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ASYMMETRY OF THE SCATTERING OF POLARIZED ELECTRONS BY POLYCRYSTALLINE GOLD

A Thesis presented to the School of
Graduate Studies
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by
BEREKET NEWAY

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ASYMMETRY OF THE SCATTERING OF POLARIZED ELECTRONS BY POLYCRYSTALLINE GOLD

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ABSTRACT

The fundamental concepts of polarized electrons and the mathmatical formulations of the scattering of these electrons from spinnless atoms are reviewed.

The Theoretical investigations were made of the asymmetry of the scattering on the surface of polycrystalline gold. Atomic data for a single scattering process were used to calculate asymmetry and intensity as a function of the scattering angle for multiple collisions. The specific influence of a solid was taken into account. The asymmetry of the scattered electrons into a wide solid angle was calculated and a comparison with some experimental data for the scattering of polarized electrons of energy Ep from 100 to 500 eV was made.

Satisfactory agreement has been obtained between the calculated and experimental results.

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INTRODUCTION

Polarization effects in elastic electron scattering were predicted for the first time by Mott [1,2], where the scattering process is described on the basis of Dirac equation.

In conventional electron scattering experiments, spin dependent interactions are often masked by the much stronger coulomb interaction. They can, however, be unmasked by collision studies with polarized electron [3]. Investigation carried out on the last two decades have established that participation of spin state in the interaction of electrons with a solid can provide additional information on the scattering mechanisms, characteristics of the potential barrier at a solid vacuum interface and physicochemical properties of the surface [4,5,6].

The study of polarized electrons scattering is widely used at present for investigations of magnetic, electronic and even geometrical properties of the surface of solids [7]. This knowledge is very important for the development of new electronic devices, but the exact mechanism of the interaction of polarized electrons with the surface is not well known.

The results of the scattering asymmetry exhibited by elastic scattering of polarized electrons of primary incident energy(E_p) less than 500 eV from the surface of polycrystalline gold is presented. The choice of polycrystalline gold as a target is due to the fact that [8]:

1) it is a heavy material and has a strong spin-orbit interaction,

2) easy to fabricate as opposed to crystalline material,

and inert to contaminate in vaccum, and

3) the observed effects are not modulated by diffraction as in crystalline solids.

Chapter I introduces fundamental concepts of polarized electrons that are scattered not only by coulomb scattering forces but also by spin-dependent forces. Chapter II covers the scattering of electrons from the spineless atoms, where the spin-dependent effects are caused by the spin orbit interaction. The spin polarization in the elastic scattering processes, arising from the spin-orbit coupling also discussed. The mathematical expressions of the differential scattering cross sections, the asymmetry of scattering polarized electrons and the polarization of the beam scattered electrons acquired after scattering by free atoms are included in this chapter.

Chapter III deals with the theoretical investigation of the asymmetry of scattering polarized electrons by a solid material (in particular gold). Based on the adopted model of multiple scattering effects, the asymmetries and differential cross sections for $n(n\geq 2)$ fold multiple scattering was calculated and finally obtained the asymmetry of the scattered polarized electrons for the investigated substances. In this analysis, theoretical values of the differential cross sections and asymmetries of elastic scattering by free atoms were used. All the calculations were carried out by standard method of numerical integration on a computer. A comparison of the calculated results and experimentally measured values[9] of the scattering asymmetries have been done for polarized electrons $Ep \leq 500$ eV.

Finally, concluding remarks are presented.

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CHAPTER I

1. BASIC PRINCIPLES AND THE THEORY OF ELECTRONS SCATTERING AND POLARIZATION

1.1. The Spin Of The Electron

The concept of spinning electron was first suggested by Compton in 1921. Shortly later in 1925, Uhlenbeck and Goudsmit proposed the electron as a point magnet with intrinsic spin in order to clarify the anomalous Zeeman effect. The main result of the arguments were [10].

1) The electron must have an intrinsic spin $\frac{1}{2}\hbar$. Hence a single electron atomic levels must be characterized by half-integral angular momentum.

2) The electron magnetic moment arising from the spin must have a magnitude equal to the Bohr magneton

$$\mu_B = \frac{\epsilon\hbar}{2mc} \tag{1.1}$$

where m is the mass of the electron and $\epsilon = -e$ is its charge.

1.1.1. Electron Wave Function

When an electron is in a magnetic field, it occupies two spectral lines [Zeeman effect], so that its spin angular momentum has two values, $\frac{1}{2}\hbar$ or $-\frac{1}{2}\hbar$. Due to this fact in measuring any component (for instance the Z- component) of the spin angular momentum of an electron one can obtain only the two numerical values $\frac{1}{2}\hbar$ or $-\frac{1}{2}\hbar$.

