb2_[i0]=S;
    printf("\a\nRFB2_ = %7.4e ",rfb2_[i0]);
   }
/*  Table  */
  printf("\n\nS      fb1      ReFB2_         ");
  printf("\n_____________________________\n\n");

  for(i=1,t=iv;t<=lp2;++i,t+=ic)
  printf("%1.2f  %7.4f  %e \n",(float)t,fb1[i],rfb2_[i]);

getch();
}
□
```

```
/* Gaussian points for integration GJ0.p */


x[1]=.0198550718;  w[1]=.0506142681;
x[2]=.1016667613;  w[2]=.1111905172;
x[3]=.2372337950;  w[3]=.1568533229;
x[4]=.4082826788;  w[4]=.1813418917;
x[5]=.5917173212;  w[5]=.1813418917;
x[6]=.7627662050;  w[6]=.1568533229;
x[7]=.8983332387;  w[7]=.1111905172;
x[8]=.9801449282;  w[8]=.0506142681;

/* Bessel's zeroes for integration limits */

l[0]=0.000000000;l[1]=2.4048255577;
l[2]=5.5200781103;l[3]=8.6537279129;
l[4]=11.7915344391;l[5]=14.9309177086;
l[6]=18.0710639679;l[7]=21.2116366299;
l[8]=24.3524715308;l[9]=27.4934791320;
l[10]=30.6346064684;l[11]=33.7758202136;
l[12]=36.917098353;l[13]=40.0584257646;
l[14]=43.1997917132;l[15]=46.3411883717;
l[16]=49.482609897;l[17]=52.6240518411;
l[18]=55.7655107550;l[19]=58.9069839261;
l[20]=62.0484691902;

/* Parameters for the target pmt.He */

a1[1]=-.2259;a1[2]=1.2259;
b1[1]=5.5272;b1[2]=2.3992;

/* Parameters to calculate refB2_ x1.He */


arf[1]=b1[1];brf[1]=b1[1];arf[3]=b1[2];brf[3]=b1[1];
arf[2]=b1[1];brf[2]=b1[2];arf[4]=b1[2];brf[4]=b1[2];

crf[1]=a1[1]* a1[1];      crf[3]=a1[2]* a1[1];
crf[2]=a1[1]* a1[2];      crf[4]=a1[2]* a1[2];

```

2.4 WALLACE CORRECTION :

Eikonal amplitude is effectively corrected by real part of the second Born term as discussed in section 2.3. Another way of obtaining improvement over eikonal amplitude in potential scattering has been proposed by Wallace[47]. The potential experienced by the incident particle depend on the coordinate $\underline{r}$ of the target particles and the phase shift of projectile wave is the sum of phase shifts from interaction of each target particles. Wallace used a technique introduced by Aberbanel and Itzkson [48] to obtain the leading correction to the eikonal amplitude. He has incorporated the trajectory correction in the expansion of the Green's function of the eikonal approximation by considering velocity of incident particle v by $|k|/m = v\cos\theta/2$ and carried out further analysis of the perturbation series. The Wallace improved eikonal amplitude containing leading correction for a central potential is given by [35,34]

$$f_W = \frac{k}{i}\int_0^\infty db\, b\, J_0(\Delta b) \times \left\{ \exp[i(\frac{\chi_0(b)}{k} + \frac{\chi_1(b)}{k^3})] - 1 \right\} \tag{2.4.1}$$

where $\chi_0(b) = -\frac{1}{2}\int_{-\infty}^{\infty} U(b,z)\,dz$; $U(r) = \frac{2m}{\hbar^2}V(r)$, (2.4.2)

$$\chi_1(b) = -\frac{1}{4}\int_{-\infty}^{\infty} U(r)\left[U(r) + r\frac{d}{dr}U(r)\right]dz$$

$$= -\frac{1}{4}\int_{-\infty}^{\infty} U^2(r)dz - \frac{1}{4}\int_{-\infty}^{\infty} U(r) r \frac{dU(r)}{dr} dz \tag{2.4.3}$$

Now

$$f_W = \frac{k}{i}\int_0^\infty db\, b\, J_0(\Delta b)\left[Cos\{\frac{\chi_0(b)}{k} + \frac{\chi_1(b)}{k^3}\} - 1 + i\, Sin\{\frac{\chi_0(b)}{k} + \frac{\chi_1(b)}{k^3}\} \right]$$

$$\therefore \mathrm{Re}\, f_W = k\int_0^\infty db\, b\, J_0(\Delta b)\, Sin(\chi_W) \quad \text{and}$$

$$\mathrm{Im}\, f_W = k\int_0^\infty db\, b\, J_0(\Delta b)\left[Cos(\chi_W) - 1\right], \text{ where } \chi_W = \frac{\chi_0(b)}{k} + \frac{\chi_1(b)}{k^3}. \tag{2.4.4}$$

excluding minus sign in the last integral.

Let us consider the case of Yukawa potential of the form $U(r) = -U_0\frac{e^{-\lambda r}}{r}$;

$\therefore \chi_0(b) = U_0 K_0(\lambda b)$ and $\chi_1(b) = \frac{1}{2} U_0^2 K_0(2\lambda b)$;

where K_0 is the modified Bessel function of zero order.

For superposition of Yukawa potential : $U(r) = -\frac{U_0}{r}\sum_{i=1}^{2}\gamma_i e^{-\lambda_i r}$

$$\chi_0(b) = \frac{U_0}{2}\sum_i \gamma_i \int_{-\infty}^{\infty} \frac{e^{-\lambda_i r}}{r} dz$$

Now $\int_{-\infty}^{\infty} \frac{e^{-\lambda_i r}}{r} dz$; $r^2 = b^2 + z^2 \Rightarrow \frac{r\,dr}{z} = dz$.

$$= 2\int_b^{\infty} \frac{e^{-\lambda_i r}}{r}\frac{r\,dr}{z} = 2\int_b^{\infty} \frac{e^{-\lambda_i r}\,dr}{\sqrt{r^2 - b^2}} = 2K_0\{b\lambda_i\}$$

$$\therefore \chi_0(b) = \frac{U_0}{2}\sum_i \gamma_i [2K_0(b\lambda_i)] = U_0 \sum_i \gamma_i K_0(b\lambda_i) \qquad (2.4.5)$$

Now $U^2(r) = U_0^2[\gamma_1 \frac{e^{-\lambda_1 r}}{r} + \gamma_2 \frac{e^{-\lambda_2 r}}{r}]^2 = \frac{U_0^2}{r^2}\sum_{i,j=1}^{2'} \gamma_i \gamma_j e^{-(\lambda_i + \lambda_j) r}$ and

$$U(r) = -U_0 \sum_{i=1}^{2} \gamma_i \frac{e^{-\lambda_i r}}{r} \quad \Rightarrow \quad \frac{dU}{dr} = -U_0 \sum_{i=1}^{2} \gamma_i [-\frac{e^{-\lambda_i r}}{r^2} - \lambda_i \frac{e^{-\lambda_i r}}{r}]$$

$$\Rightarrow r\frac{dU}{dr} = U_0 \sum_{i=1}^{2} \gamma_i \frac{e^{-\lambda_i r}}{r} + U_0 \sum_{j=1}^{2} \gamma_i \lambda_i e^{-\lambda_i r}$$

$$\Rightarrow U r \frac{dU}{dr} = -U_0^2 \sum_{i,j} \gamma_j \gamma_i \frac{e^{-(\lambda_i + \lambda_j) r}}{r^2} - U_0^2 \sum_{i,j} \gamma_j \gamma_i \lambda_i \frac{e^{-(\lambda_i + \lambda_j) r}}{r}$$

$$\Rightarrow U^2 + Ur\frac{dU}{dr} = -U_0^2 \sum_{i,j} \gamma_j \gamma_i \lambda_i \frac{e^{-(\lambda_i + \lambda_j) r}}{r}$$

$$\Rightarrow \chi_1(b) = \frac{U_0^2}{4}\sum_{i,j} \gamma_j \gamma_i \lambda_i \int_{-\infty}^{\infty} \frac{e^{-(\lambda_i + \lambda_j) r}}{r} dz$$

$$= \frac{U_0^2}{4}\sum_{i,j} \gamma_j \gamma_i \lambda_i \, [2K_0\{b(\lambda_i + \lambda_j)\}]$$

$$= \frac{U_0^2}{2}\sum_{i,j} \gamma_i \gamma_j \lambda_j \, K_0\{b(\lambda_i + \lambda_j)\} \qquad (2.4.6)$$

Thus Wallace corrected eikonal phase is

$$\chi_W = \frac{U_0}{k}\sum_i \gamma_0 K_0(\lambda_i b) + \frac{U_0^2}{2k^3}\sum_{i,j}\gamma_i \gamma_j \lambda_j \; K_0\{(\lambda_i + \lambda_j)b\}\,. \tag{2.4.7}$$

We rewrite equation (2.3.7) and (2.3.14) as

$$f_{EBS} = f_W + \mathrm{Re}\,\overline{f}_{B2},$$

$$f_W = \left| \mathrm{Re}\, f_W^2 + \mathrm{Im}\, f_W^2 \right|^{1/2} \tag{2.4.8}$$

The differential cross-section is obtained from (2.2.14) and (2.4.4)

$$\frac{d\sigma}{d\Omega} = |f_{EBS}|^2 = \left|\mathrm{Re}\, f_W + \mathrm{Re}\,\overline{f}_{B2}\right|^2 + \left|\mathrm{Im}\, f_W\right|^2. \tag{2.4.9}$$

Equations in (2.4.4) are evaluated numerically by taking care for Bessel's zeroes and using the Euler's transform as in previous section.

Program : fw1.f

The function program evaluates Wallace amplitude through block wise integration.

/* calculation of Wallace amplitude */