This means that the values of $\frac{1}{2}\hbar$ or $-\frac{1}{2}\hbar$ are the sole eigen

values of the operator Σ_z of the z component of the spin angular momentum. The matrix representative Σ_z of the operator Σ_z in its set of eigen values has the form

$$\sum_z = \tfrac{1}{2}\hbar \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1.2}$$

On the basis of the general postulates of quantum mechanics, the square absolute value of the elements of this matrix determines the probability of measuring each of the two eigen values $\frac{1}{2}\hbar$ or $-\frac{1}{2}\hbar$. The probability of finding an electron with spin angular momentum $\frac{1}{2}\hbar$ will differ from the corresponding one angular momentum $-\frac{1}{2}\hbar$. Thus one would be compelled to use two wave functions $\Psi_+(x,y,z,\frac{1}{2}\hbar,t)$ and $\Psi_-(x,y,z,-\frac{1}{2}\hbar,t)$. A matrix consisting of both these functions

$$\begin{bmatrix} \psi_+(x,y,z,\tfrac{1}{2}\hbar,t) \\ \psi_-(x,y,z,-\tfrac{1}{2}\hbar,t) \end{bmatrix} \tag{1.3}$$

should be regarded as the position-spin representative of the state of an electron.

Using the operator (1.2) and the wave function (1.3) one can consider the eigen value problem of the operator (1.2).

$$\sum_z \psi = \lambda \Psi$$

Since with regard to the normalization, ψ_+ and ψ_- can not vanish simultaneously, the eigen value problem has two solutions.

$$\lambda = \tfrac{1}{2}\hbar \quad , \quad \psi_- = 0 \quad , \quad \psi = \begin{bmatrix} \Psi_+ \\ 0 \end{bmatrix} \tag{1.4a}$$

$$\lambda = -\tfrac{1}{2}\hbar \quad , \quad \Psi_{+} = 0 \quad , \quad \Psi = \begin{bmatrix} 0 \\ \Psi_{-} \end{bmatrix} \qquad (1.4b)$$

In the first case, the spin angular momentum is in the direction of the positive Z - axis, and in the second case, of the negative z - axis [11,12].

1.1.2. **Spin Operators**

The following facts can be drawn from text books on **quantum mechanics : the observable " spin " is represented by the operator Σ which satisfies the commutation relations** characteristic of angular momenta [10,11,12].

$$\begin{aligned} \Sigma_x\Sigma_y - \Sigma_y\Sigma_x &= i\hbar\Sigma_z \\ \Sigma_y\Sigma_z - \Sigma_z\Sigma_y &= i\hbar\Sigma_x \\ \Sigma_z\Sigma_x - \Sigma_x\Sigma_z &= i\hbar\Sigma_y \end{aligned} \qquad (1.5^{\cdot})$$

One can understand that the operators Σ_x, Σ_y, Σ_z do not commute with each other. Therefore, one can not assert that x, y, z components of the electron spin simultaneously have exactly determined value.

It can be easily checked that in accordance with these relations (1.5˙) one can choose Σ_x, Σ_y for the spin-component operators to suit Σ_z of expression (1.2) in the following manner.

$$\sum_x = \tfrac{1}{2}\hbar \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad , \sum_y = \tfrac{1}{2}\hbar \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad (1.5$$

In our considerations further on we shall frequently use the operators σ_x, σ_y, σ_z which are connected with the operators Σ_x, Σ_y, Σ_z by equations

$$\Sigma_i = \tfrac{1}{2}\hbar\sigma_i \qquad \text{where i = x, y, and z}$$

Hence, because of equations (1.2) and (1.5), these operators

have the representative

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad , \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad , \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1.6}$$

These matrices are known as Pauli spin matrices. It can be easily verified by calculation , the relations

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I \text{ (unit matrix)} \tag{1.7a}$$

$$\sigma_x = -i\sigma_y\sigma_z = i\sigma_z\sigma_y \quad , \quad \sigma_y = -i\sigma_z\sigma_x = i\sigma_x\sigma_z \quad | \tag{1.7b}$$

$$\sigma_z = -i\sigma_x\sigma_y = i\sigma_y\sigma_x \quad |$$

are satisfied for these matrices.

Eqn. (1.7a) states that the squares of the Pauli matrices are given by unit matrices , and eqn. (1.7b) implies that these matrices anti - commute.

According to eqn. (1.6) , $\sigma_x^2 = \sigma_y^2 = \sigma_z^2$ is equal to unit matrix. Consequently, owing to eqn. (1.5) one obtains

$$\Sigma_x^2 = \Sigma_y^2 = \Sigma_z^2 = \tfrac{1}{4}\hbar^2 \text{, and}$$

$$\Sigma_x^2 + \Sigma_y^2 + \Sigma_z^2 = 3/4\hbar^2$$

This implies that one always obtains one and the same value, $\frac{1}{4}\hbar^2$ or $3/4\hbar^2$, for the square of the electron spin component in any direction or for the square of the total electron spin.

1.1.3. Pure Spin State

It is inconvenient to write wave functions with spin in matrix form when the system contains more than one electron. The matrix (1.3), however, is determined if one gives both elements either separately or collecively in the expression

$$\psi(x, y, z, s_z, t) = \chi_+(s_z)\psi_+ + \chi_-(s_z)\psi_- \tag{1.8}$$

The symbol $\chi_+(S_z)$ and $\chi_-(S_z)$ thereby depend on the magnetic quantum number of the electron spin S_z. Thus S_z may take on the value of $+\frac{1}{2}$ or $-\frac{1}{2}$. When $S_z=\frac{1}{2}$ (or $S_z=-\frac{1}{2}$), then ψ should be equal

to $\psi_+(\psi_-)$, so that in eqn. (1.8) the symbols $\chi_+(s_z)$ and $\chi_-(s_z)$ denote

$$\chi_+(S_z) = \delta_{+\frac{1}{2}, S_z}, \tag{1.9}$$

$$\chi_-(S_z) = \delta_{-\frac{1}{2}, S_z}, \tag{1.10}$$

These symbols may be regarded as eigen functions of the spin, the role of spin coordinate being assigned to the quantum number S_z. Note that χ_+ and χ_- defined in this way are both normalized and are orthogonal to each other. Thus the function (1.8) can be re-written as

$$\psi(x, y, z, s_z, t) = \delta_{\frac{1}{2}, s_z}\, \psi_+ + \delta_{\frac{1}{2}, s_z}\, \psi_-$$

The two wave functions χ_+ and χ_- describe the two stationary states of the system i.e. the two states in which the spin eigen value is known. The general state of the pure spin system will be described by a wave function

$$\chi = a\chi_+ + b\chi_-$$

where a and b are arbitrary complex numbers and χ is assumed to be normalized, i.e.

$$\langle \chi \mid \chi \rangle = |a|^2 + |b|^2 = 1$$

From eqns. (1.9) and (1.10), the symbols χ_+ and χ_- were replced by the matrices

$$\begin{vmatrix} 1 \\ 0 \end{vmatrix} \text{ and } \begin{vmatrix} 0 \\ 1 \end{vmatrix} ,$$

respectively , that is by the representative of the states of electrons with spin eigen values of $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$.

Similarly, the general pure spin state of the system in the matrix form is given by

$$\chi = \begin{bmatrix} a \\ b \end{bmatrix} = a \begin{bmatrix} 1 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad (1.11)$$

So far we have discussed the spin of an electron in Z - direction. Now, we would like to get the spin function describing the spin in any arbitrary direction.

The spin direction of a state which is described by $\chi = \begin{vmatrix} a \\ b \end{vmatrix}$ is specified by a and b. Let $\vec{e} = (e_x, e_y, e_z)$ be the unit vector in the direction ϑ, φ [see Fig 1.1].

$$e_x = \sin\vartheta\cos\varphi \ , \ e_y = \sin\vartheta\sin\varphi \ , \ e_z = \cos\vartheta$$

we now ask what the spin function that describe a spin in the direction ϑ, φ would look like. For this we must solve the eigen value equation $(\vec{\sigma}.\vec{e})\chi = \lambda\chi$, since $\vec{\sigma}.\vec{e}$ is the projection of the spin operator in the specified direction. Since

$$\sigma_x \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} b \\ a \end{bmatrix} \ , \qquad \sigma_y \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} -ib \\ ia \end{bmatrix} \ , \qquad \sigma_z \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a \\ -b \end{bmatrix}$$

One obtains

$$(\vec{\sigma}.\vec{e})\chi = \begin{bmatrix} a\cos\vartheta + b\sin\vartheta e^{-i\varphi} \\ a\sin\vartheta e^{i\varphi} - b\cos\vartheta \end{bmatrix}$$

The attempt of finding the eigen function of the component of the spin operator in the $\vec{e}$ direction, i.e. to solve the equation $(\vec{\sigma}.\vec{e})\chi = \lambda\chi$, thus gives

$$\begin{aligned} a(\cos\vartheta - \lambda) + b\sin\vartheta e^{-i\varphi} &= 0 \\ a\sin\vartheta e^{i\varphi} - b(\sin\vartheta + \lambda) &= 0 \end{aligned} \qquad (1.12)$$

The condition for a non trivial solution (disappearance of the determinant) is

$$-\cos^2\vartheta + \lambda^2 - \sin^2\vartheta = 0 \ , \ or \ \ \lambda = \pm 1$$

a) For $\lambda = +1$, one obtains from eqn. (1.12)

$$\frac{b}{a} = \tan\frac{\vartheta}{2}e^{i\varphi} \qquad (1.13a)$$

b) and for $\lambda = -1$

$$\frac{b}{a} = -\cot\frac{\vartheta}{2}e^{i\varphi} \qquad (1.13b)$$

The probability, therefore, that the electron will take up the spin angular momentum $\frac{1}{2}\hbar$ in the new system is $\cos^2\frac{1}{2}\vartheta$, and that it will take up $-\frac{1}{2}\hbar$ is $\sin^2\frac{1}{2}\vartheta$.