```
void Fw1()
{
int i0,i1,j0,j1,n,b0,c0,c1,c2,c3;
double f,a,b,m,y,k1,xy;
double fi,s0,s0i,s,si,k0;
double s1,s1i,s2,s2i,t0,t0i,t1,t1i,p;
double f0[20][20],f0i[20][20];

#include "GJ0.P"
i0=1;i=0;
for(t=lp1;SAo<lp2;t +=lp3,++i0){h=t;
   h=h* PI/180;
    del=2* k* sin(h/2);d1=del;d2=d1* d1;
    SAo=del* 96.18/50.73;
    f=(double)0;                                    /* First Born */
    fb1[i0]=(double)0;
    for(i=1;i<=2;++i)
    f=f+a1[i]/(b1[i]* b1[i]+d2);f=u0* f;fb1[i0]=f;
    printf("\n\n@ = %.4f  SAo = %.2f k = %.2f u0 = %.2f ",
                                        (float)t,SAo,(float)k,u0);
    printf("\nfb1  = %.4f (a.u.) ",fb1[i0]);

    b0=11;
    for(j=0;j<=b0;++j){
     a=l[j];b=l[j+1];
     m=b-a;
     s0=s0i=(double)0;
     for(i=1;i<=8;++i){
         x0=x[i];w0=w[i];
          y=x0* (b-a)+a;              /* Transformation */
```

```
          k0= a1[1]* K0(b1[1]* y/d1)+a1[2]* K0(b1[2]* y/d1);
          k1=(double)0;
          for(i1=1;i1<3;++i1)
           for(j1=1;j1<3;++j1){
            s =a1[i1]* a1[j1]* b1[j1]* K0((b1[i1]+b1[j1])* y/d1);
            k1=k1+s;}

          xy=(u0* k0/k)+(u0* u0* k1/(2* k* k* k));

          f =m* y* J0(y)* sin(xy);f =k* f/d2;
          fi=m* y* J0(y)* (cos(xy)-1);fi=k* fi/d2;
          s0 = s0+f* w0;
          s0i= s0i+fi* w0;
         }
      if(s0<0)s0=-s0;f0[j][0]=s0;
      if(s0i<0)s0i=-s0i;f0i[j][0]=s0i;}          /* 0th column */

    n=8;c0=b0-n;
    for(j=1;j<=c0;++j)
      for(i=0;i<=b0;++i) f0[i][j]=f0i[i][j]=(double)0;
for(i=n;i<=b0-1;++i){f0[i][1]=f0[i+1][0]-f0[i][0];/*1st column */
                     f0i[i][1]=f0i[i+1][0]-f0i[i][0];}
for(j=1;j<=c0;++j){ c1=b0-j-1;                /* 2nd,3rd column */
      for(i=n;i<=c1;++i){f0[i][j+1]=f0[i+1][j]-f0[i][j];
                   f0i[i][j+1]=f0i[i+1][j]-f0i[i][j];}
}
    s1=s1i=(double)0;
    for(i=0;i<n;++i) {p=pow(-1,i);s1 =s1+p* f0[i][0];
                        s1i=s1i+p* f0i[i][0];}
/*  Euler transform to remaining series  */
    s2=s2i=(double)0;c3=b0-n;
    for(j=0;j<=c3;++j) { p=pow(-1,j);
      t0 =f0[n][j]/pow(2,j+1); t1 =p* t0;
      t0i=f0i[n][j]/pow(2,j+1);t1i=p* t0i;
      s2 =s2+t1;
      s2i=s2i+t1i; }
 rfe[i0]=(s1+s2);ife[i0]=(s1i+s2i);fe[i0]=sqrt(pow(rfe[i0],2)
                                              +pow(ife[i0],2));
 printf("\a\nRefE = %7.4e ImfE = %7.4e \nfE = %7.4e",rfe[i0],
                                               ife[i0],fe[i0]);
}
/* Table  */
  printf("\n\nS(Ao-1)  fb1      Fw1       ");
  printf("\n_____________________________\n\n");
  for(i=1,t=iv;t<=lp2;++i,t+=ic)
  printf("%1.2f  %7.4f  %e \n",(float)t,fb1[i],fe[i]);
getch();
}
```

2.5 DAS METHOD :

To obtain reliable scattering amplitude higher order Born terms described by equation (2.3.1) should be involved in the scattering amplitude. The evaluation of higher order more than 2nd is very difficult. J.N.Das has suggested a simpler method to include higher order Born terms in the scattering amplitude in which the second Born term is multiplied by variationally determined complex number to compensate for the missing higher order Born terms [27]. In this method first the Born series is represented by Fredholm integral equation (1.5.2) than the equation is evaluated by iteration method for elastic scattering (1.5.3). To solve this equation trial input function for the scattering amplitude is used. The input scattering function is considered as

$$f^{(in)}(q,k_i) = (a^D + i\,b^D)\,f_{B1}(q,k_i), \tag{2.5.1}$$

where a^D and b^D are energy dependent variational parameters, which are coming through the asymptotic form of the scattering amplitude given in (1.5.3) and satisfy the limiting conditions (1.5.4). With this choice of input trial function Das obtained output scattering amplitude as

$$f^{(out)} = f_D = f_{B1} + (a^D + i\,b^D)\,\overline{f}_{B2}. \tag{2.5.2}$$

Denoting real and imaginary parts of $\overline{f}_{B2}$ by $\overline{f}_{B2R}$ and $\overline{f}_{B2I}$, respectively the above equation reads

$$\begin{aligned} f_D &= f_{B1} + (a^D + i\,b^D)(\overline{f}_{B2R} + \overline{f}_{B2I}) \\ &= f_{B1} + (a^D\overline{f}_{B2R} - b^D\overline{f}_{B2I}) + i\,(a^D\overline{f}_{B2I} + b^D\overline{f}_{B2R}) \end{aligned} \tag{2.5.3}$$

The parameters a^D and b^D are independent of the scattering angle, obtained by minimizing the norm $|f^{(out)} - f^{(in)}|^2$ integrated over the whole angular region of the scattering angle with respect to a^D and b^D. The calculation with equation (2.5.1) and (2.5.2) yields equation

$$a_D = \frac{\int d\theta\, Sin\theta\; f_{B1}(f_{B1} - \overline{f}_{B2R})}{\int d\theta\, Sin\theta\; [(f_{B1} - \overline{f}_{B2R})^2 + \overline{f}^2_{B2I}]} \tag{2.5.4}$$

$$b_D = \frac{\int d\theta\, Sin\theta\, f_{B1}\overline{f}_{B2I}}{\int d\theta\, Sin\theta\; [(f_{B1} - \overline{f}_{B2R})^2 + \overline{f}^2_{B2I}]} \tag{2.5.5}$$

The analysis carried out by Byron and Joachain [36] show that at large energies a^D increases with energy and go to its asymptotic value of unity. On the other end at large energies b^D decreases with energy and it varies between $\ln k_i / k_i$ and $1/k_i$. Thus in this method higher order Born terms are included in the scattering amplitude by multiplying second order Born term with complex parameter.

Calculation of a^D, b^D:

Denote integral of equation (2.5.4) in numerator as

$$I_1 = \int d\theta \, Sin\theta \; f_{B1}(f_{B1} - \overline{f}_{B2R})$$

$$= \int_0^{\pi} f_{B1}(f_{B1} - \overline{f}_{B2R}) Sin\theta \; d\theta$$

Now consider half angle formula and change the variable of the integral as

$$Sin\theta = 2Sin\theta/2 Cos\theta/2$$

Let $t = Sin\theta/2 \quad \Rightarrow d\theta = 2dt/Cos(\theta/2)$,

$$Sin\theta = 2tCos\theta/2 \text{ and } q = 2kSin\theta/2 = 2kt$$

$$\therefore I_1 = 4\int_0^1 f_{B1}(f_{B1} - \overline{f}_{B2R})\, t\, dt. \qquad (2.5.6)$$

Similarly,

$$I_2 = \int d\theta \, Sin\theta \; [(f_{B1} - \overline{f}_{B2R})^2 + \overline{f}^2_{B2I}]$$

$$= 4\int_0^1 [(f_{B1} - \overline{f}_{B2R})^2 + \overline{f}^2_{B2I}]\, dt \qquad \text{and (2.5.7)}$$

$$I_3 = \int d\theta \, Sin\theta \, f_{B1} \overline{f}_{B2I}$$

$$= 4\int_0^1 f_{B1} \overline{f}_{B2I} \, dt. \quad (2.5.8)$$

These integrals are evaluated numerically by Gaussian integration.

Finally we have

$$a^D = \frac{I_1}{I_2} \; ; \; b^D = \frac{I_3}{I_2} \qquad (2.5.9)$$

2.6 Modified Das Method :

The Das technique was improved further by including the second Born term in the input trial function [28] as

$$f^{(in)} = (a_p + ib_p)(f_{B1} + \bar{f}_{B2}) \tag{2.5.10}$$

Putting this in equation (1.5.3) and proceeding as before, the derivation of direct out put scattering amplitude is given by

$$f^{(out)} = f_{MD} = f_{B1} + (a_p + ib_p)(\bar{f}_{B2} + \bar{f}_{B3}), \tag{2.5.11}$$

where $a_p = \dfrac{f_{B1}}{(f_{B1} - \bar{f}_{B3R}) + \dfrac{\bar{f}^{\,2}_{B3I}}{f_{B1} - \bar{f}_{B3R}}}$.

According to the analysis of Byron and Joachain [36] at large energies a_p is independent of energy and converge to unity, whereas b_p varies with energy as k_i^{-3}. So the terms $\bar{f}_{B3I}$ and b_p which fall faster than k_i^{-2} asymptotically are neglected. Here we replace the $\bar{f}_{B3R}$ by the equivalent term $\bar{f}_{E3}$ due to equivalence of eikonal and Born series for large k. Thus f_{MD} correct up to the order k_i^{-2} is given by

$$f_{MD} = f_{B1} + a_p(\bar{f}_{B2R} + \bar{f}_{E3}) + ia_p\,\bar{f}_{B2I}, \tag{2.5.12}$$

and a_p reduces to

$$a_p = \frac{f_{B1}}{f_{B1} - \bar{f}_{B3R}}$$

$$\therefore\ a_p = \frac{f_{B1}}{f_{B1} - \bar{f}_{E3}} \tag{2.5.13}$$

Thus using better trail input scattering amplitude $f^{(in)}$ in the Das technique the obtained out put scattering amplitude $f^{(out)}$ contains Third order Born terms also and the higher order terms are included through the parameter a_p and b_p.

Program description :

Energy 35 KeV; k in Hartree a.u.

Potential : DHFS;

Method : Das

Program : He16.c

Calculation : $f^{(out)} = f_D = f_{B1} + (a^D + i\,b^D)\overline{f}_{B2}$

Das amplitude given by equation (2.5.2) is evaluated for the He atom target.

Program structure :

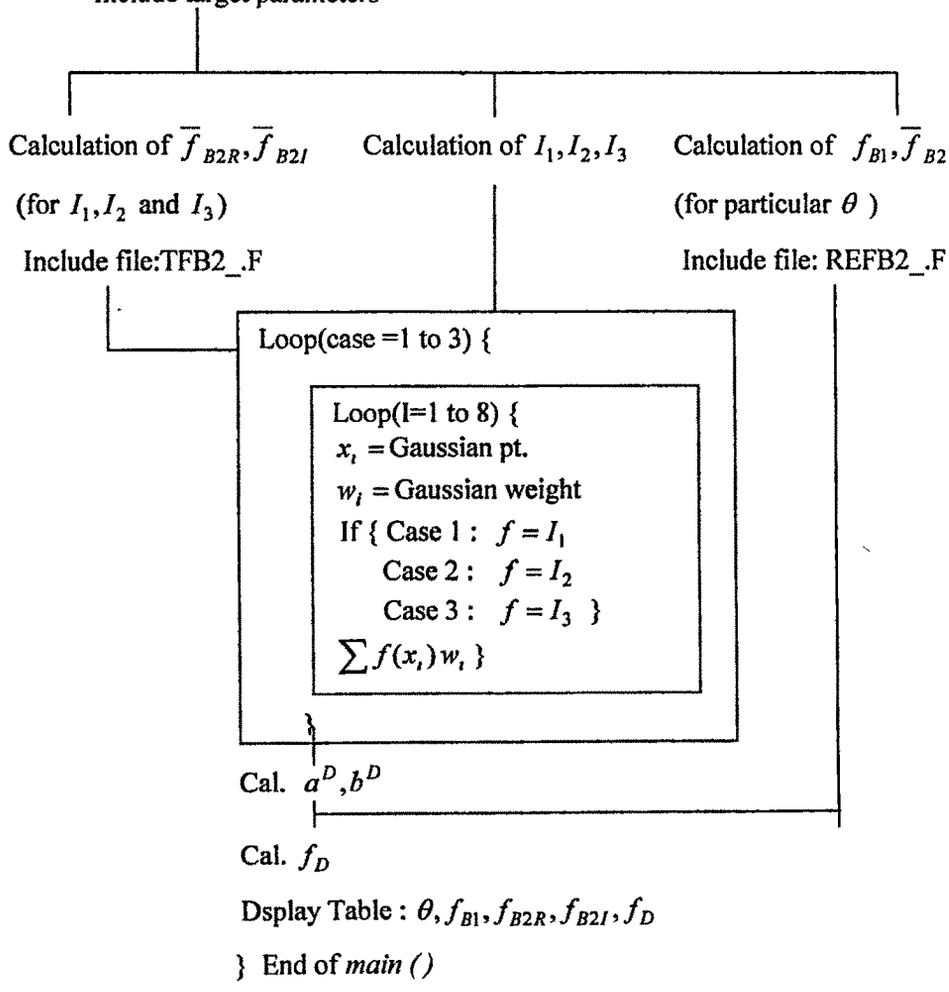
Global declaration of variables & array.

Include files for different function programs.

Function main( ) {

Declaration of variables

Include target parameters