The phases are chosen as follows:

$$\lambda = 1 : a = \cos\frac{\vartheta}{2} \quad , b = e^{i\varphi}\sin\frac{\vartheta}{2} \qquad (1.14a)$$

$$\lambda = -1 : a = \sin\frac{\vartheta}{2} \quad , b = -\cos\frac{\vartheta}{2}e^{i\varphi} \qquad (1.14b)$$

Therefore, the spin functions which diagonalize $\vec{\sigma}.\vec{e}$ with eigen value ± 1 are

$$\lambda = +1 \quad : {}^{+}\chi = \begin{bmatrix} \cos\frac{\vartheta}{2} \\ e^{i\varphi}\sin\frac{\vartheta}{2} \end{bmatrix}$$

$$\lambda = -1 \quad : {}^{-}\chi = \begin{bmatrix} \sin\frac{\vartheta}{2} \\ -\cos\frac{\vartheta}{2}e^{i\varphi} \end{bmatrix}$$

These are a complete orthonormal set of spin functions. For $\vartheta, \varphi \to 0$ the function ${}^{\pm}\chi$ reduces to $\chi_{\pm}$. One can immediately see that the solutions (1.13a) and (1.14a) are none other than the solutions (1.13b) and (1.14b), respectively, for the direction $-\vec{e}$ which is described by the angles $\pi - \vartheta, \varphi + \pi$. Thus it is sufficient to use only the solutions (1.13a) or (1.14a).

If electrons are in the same spin state the system of electrons is said to be in a pure spin state [4,10].

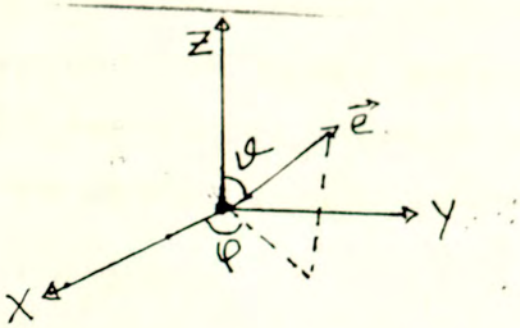


Fig 1.1 Spin direction

1.2 Description of Polarization of Primary Beam in Terms of the Density Matrix

Definition : An ensemble of electrons is said to be polarized if the electrons spin have a preferential orientation so that there exists a direction for which the two possible spin states are not equally populated [3,4].

$$P = \frac{N\uparrow - N\downarrow}{N\uparrow - N\downarrow}$$

where N↑ and N↓ are the numbers of the electrons with spin parallel and anti parallel and anti parallel of the two possible states.

If all spins have the same direction one has the extreme case of a totally polarized ensemble of electrons. If not all, but only a majority of the spin has the same direction, the ensemble is called partially polarized. Fig (1.2) illustrates

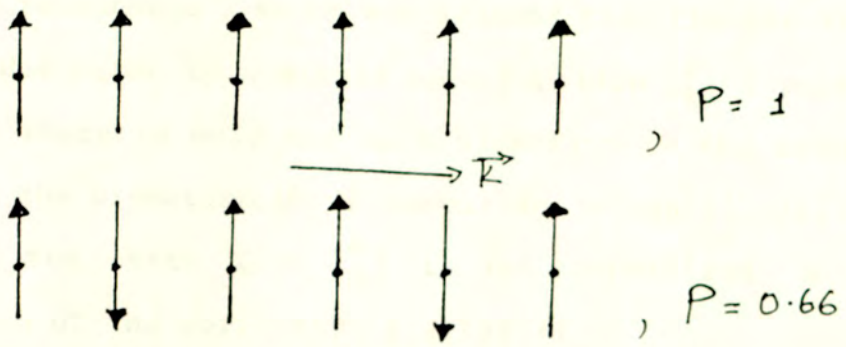


Fig.1.2 Definition of electron polarization

the case of total and partial polarization (for transverse polarization case). Let the pure spin state of the electrons is given by $\left|\begin{matrix}a\\b\end{matrix}\right|$. From quantum mechanics approach polarization is defined as the expectation value of the Pauli spin operator

$$\vec{P} = \langle\vec{\sigma}\rangle = \langle\chi|\vec{\sigma}|\chi\rangle \qquad (1.15$$

with this definition, the components of the polarization are

$$\vec{P} = \langle\vec{\sigma}\rangle = \langle\chi|\vec{\sigma}|\chi\rangle \qquad (1.15$$

$$P_x = [a^*, b^*]\begin{bmatrix}a\\b\end{bmatrix} = a^*b + ab^* = 2Re(ab^*) = \sin\vartheta\cos\varphi \qquad (1.16)$$

$$P_y = [a^*, b^*]\begin{bmatrix}-ib\\ia\end{bmatrix} = i(ab^* - a^*b) = 2Im(a^*b) = \sin\vartheta\sin\varphi \qquad (1.17)$$

$$P_z = [a^*, b^*]\begin{bmatrix}a\\-b\end{bmatrix} = a^*a - bb^* = \cos\varphi \qquad (1.18)$$

It can be seen from these equations that the polarization has the direction ϑ , φ and the degree of polarization which is defined by

$$P = \sqrt{P_x^2 + P_y^2 + P_z^2} = 1$$

This is reasonable , as it was assumed that the electron spins can be described by a single spin function $\left|\begin{matrix}a\\b\end{matrix}\right|$ (pure state) so that there is only one spin direction in the beam, namely that in the direction ϑ , φ specified in eqn.(1.14a).