```
/* Das Method :     aD,bD  by taking @ = 0  to  180
   35 Kev         @ = .059  to  .59          he16.c */

#define PI 3.142
#define Ao .529
#include <math.h>

/* Globle declaration of array & variables */
int i,j,i0;
static float       iv = .1,            ic = .1;/*Change theta*/
static float SAo=0,lp1=.0595636,lp2=1,lp3=.0595636;
float  h,t,th,ar1,br1;
double k,del,d1,d2,fb,u0,z;
static double a1[10],b1[10];
double x1,w1,x[10],w[10];
static float arf[20],brf[20],crf[20];
double r0,r1,r2,d2,f,fi,s,si,S,Si;
static double fb1[50],rfb2_[50],ifb2_[50];

/* Different function programms are included */
#include "tfb2_.f"
#include "thfb2_.f"

main()
{

/*  Declaretion of variables       */
int i,n;
static float SAo;
double f,S,I1,I2,I3,I[4];
double aD,bD,rfb2,fb2,fD[50],rfD[50],ifD[50],fd[50];
clrscr();

/* Input Data */
z=2.0;                          /* He  Atom    */
u0=2* z;
k=sqrt(2* 35000/(2* 13.6)); /* Hartree A.U. */
for(i=0;i<=10;++i)a1[i]=0;
#include "pmt.He"

/* Calculation of fB2_ for theta  0 to 180  */

tfb2_();

/* Calculation of Integrals I1,I2,I3 */
for(n=1;n<4;++n){
S=(double)0;
for(i=1;i<9;++i){ x1=x[i];w1=w[i];  /* use of switch st. */
    switch(n){
    case 1:f=x1* fb1[i]* (fb1[i]-rfb2_[i]);   /* I1 1st int. */
           break;                              /* I2 2nd int. */
    case 2:f=x1* (pow(fb1[i]-rfb2_[i],2)+pow(ifb2_[i],2));
           break;
    case 3:f=x1* fb1[i]* ifb2_[i];            /* I3 3rd int. */
   }S=S+f* w1;
```

```
  } I[n]=4* S; printf("\nI%d = %e",n,I[n]);
 }
/* Calculation of Das parameters aD, bD  */
aD=I[1]/I[2];bD=I[3]/I[2];
printf("\n\naD = %.3f bD = %.3f\n",aD,bD);

/* Calculation of  fb1, fb2_  for particular  @  */
thfb2_();

/* Out put Table heading  */
printf("\nS(Ao-1) fb1(Ao)    RfB2_(Ao)    IfB2_(Ao)    RefD(Ao)
ImfD(Ao)   DCS(Ao^2) \n");
printf("_____________________________________________\n\n");

/* Calculation of Das amplitude fD out   */

for(i=1,t=lp1;SAo<=lp2;t +=lp3,++i){
    del=2* k* sin((t* PI/180)/2);SAo=del* 96.18/50.73;
    rfb2=fb1[i]+rfb2_[i];
    fb2=sqrt(pow(fb1[i]+rfb2_[i],2)+ifb2_[i]* ifb2_[i]);
    rfD[i]=fb1[i]+aD* rfb2_[i]-bD* ifb2_[i];
    ifD[i]=aD* ifb2_[i]+bD* rfb2_[i];
    fd[i]=sqrt(rfD[i]* rfD[i]+ifD[i]* ifD[i]);

printf(" %1.1f %.4f  %7.4e  %7.4e  %.4f   %.5f   %.4f\n",
      SAo,(float)fb1[i]* Ao,rfb2_[i]* Ao,ifb2_[i]* Ao,
      rfD[i]* Ao,ifD[i]* Ao,pow(fd[i]* Ao,2));}
getch();
}
/* Calculation  of  fB2_ for aD, bD  tfb2_.f */
void tfb2_()
{
#include "x1.He"
#include "G.P"

for(i0=1;i0<9;++i0){t=x[i0];h=(float)t;
    k=50.73;
    del=2* k* h;
    fb=(double)0;
    for(i=1;a1[i]!=0;++i)fb=fb+(a1[i]/(b1[i]* b1[i]+del* del));
    fb=u0* fb;fb1[i0]=fb;
    S=Si=(double)0;
    for(j=1;j<5;++j){ ar1=arf[j];br1=brf[j];
     s=si=(double)0;
     for(i=1;i<=8;++i){
        x1=x[i];w1=w[i];
        r0=ar1* ar1* x1+(br1* br1* (1-x1));
        r2=r0+(x1* (1-x1)* del* del);
        r1=sqrt(r2);
         f=r0/(r1* (r0* r0+4* k* k* r2));
        fi=2* k/(r0* r0+4* k* k* r2);
        si=si+w1* fi;
         s=s +w1* f;}
     Si=Si+si* u0* u0* crf[j]/2;
     S =S + s* u0* u0* crf[j]/2;
```