If the state $\chi = \left|\begin{matrix}a\\b\end{matrix}\right|$ is not normalized, a sensible extension of the definition (1.15) is

$$\vec{P} = \frac{\langle \chi | \vec{\sigma} | \chi \rangle}{\langle \chi | \chi \rangle} \qquad (1.19)$$

Thus the magnitude of the components of $\vec{P}$ remains between 0 and +1.

The definition of density matrix is stated in order to describe polarization interms of density matrix. For a single (pure) spin state $\begin{vmatrix} a \\ b \end{vmatrix}$, the density matrix is defined as [13]

$$\chi\chi^{*} = \begin{bmatrix} aa^{*} & ab^{*} \\ b^{*}a & bb^{*} \end{bmatrix} = \rho \qquad (1.20a)$$

This matrix is defined as the spin - density matrix for the beam.

The intensity of the beam $|a|^2 + |b|^2$ which may be written

$$\langle \chi | \chi \rangle = tr(\chi\chi^{*}) = Tr(\rho) = U \qquad (1.20)$$

where Tr denotes the trace or sum of the diagonal elements of the square matrix ρ. For normalized pure state $tr(\rho) = 1$

Together with the intensity, the three components of the polarization (1.16 - 1.18) define the observable properties of the beam. All may be represented simply in terms of the density matrix.

The spin orientation is represented by a density matrix with the two rows and columns, corresponding to two pure states of opposite spin direction (e.g. up and down). Using (1.6) and (1.20) one sees immediately that these equations are correct. For example, one gets

$$\rho\sigma_x = \begin{bmatrix} ab^{*} & |a|^2 \\ |b|^2 & a^{*}b \end{bmatrix} \qquad (1.21$$

and thus

$$tr(\rho\sigma_x) = ab^* + a^*b = 2Re(ab^*) = P_x$$

where use has been made of eqn.(1.16). Similarly, $tr(\rho\sigma_y) = 2Im(a^*b) = P_y$, and $tr(\rho\sigma_z) = P_z$. Thus from the above facts, the density matrix is connected to the polarization by the relation

$$\langle\vec{\sigma}\rangle = \vec{P} = tr(\rho\vec{\sigma}), \qquad and \quad P_i = tr(\rho\sigma_i) \tag{1.22}$$

Knowledge of $\vec{P}$ is sufficient to identify the density matrix, [14,15] considering

1) that any 2x2 Hermitian matrix can be represented as a linear combination of $\sigma_x, \sigma_y, \sigma_z$ and of the unit matrix I

i.e. $\rho = AI + B\sigma_x + C\sigma_y + D\sigma_z$

2) that the Pauli matrix have the properties

$$Tr\ \sigma_i = 0\ ,\ Tr(\sigma_i\sigma_k) = 2\delta_{ik}$$

3) that $Tr(\rho) = 1$ for normalized state and $tr(I) = 2$ require the coefficients of (I) to be $\frac{1}{2}$

That is , $tr(\rho) = 2A$

$$A = \tfrac{1}{2}$$

and using the above facts one obtains ,

$$B = P_x/2 \quad , \quad C = P_y/2 \quad , \quad D = P_z/2$$

so that the density matrix can be written as

$$\begin{aligned}\rho &= \tfrac{1}{2}(I + P_x\sigma_x + P_y\sigma_y + P_z\sigma_z) \\ &= \tfrac{1}{2}\begin{bmatrix} 1+P_x & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{bmatrix} \\ &= \tfrac{1}{2}(I + \vec{P}.\vec{\sigma})\end{aligned} \tag{1.23}$$

If the state $\chi = \begin{vmatrix} a \\ b \end{vmatrix}$ is not normalized, then $tr(\rho) \neq 1$. In this case eqns.(1.22) and (1.23) should have some modification. Instead of (1.22) one can obtained

$$\vec{P} = \frac{tr(\rho\vec{\sigma})}{tr(\rho)} \tag{1.24}$$

The denominator

$$\langle\chi/\chi\rangle = |a|^2 + |b|^2 = tr(\rho) = U$$

now appearing in the polarization formula (1.19) and (1.23) must also be taken into account on the left hand side of (1.23), so that the corresponding relation is

$$\frac{\rho}{tr(\rho)} = \tfrac{1}{2}\begin{bmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{bmatrix} = \tfrac{1}{2}(I + \vec{P}.\vec{\sigma}) \tag{1.25}$$

So far it has been dealing with a beam in which the electrons are in a definite state. There is no difficulty in generalizing the analysis the case in which there is a distribution of electron beams between the different states [mixture of pure spin states]. All that is necessary is to average the density matrix over the probability distribution [4].