```
        }
     printf("\a");ifb2_[i0]=Si;rfb2_[i0]=S;
    }
}□

/* Calculation of fB2  for  particular theta    */

void thfb2_()
{
int i0;
float ar1,br1;
static float arf[20],brf[20],crf[20];
double r0,r1,r2,f,fi,s,si,S,Si;

#include "x1.He"
i0=1;SAo=(float)0;
for(t=lp1;SAo<=lp2;t +=lp3,++i0){h=(float)t;

    h=h* PI/180;
    del=2* k* sin(h/2);SAo=del* 96.18/50.73;
    fb=(double)0;
    for(i=1;a1[i]!=0;++i)fb=fb+(a1[i]/(b1[i]* b1[i]+del* del));
    fb=u0* fb;fb1[i0]=fb;
    printf("\n@ = %.4f  SAo = %.2f k = %.2f u0 = %.2f ",
                                    (float)t,SAo,(float)k,u0);
    printf("\nfb1  = %.4f (a.u.) ",fb1[i0]);
    S=Si=(double)0;
    for(j=1;j<5;++j){ ar1=arf[j];br1=brf[j];
      s=si=(double)0;
      for(i=1;i<=8;++i){
         x1=x[i];w1=w[i];
         r0=ar1* ar1* x1+(br1* br1* (1-x1));
         r2=r0+(x1* (1-x1)* del* del);
         r1=sqrt(r2);
         f =r0/(r1* (r0* r0+4* k* k* r2));
         fi=2* k/(r0* r0+4* k* k* r2);
         si=si+w1* fi;
         s =s +w1* f ;}
      Si=Si+si* u0* u0* crf[j]/2;
      S=S+s* u0* u0* crf[j]/2;
        }
    ifb2_[i0]=Si;rfb2_[i0]=S;
     fb2_[i0]=sqrt(rfb2_[i0]* rfb2_[i0]+ifb2_[i0]* ifb2_[i0]);