In this case the polarization of the total system is the average of the polarization value $\vec{P}^{(n)}$ of the individual systems which are in pure spin states $\chi^{(n)}$

$$\vec{P} = \sum_n w^{(n)}\,\vec{p}^{(n)} = \sum_n w^{(n)} \langle \chi^{(n)} | \vec{\sigma} | \chi^{(n)} \rangle \tag{1.26}$$

where the weighting factor $w^{(n)}$ takes in to account the relative proportion of the states $\chi^{(n)}$.

$$w^{(n)} = N^{(n)}/\Sigma N^{(n)}$$

where $N^{(n)}$ is the number of electrons in the state $\chi^{(n)}$. The $\chi^{(n)}$ have been assumed to be normalized here. And the average density matrix is

$$\bar{\rho} = \sum_n w^{(n)} \rho^{(n)} = \sum_n w^{(n)} \chi^{(n)} \chi^{*(n)} \qquad (1.27)$$

where $\rho^{(n)}$ the density matrix of individual system which are in pure spin states $\chi^{(n)}$.

Following the same procedure as the previous eqns. (1.21 - 1.25), there is no difficulty in showing that the mean values of the quantities U, $\vec{P}$ are given by

$$U = tr(\bar{\rho}) \quad , \quad \vec{P} = tr(\vec{\sigma}\bar{\rho}) \qquad (1.28$$

and that

$$\bar{\rho} = \tfrac{1}{2}(I + \vec{P}.\vec{\sigma}) \qquad (1.29$$

In the above consideration it was assumed that the states $\chi^{(n)}$ were normalized, the relative proportions of the single states were taken into account by using weighting factors. One can also start unnormalized $\chi^{(n)}$. Then weighting factors are unnecessary, since the relative proportion of the n^{th} state is already expressed by the unnormalized amplitude $\chi^{(n)}$, it is given as

$$\frac{\langle \chi^{(n)} | \chi^{(n)} \rangle}{\sum_n \langle \chi^{(n)} | \chi^{(n)} \rangle} \qquad (1.30)$$

In this case the polarization is

$$\vec{P} = \frac{\sum_n \langle \chi^{(n)} | \vec{\sigma} | \chi^{(n)} \rangle}{\sum_n \langle \chi^{(N)} | \chi^{(N)} \rangle} \qquad (1.31)$$

and the density matrix has the form

$$\bar{\rho} = \sum_n \rho^{(n)}$$

Then, eqns. (28) and (29) may be re-written as

$$\vec{P} = \frac{tr(\vec{\sigma}\bar{\rho})}{tr(\bar{\rho})} \quad , \text{ and} \tag{1.32}$$

$$\bar{\rho} = \tfrac{1}{2} I tr(\bar{\rho}) = \tfrac{1}{2} IU \tag{1.33}$$

If the beam is unpolarized, P = 0 so that

$$\bar{\rho} = \frac{1}{2} I tr(\bar{\rho}) = \frac{1}{2} IU$$

1.3 Spin - Dependent Interaction

The Uhlenbeck - Goudsmit hypothesis was that an electron possessed a spin angular momentum $\vec{S}$ (which could take an quantized values of $\hbar/2$ along any axis) and a magnetic moment $\vec{\mu}$ related to $\vec{S}$ by

$$\vec{\mu} = \frac{\epsilon \vec{S}}{mc} \tag{1.34}$$

with the electron charge $\epsilon = -e$.

Suppose that an electron moves with a velocity $\vec{V}$ in external fields $\vec{E}$ and $\vec{B}$, the equation of motion of the spin angular momentum in the rest frame is

$$\left(\frac{d\vec{S}}{d\vec{t}}\right)_{rest\ frame} = \vec{\mu} \times \vec{B}' \tag{1.35}$$

where $\vec{B}'$ is the magnetic induction in the rest frame of the electron.

For a coordinate system moving with the electron, with terms up to the order V^2/c^2, the magnetic induction is given by

$$\vec{B}' = \left(\vec{B} - \frac{\vec{V}}{c} x \vec{E} \right) \tag{1.36}$$

Then, eqn. (1.35) becomes

$$\left(\frac{d\vec{s}}{dt}\right)_{rest\ frame} = \vec{\mu} \times \left(\vec{B} - \frac{\vec{v}}{c} \times \vec{E} \right) \qquad (1.37$$

On the other hand the interaction energy of the electron spin in the magnetic field is given by

$$U' = -\vec{\mu}.\vec{B}' = -\vec{\mu}.\left(\vec{B} - \frac{\vec{v}}{c} \times \vec{E} \right) \qquad (1.38)$$

In an atom the electric force $\epsilon\vec{E}$ can be approximated as the negative gradient of a spherically symmetry average potential energy U(r). For one - electron atom this is of course exact.