    printf("\a\nRFb2_= %7.4e IFb2_ = %7.4e \n",rfb2_[i0],
                                                ifb2_[i0]);
  }
/*  Table                                  */
printf("\nS     fb1     rfb2_       ifb2_       Fb2_ ");
printf("\n_____________________________________________\n\n");
for(i=1,t=iv;t<=lp2+ic;++i,t+=ic)
printf("%.1f  %.4f  %7.5e  %7.5e  %7.5e \n",\
     (float)t,fb1[i],rfb2_[i],ifb2_[i],fb2_[i]);
getch();
}□
```

2.6 PARTIAL WAVE ANALYSIS :

Problem of particle scattered by central field plays a role in different branches of the physics. Fully analytical solutions are not known except coulomb field, so one has to rely on the approximations that in the most favorable cases are only valid in limited energy ranges. Thus partial wave analysis is the alternative solution for any energy rage, which gives most accurate results for the problem.

In the beginning work we have employed PWA for small k and phase shifts were obtained from radial solution of Schrodinger equation by Numerov method according to elementary description given in chapter one.

To calculate phase shift and differential cross sections in the present work for different atomic target and energies cross-sections we have used FORTRAN code PWADIR (Partial Wave Analysis, DIRac) [30]. The Method of solution of Dirac equation and program description is given here.

Elastic scattering of electrons by neutral atoms in a central field $V(r)$ such that $rV(r) \to 0$ when r goes to infinity. Where charge cloud polarization effects are neglected and local exchange potential is considered i.e.

$V(r) = -\phi(r) + V_{ex}(r)$;

$$\phi(r) = \frac{Z}{r}\sum_{i=1}^{N} A_i \exp(-\alpha_i r), \tag{2.6.1}$$

where $\sum A_i = 1$ for neutral atoms. Expression (2.6.1) if the form of superposition of Yukawa type potential and it is obtained from self-consistent calculations. The parameters (with N=3) are obtained by salvat et al [38] from Dirac-Hartree-Fock-Slater (DHFS) field. Considering scattering of electron in a central field $V(r)$ Dirac phase shifts are determined by solving the radial wave equations [44]

$$\frac{dR}{dr} = -\frac{K}{r}R - \frac{E - V(r) + 2c^2}{c}Q \quad \text{and}$$

$$\frac{dQ}{dr} = \frac{E - V(r)}{c}R + \frac{K}{r}Q, \tag{2.6.2}$$

where $K = (l - j)(2j + 1)$ is the relativistic angular momentum quantum number, j and l are total and orbital angular momentum quantum number respectively. $E + c^2$ is the total energy, c is the speed of light in the vacuum, $R(r)$ and $Q(r)$ are the radial functions. In

the numerical procedure $rV(r)$ is replaced by the natural cubic spline that interpolates the values of this function. The grid is dense enough to have minimum interpolation errors, which do not affect the computed phase shifts. The solution of the radial equation (2.6.2) is obtained by Buhring power series method [45]. The accuracy of the solution can be controlled by the input parameter $\in$. The Phase shifts are determined by matching the outward radial solutions to the free spherical waves, so that scattering field is assumed to vanish outside the matching radius.

Elastic scattering amplitude of relativistic electron scattered from the atom for central field is defined by [42]

$$f(\theta)=\frac{1}{2ik}\sum_{l=0}^{\infty}\{(l+1)[\exp(2i\delta_{l+})-1]+l[\exp(2i\delta_{l-})-1]\}P_l(Cos\theta),$$

$$g(\theta)=\frac{1}{2ik}\sum_{l=0}^{\infty}\{\exp(2i\delta_{l-})-\exp(2i\delta_{l+})\}P_l^1(Cos\theta). \qquad (2.6.3)$$

Where $|k_l|=k$ is the wave number of the incident electron and δ_{l+},δ_{l-} are the phase shift of order l. $P_l(Cos\theta)$ and $P_l^1(Cos\theta)$ are Legender and associated Legender polynomials respectively.