Thus,

$$\vec{F} = \epsilon\vec{E} = -\frac{\vec{r}}{r}\,\epsilon\,\frac{dV(r)}{dr} = -\frac{\vec{r}}{r}\,\frac{du}{dr}(r) \qquad (1.39)$$

where $U(r) = \epsilon V(r)$, V(r) is the electrostatic scattering potential of the electron.

Then the spin - interaction energy eqn. (1.38) can be written as

$$U' = \frac{-\epsilon}{mc}\vec{S}.\vec{B} + \frac{1}{m^2c^2}(\vec{S}.\vec{L})\ \frac{1}{r}\frac{du(r)}{dr} \qquad (1.40)$$

where $\vec{L} = m(\vec{r}x\vec{v})$ is the electron's orbital angular momentum. This interaction energy gives the anomalus Zeeman effect correctly, but has a spin - orbit interaction that is twice too large.

The error in eqn. (1.40) can be traced to the incorrectness of eqn. (1.35) as an equation of motion for the electron spin. The left hand side of eqn. (1.35) gives the rate of change of spin in the rest frame of the electron.If a coordinate system rotates, then the total time rate of change of spin, or more generally, any vector $\vec{G}$ is given by [16]

$$\left(\frac{d\vec{G}}{dt}\right)_{non.\ rot} = \left(\frac{d\vec{G}}{dt}\right)_{rest\ frame} + \vec{\omega}_T \times \vec{G} \qquad (1.41)$$

where $\vec{\omega}_T$ is the angular velocity of rotation found by Thomas when applied to the electron spin, eqn. (1.41) gives an equation of motion

$$\left(\frac{d\vec{S}}{dt}\right)_{non\text{-}rot} = \vec{S} \times \left(\frac{\epsilon}{mc}\vec{B}' - \vec{\omega}_T\right) \qquad (1.42)$$

The corresponding energy of interactions is

$$U = U' + \vec{\omega}_T . \vec{S} \qquad (1.43)$$

where U′ is the electromagnetic spin interaction eqn. (1.38) or eqn. (1.40)

For electrons in atoms the acceleration is caused by coloumb (screened) fields (1.39), and thus the Thomas precession [16] is given by

$$\vec{\omega}_T = -\frac{\vec{L}}{2c^2m^2r}\frac{du(r)}{dr} \qquad (1.44)$$

It is clear from eqns. (1.43) and (1.42) that the extra contribution to the energy reduces the spin-orbit coupling, yielding

$$U = \frac{-\epsilon\ \vec{S}.\vec{B}}{2mc} + \frac{\vec{S}.\vec{L}}{2m^2c^2r}\frac{d\mathcal{U}(r)}{dr} \qquad (1.45)$$

or

$$U = \alpha\vec{S}.\vec{B} + \xi(r)\vec{S}.\vec{L}$$

where

$$\alpha = \frac{-\epsilon}{2mc}\ ,\ \xi(r) = \frac{1}{2m^2c^2r}\frac{du(r)}{dr}$$

The term $\alpha\vec{S}.\vec{B}$ is known as exchange interaction, and

$\xi(r)\vec{S}.\vec{L}$ is the spin orbit interaction

$\vec{S}$ is the spin of the incident electrons and $\vec{L}$ its orbital angular momentum with respect to the scattering center.

For a spinneless (unpolarized) scattering atom $\vec{B} = 0$, eqn. (1.45) reduces to

$$U_{so} = \frac{1}{2m^2c^2} \frac{1}{r} \frac{du(r)}{dr} \vec{S}.\vec{L} \qquad (1.46)$$

or

$$V_{so} = \frac{1}{2m^2c^2} \frac{1}{r} \frac{dv(r)}{dr} \vec{S}.\vec{L} \qquad (1.47)$$

where V_{so} is the spin-orbit scattering potential.

From this result one can learn that the scattering potential of an electron during its motion near the nucleus consists of the electrostatic and the spin orbit potential (for unpolarized target) $V = V_o + V_{so}$ respectively. Since V_{so} contains the scalar product L.S , it has different signs for electrons of the same orbit but different spin directions. As Fig. (1.3) shows, the resulting scattering potential will therefore be higher or lower for spin-up electrons (e↑) than for spin-down electrons (e↓), depending on which side of the atom they pass [3,4,7].