For high-energy the direct summation of the partial wave series given in above equation require large number of terms. In the code phase shift of order l less than a finite value NDELTA can be computed only. So the value of NDELTA given as input should be large enough to enable convergence of the partial wave series. It must be less than the dimension of the phase shift array [i.e. 2000]. The magnitude of truncation errors can be systematically reduced by using the "reduced" series method [57]. This method makes the Legender expansion rapidly convergent.

The outward numerical solution and asymptotic solution of radial function must join smoothly at some point r_∞ This requirement leads to the following value of phase shift [46],

$$\tan\delta=\frac{kj_l'(kr_\infty)-\beta j_l(kr_\infty)}{kn_l'(kr_\infty)-\beta n_l(kr_\infty)} \qquad (2.6.4)$$

with

$$\beta=\frac{R'(r_\infty)}{R(r_\infty)}-\frac{1}{r_\infty},$$

$$k = \left(\frac{E(E+2c^2)}{c^2} \right)^{1/2}.$$

j_l and n_l are the spherical Bessel and Neumann functions respectively.

For an unpolarized incident beam resultant scattering amplitude is

$$f_{num}(\theta) = [|f|^2 + |g|^2]^{1/2}. \qquad (2.6.5)$$

Generalized atomic units[$\hbar = e = m = 1$] are used in the calculations throughout.

The unit of length is for electron is the Bohr radius $a_0 = 5.29177 \times 10^{-11} m$.

The unit o energy ($me^4/\hbar^2$) is the Hartree energy $E_H = 27.2114\, eV$.

In put data *: ACJX.DAT*

92	ATOMIC NUMBER
-1	MUFFIN-TIN RADIUS (-VE FOR FREE ATOM)
-1	INCIDENT PARTICLE (-1 FOR ELECTRON)
1.0E-8	EPSILON (FOR ERROR CONTROL).
1000 1	NUMBER OF PHASE SHIFT (NDELTA), IWR
1	SCATTERING FIELD (1 FOR ANALYTICAL)
30.0000E+03	K.E. OF PROJECTILE.

□

2.8 *TABLES*

Table 2.1 E = 35 keV .

Differential cross-sections in atomic unit.

He-Atom			Ar-Atom	
θ (deg.)	W	MD	W	MD
0.20	0.753	0.669	65.607	62.262
0.30	0.688	0.659	63.004	60.283
0.40	0.662	0.647	60.196	58.249
0.50	0.641	0.631	57.350	55.996
0.60	0.619	0.612	54.504	53.505
0.70	0.597	0.592	51.593	50.805

W: DCS using the Wallace method (Eq. 2.4.9).

MD: DCS using the Modified Das method (Eq. 2.5.12).

Table 2.2 E = 35 keV .

Differential cross-sections in atomic unit.

Ne Atom		
θ (deg.)	W	MD
0.20	10.257	8.763
0.40	8.754	8.420
0.60	8.189	8.026
0.80	7.640	7.535
1.00	7.046	6.968
1.20	6.420	6.357
1.40	5.786	5.734
1.60	5.166	5.121
1.80	4.578	4.539
2.00	4.032	3.998

W: DCS using the Wallace method (Eq. 2.4.9).

MD : DCS using the Modified Das method (Eq.2.5.12)

Table– 2.3

Partial wave phase-shifts $|\delta_l|$ for Argon at 40 keV.

l	Born [a]	WKBJ [b]	numerical [c]
0	1.2899	1.3228	1.2861
1	0.9430	0.9550	0.9412
2	0.7739	0.7802	0.7691
3	0.6645	0.6678	0.6572
4	0.5849	0.5863	0.5760
5	0.5230	0.5232	0.5132
6	0.4728	0.4722	0.4628
7	0.4309	0.4298	0.4211
8	0.3952	0.3939	0.3860
9	0.3644	0.3629	0.3559
10	0.3375	0.3359	0.3297
11	0.3137	0.3120	0.3067
12	0.2927	0.2908	0.2864
13	0.2739	0.2718	0.2682
14	0.2571	0.2547	0.2518

Partial wave phase-shifts $|\delta_l|$ for Uranium at 40 KeV.

l	Born [b]	WKBJ [b]	numerical [c]
0	5.7234	5.2815	5.7356
1	3.9818	4.1405	4.1707
2	3.1518	3.3489	3.2971
3	2.6261	2.7915	2.7284
4	2.2514	2.3828	2.3287
5	1.9662	2.0704	2.0302
6	1.7399	1.8233	1.7966
7	1.5549	1.6224	1.6073
8	1.4004	1.4556	1.4500
9	1.2694	1.3149	1.3166
10	1.1567	1.1946	1.2017
11	1.0589	1.0906	1.1017
12	0.9733	1.0000	1.0137
13	0.8978	0.9204	0.9358
14	0.8307	0.8500	0.8663
16	0.7173	0.7314	0.7479
18	0.6252	0.6358	0.6512
20	0.5495	0.5574	0.5711

a,b HF and TFD potential respectively; Ref. 13.
c present work; using numerical integration, from Eq. 2.6.5

2.8 **Table – 2.4**

Scattering factor $f(\theta)$ for Argon-atom at 40 keV (a. u.).

	Method			
$\Delta(\text{Å}^{-1})$	numerical [a]	numerical [c]	EBS [c]	Wallace [f]
0	4.828	4.504	-	-
5.47	1.294	1.294	1.237	1.243
10.93	0.420	0.421	0.404	0.407
16.38	0.218	0.214	0.204	0.207
21.83	0.132	0.130	0.124	0.126
27.26	0.088	0.088	0.083	0.085
32.67	0.062	0.063	0.060	0.061
38.06	0.046	0.047	0.045	0.046
43.42	0.036	0.037	0.035	0.036
48.75	0.029	0.030	0.028	0.029
54.05	0.024	0.025	0.023	0.024

Scattering factor $f(\theta)$ for Uranium-atom at 40 keV (a. u.).

	Method			
$\Delta(\text{Å}^{-1})$	numerical [b]	numerical [c]	EBS [e]	Wallace [f]
0	12.534	16.071	-	-
5.47	3.101	3.142	3.127	3.112
10.93	1.145	1.181	1.127	1.131
16.30	0.613	0.632	0.557	0.570
21.83	0.393	0.403	0.282	0.263
27.26	0.278	0.282	0.119	0.125
32.67	0.209	0.210	0.118	0.139
38.06	0.164	0.162	0.130	0.148
43.42	0.133	0.130	0.128	0.138
48.75	0.109	0.106	0.117	0.120
54.05	0.091	0.089	0.102	0.101

a,b HF and TFD potential respectively; Ref. 13.
c present work; using numerical integration, from Eq. 2.6.5.
e,f present work; from Eq. 2.3.15 and 2.4.9 respectively.

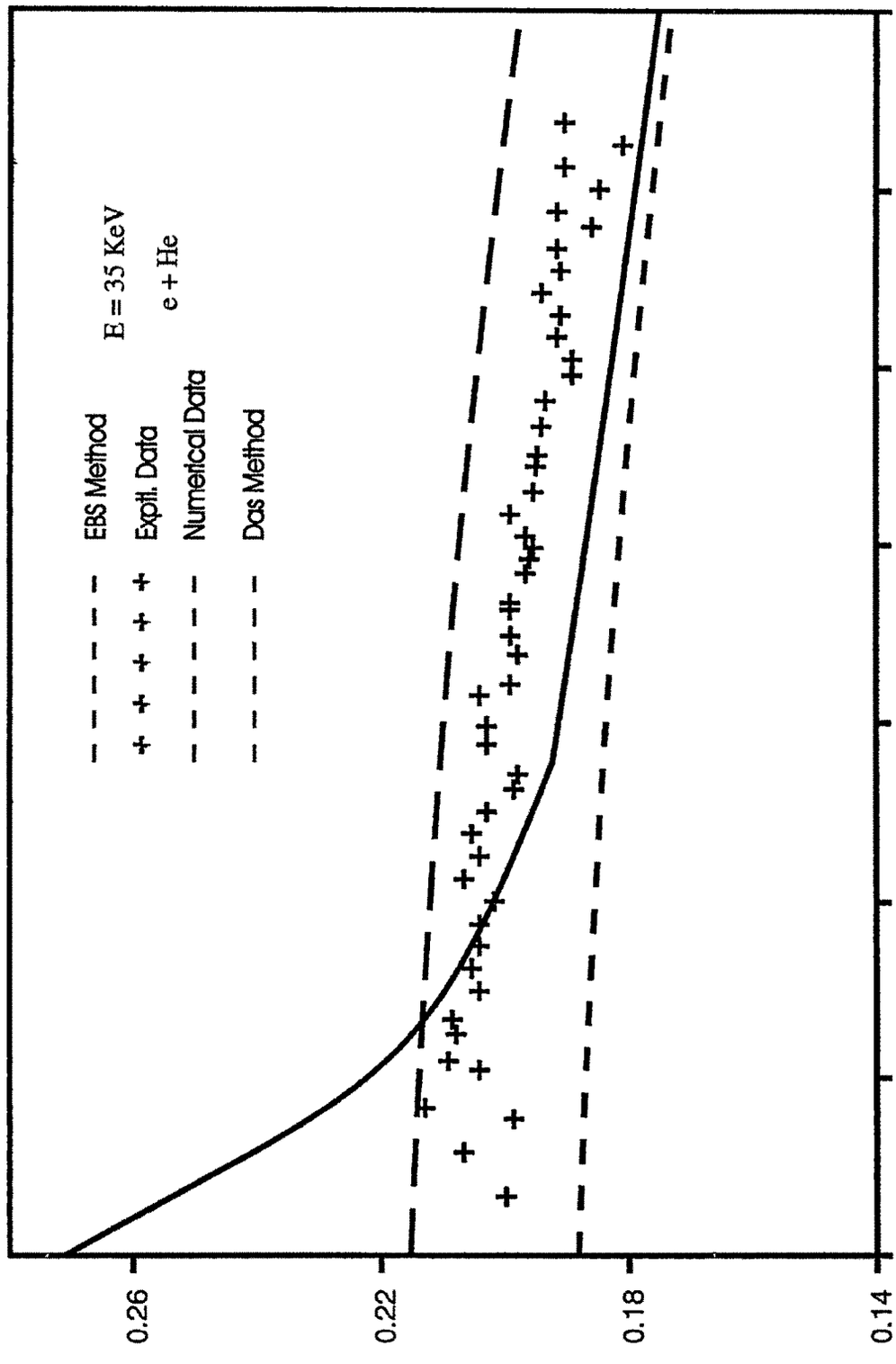

EBS Method
Expti. Data
Numerical Data
Das Method
E = 35 KeV
e + He
DIFF.CROSS SECTIONS (Å²)
S (Å⁻¹)
0.26
0.22
0.18
0.14
0.2
0.4
0.6
0.8

Fig. 2.1

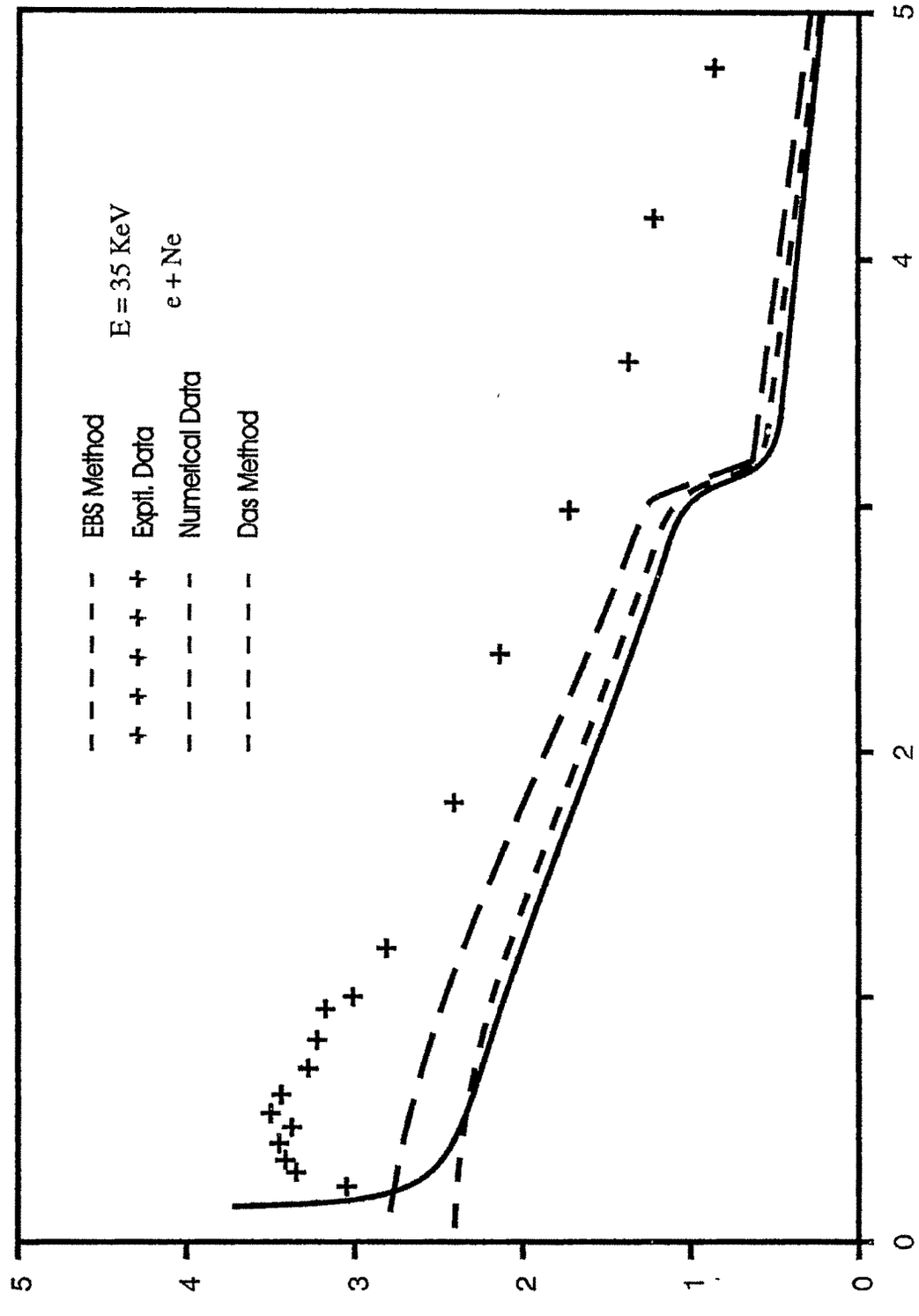

EBS Method
Expti. Data
Numerical Data
Das Method
E = 35 KeV
e + Ne
DIFF. CROSS SECTION (Å²)
S (Å⁻¹)
0
1
2
3
4
5

Fig. 2.2

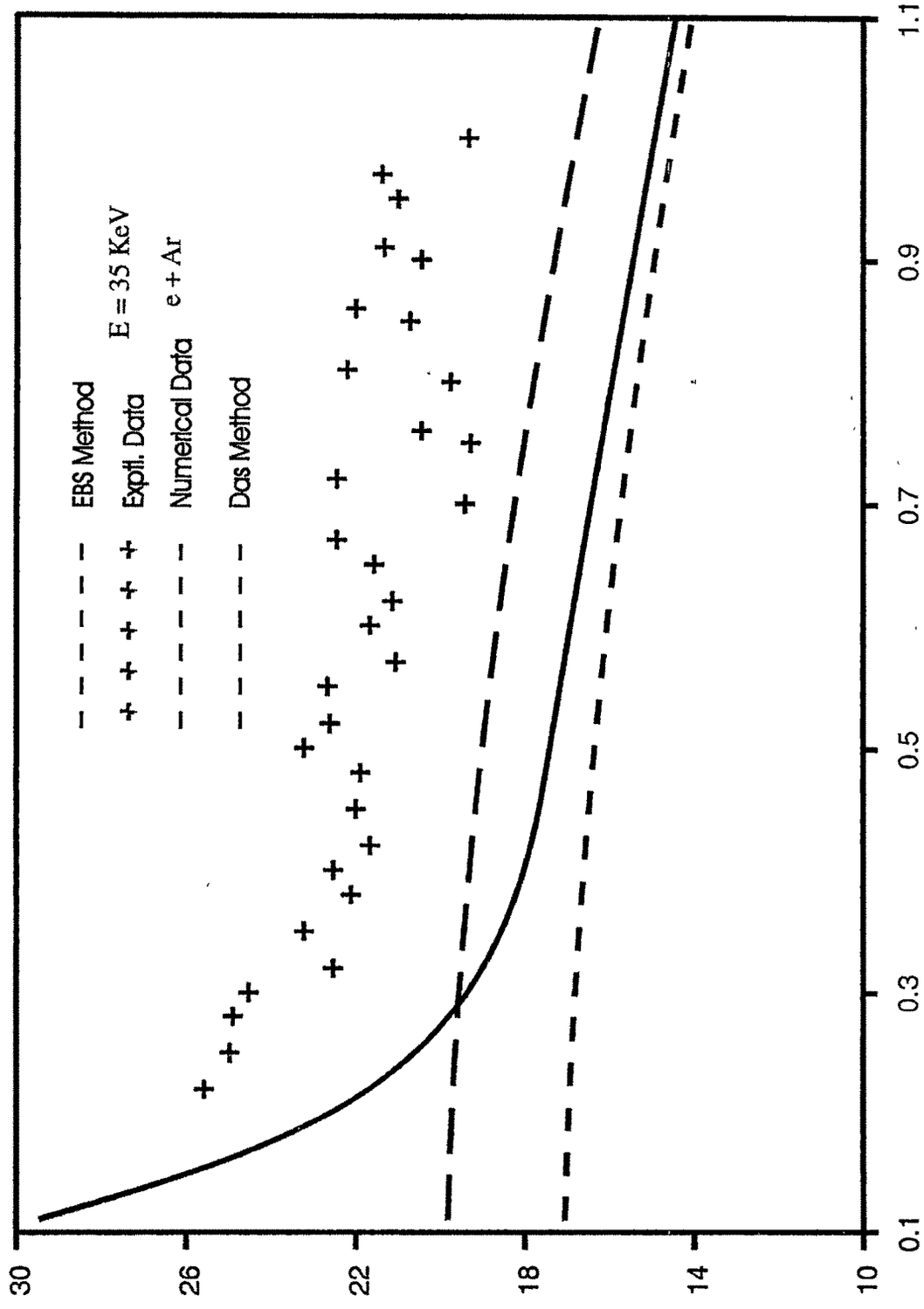

EBS Method
Expti. Data
E = 35 KeV
Numerical Data
e + Ar
Das Method
DIFF. CROSS SECTION (Å²)
S (Å⁻¹)
30
26
22
18
14
10
0.1
0.3
0.5
0.7
0.9
1.1

Fig. 2.3

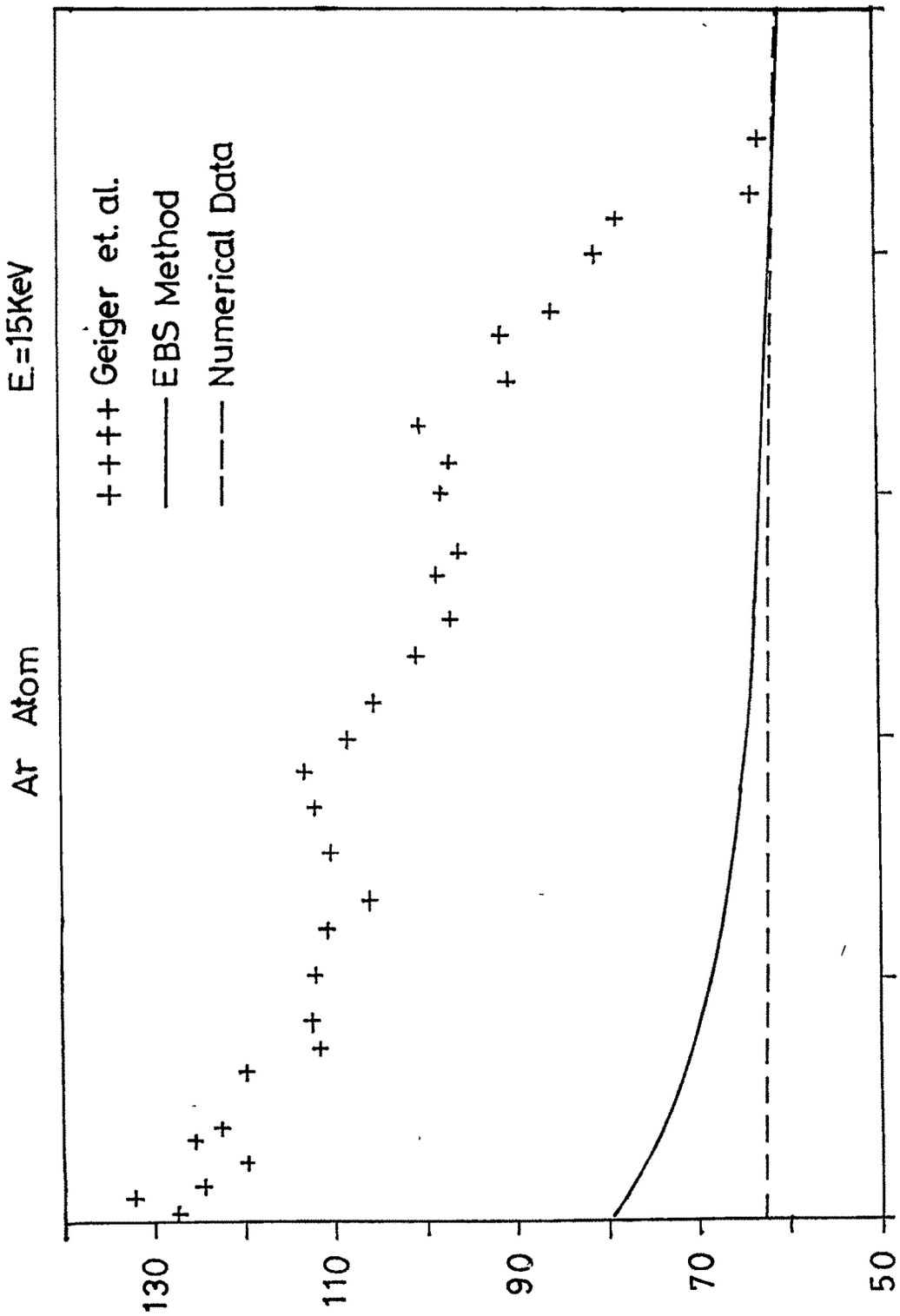

Ar Atom
E=15KeV
++++ Geiger et. al.
—— EBS Method
— — — Numerical Data
Diff. Cross Section (a.u.)
130
110
90
70
50
3
5
7
θ (mrad.)

Fig. 2.4

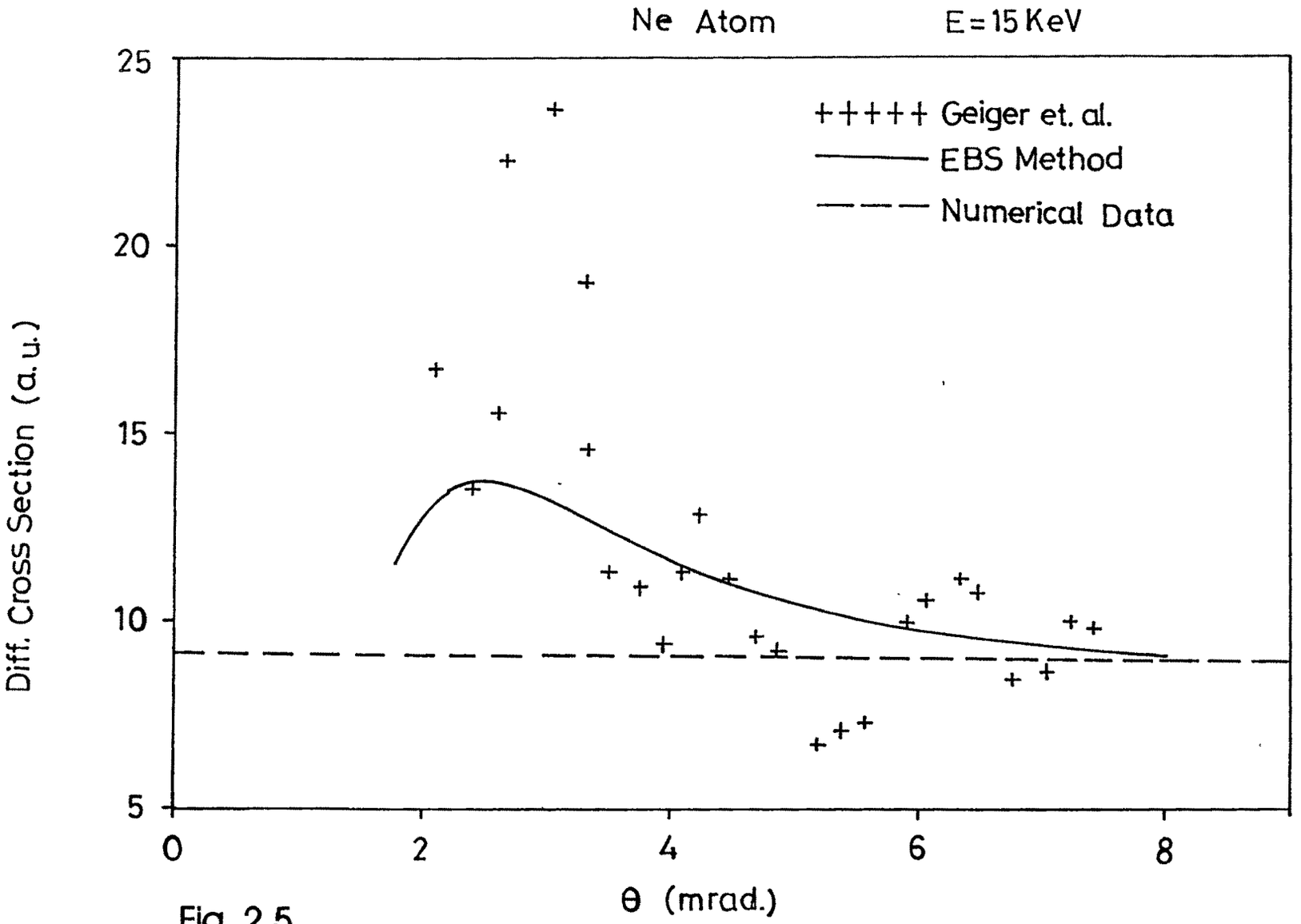
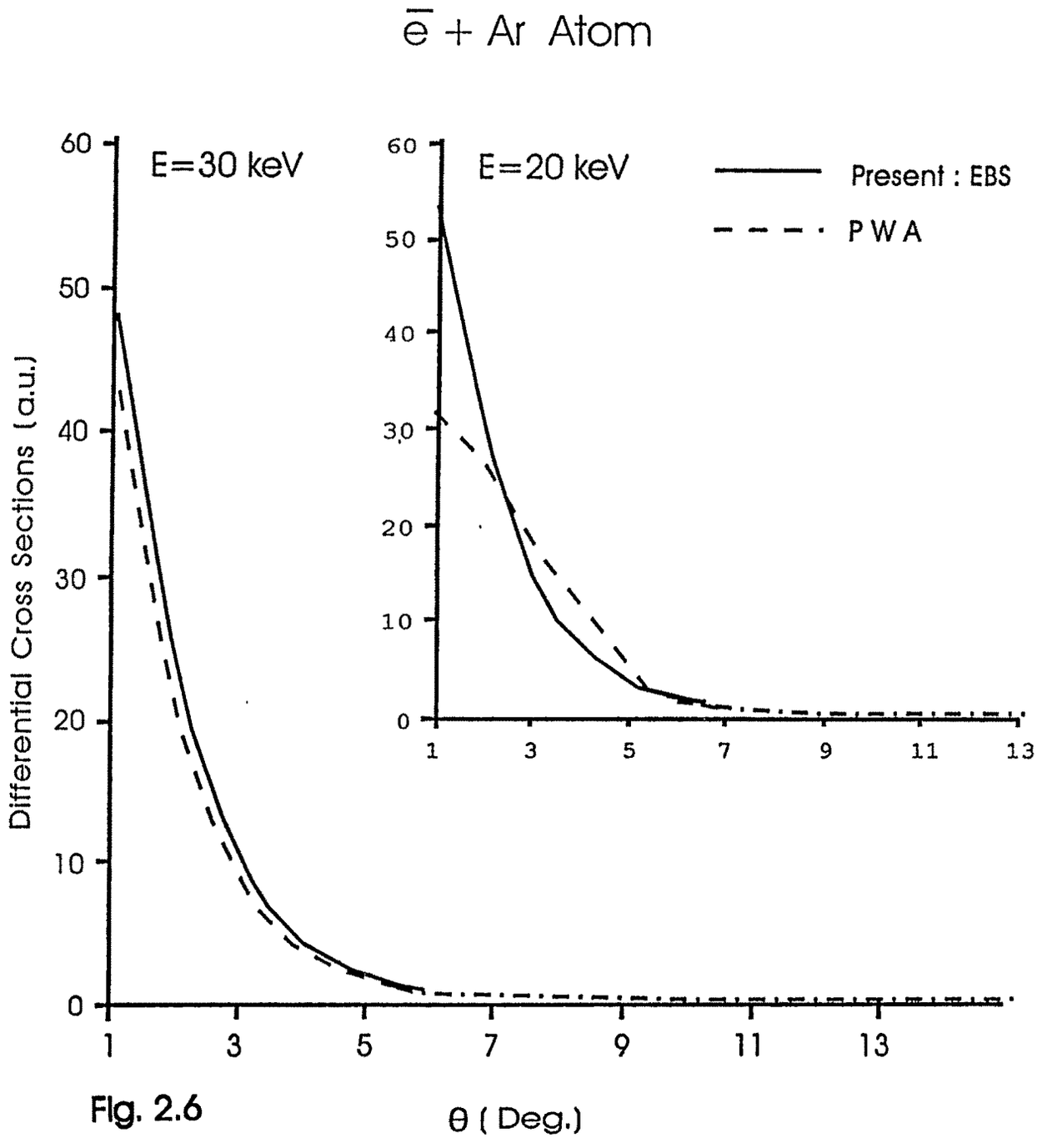
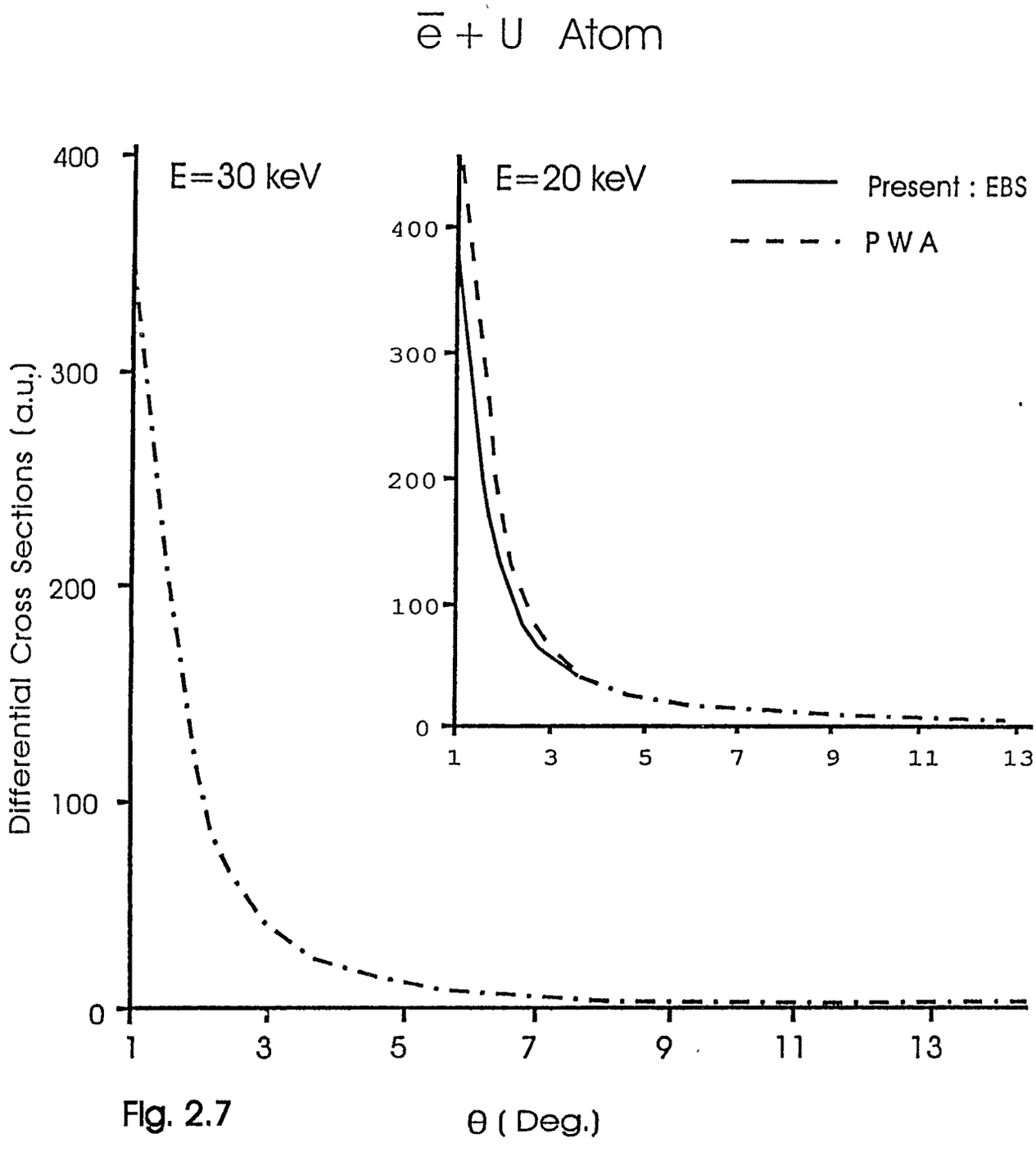

Ne Atom
E=15 KeV
+++++ Geiger et. al.
EBS Method
Numerical Data
Diff. Cross Section (a.u.)
25
20
15
10
5
0
2
4
6
8
θ (mrad.)

Fig. 2.5


$\bar{e}$ + Ar Atom
E=30 keV
E=20 keV
Present : EBS
P W A
Differential Cross Sections (a.u.)
θ (Deg.)
0
10
20
30
40
50
60
1
3
5
7
9
11
13

Flg. 2.6


$\bar{e}$ + U Atom
E=30 keV
E=20 keV
Present : EBS
P W A
Differential Cross Sections (a.u.)
400
300
200
100
0
1
3
5
7
9
11
13
θ (Deg.)

Flg. 2.7

2.8 RESULTS AND DISCUSSION :

He, Ne and Ar atoms at 35 KeV

A systematic study of the differential cross-sections for the inert gas atoms He, Ne, and Ar is reported here for the non-relativistic potential scattering. The differential cross sections for elastic scattering of electrons from these target atoms are studied for energies in the range of 15 keV to 35 keV. We did not find any strong peak in the forward direction or an oscillatory nature in differential cross sections as reported by Geiger *et al* [17]. Our results are close to the new experimental data [16]. The results are exhibited graphically in Fig. 2.1-2.3. We see that according to the EBS method the differential cross sections for He, Ne, Ar atoms at very small scattering angle differ from exact results (numerical) in the range 0.2 to 0.3 $\overset{0}{A}^{-1}$. The EBS amplitude reproduce the exact results for momentum transfer greater than 0.3 $\overset{0}{A}^{-1}$. For He-atom (Fig. 2.1), differential cross-section obtained by the numerical and Das method has similar nature but they are on either side of the experimental data, which cover all points. The EBS results are close to the experimental data with compared to the numerical and Das results beyond 0.3 $\overset{0}{A}^{-1}$. In the case of Ne atom (Fig. 2.2), differential cross sections resulting from EBS and Das method are in excellent agreement with the partial wave calculations. These results differ from the experimental results. In the case of Ar atom (Fig.2.3), the results obtained by numerical method are closer to the experimental results.

We have also reported differential cross-sections by Wallace and modified Das method at 35 keV. These results give nearly the same values as those given by EBS and Das method respectively. The strong forward peak and oscillating features in differential cross sections are lacking. The results are shown in Tables 2.1 and 2.2. The differential cross-sections calculated by Wallace method are in close agreement with the EBS results and modified Das results.

Ar and U at 40 KeV :

The calculations of δ_l and $f(\theta)$ given by various techniques are exhibited in the Table-2.3 and 2.4. At 40 keV 441 and 891 partial waves are required for convergent series in equation (2.6.3) for *Ar* and *U* atoms respectively. For large values of *l,* Dirac phase shift

is a decreasing function of l. The decrease of $|\delta_l|$ with l is not rapid as compared to low energy projectile. The scattering factors evaluated according to equation (2.6.4); (2.6.5),(2.3.14) and (2.4.8) are compared with available results [13]. The compared results were obtained theoretically with different methods.

The EBS method has been applied for He atom at intermediate and high energy (100-500eV) by Byron and Joachain [8]. In the present work this method is extended to calculate scattering amplitude for higher atomic number atoms using DHFS potential. The EBS method and Wallace correction to eikonal phase for Ar atom (see Table-2.4) give almost four-figure accuracy. This indicates that EBS method comprises summation of large number of partial waves effectively. These calculations are computationally economic and tested for heavier atoms too. These approximations are considerably good for high energy and large atomic number, since at 40 keV it appears to be valid for U atom when $17 > \Delta > 33$. Calculations utilizing the approximations mentioned in section 2.3 and 2.6 are presently being employed to compute DCS for incident electron energies at 20 and 30 keV. As shown in figure 4 and 5 the results of EBS method are in good agreement with partial wave calculations as the incident electron energy increases.

In Fig. 1-3 theoretical data of the present work is compared with the experimental data of Coffman & Fink nature of both the graphs matches. Whereas in fig. 4-5 present results are compared with experimental results of GML [17]. Form fig. 4 It is very much clear that in the EBS results oscillatory behaviour dose not exist as shown by the experimental results. EBS results, close to the exact results, indicate their validity. In Fig. 5 forward peak in the experimental results is obvious. The small peak is observed in the EBS results but it dose not support high experimental value about angle 3 mrad.

Fig. 6-7 refer to the heavy atoms at 20 & 30 KeV, where the present results are almost equal to partial wave results means accuracy of the method is very good. In other way the EBS method comprises summation of large number of partial waves. Thus the approximation is considerably good for high energies and for large atomic number.