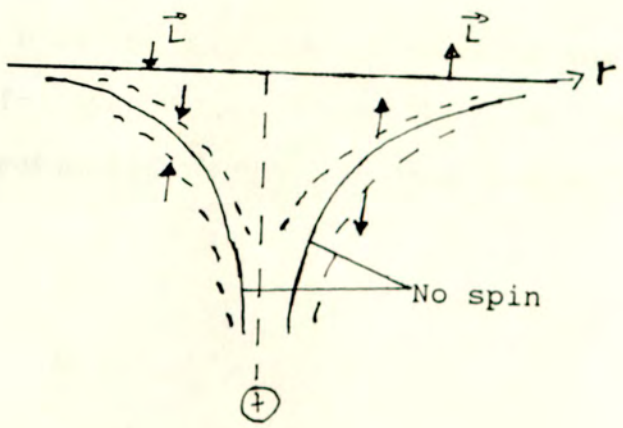


Fig (1.3) Potential curves with (...) and without (——) spin orbit coupling for electrons with spins up ↑ and down ↓.

CHAPTER II

THE EFFECTS OF POLARIZATION IN ELECTRON SCATTERING FROM UNPOLARIZED TARGETS

2.1 The Relativistic (Dirac) Wave Equation

As is well known, Dirac was able to show that it is impossible to find a wave function for an electron that is invariant with respect to Lorentz transformation, and which is linear in the time differential, unless the electron be assumed to have a fourth degree of freedom [13]. In analogy to the case of light beams, electron beams can be polarized by scattering, and the angular distribution of scattered electrons depends on the state of polarization of the incident beam. These effects can be treated by the Dirac equation, which is the basic equation for describing the electron, including its spin and its relativistic behavior [10].

The schrödinger wave equation is known as

$$H\psi = i\hbar \frac{\partial \psi}{\partial t} \tag{2.1}$$

where H is the Hamiltonian function and ψ is wave function.

In classical mechanics, in the presence of an electromagnetic field, the Hamiltonian is given by

$$H = \frac{(\vec{p} - \frac{\epsilon \vec{A}}{c})^2}{2m} + \epsilon V \tag{2.2}$$

where H and $\vec{P}$ are operators with

$$H = i\hbar \frac{\partial}{\partial t} \quad , \quad \vec{P} = -i\hbar \vec{\nabla} \tag{2.3}$$

ϵ =-e and V,$\vec{A}$ are the scalar and vector potential, respectively.

For a free particle, the Hamiltinian (eqn. (2.1)) reduces to

$$H = P^2/2m \tag{2.4}$$

By applying eqn.(2.4) to a wave function $\psi(r,t)$, one obtains the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2\psi \tag{2.5}$$

To consider the relativstic case we start with the relativstic energy law to get the corresponding Hamiltonian for a free particle and is given by

$$H^2 = c^2p^2 + m^2c^4 \tag{2.6}$$

(m = rest mass of electron). By substituting the operators (2.3) for $\vec{P}$ & H , one obtains

$$(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{1}{\lambda\!\!\!^{-2}})\ \psi = 0 \tag{2.7}$$

where $\lambda\!\!\!^{-} = h/mc$ is the compton wave length.

If one substitutes $(\vec{P} - \epsilon\vec{A}/c)$ for P ($\vec{P}$ = canonical momentum) and H- ϵV for H correspondingly, it follows (2.6) for the relativistic case ,

$$(H - \epsilon V)^2 = (c\vec{P} - \epsilon\vec{A})^2 + m^2c^4 \tag{2.8}$$

$$or\quad , \qquad H = c\sqrt{(\vec{P} - \frac{\epsilon}{c}\vec{A})^2 + m^2c^2} + \epsilon V$$

By interpreting H & $\vec{P}$ as operators, one obtains a wave function for an electron in an external electromagnetic field (the Klein - Gordon equations) .

To avoid the difficulty of using relativisitc equation, [i.e. eqn. (2.6) or eqn. (2.8)], Dirac splitted up the equation into a product of two linear expressions and of considering these individually. The equation

$$[H^2 - C^2(\sum_{i=1}^{3} P_i^2 - m^2C^2)]\,\psi = 0 \qquad (2.9)$$

($P_i = P_x, P_y, P_z$, components of the momentum operator), which follows from the force- free of (2.8) can be expressed in the form

$$[H - C(\sum_i \alpha_i P_i - \beta mc)]\ [H + (C\sum_i \alpha_i P_i + \beta mc)]\ \psi = 0 \qquad (2.10)$$

α_i and β_i are to be determined later.

If one wants to have eqns.(2.9) and (2.10) to be identical, one must require that

$$\alpha_i\alpha_{i'} + \alpha_{i'}\alpha_i = 2\delta_{ii'}$$

$$\alpha_i\beta + \beta\alpha_i = 0 \qquad \text{Where } (i, i' = x, y, z) \qquad (2.11)$$

$$\beta^2 = 1$$

This can easily be seen by multiplication. Solving eqn.(2.10), one can have

$$[H + C(\sum_i \alpha_i P_i + \beta mc)]\ \psi = 0 \qquad (2.12)$$

Or

$$H = -c\ (\Sigma_i\ \alpha_i P_i + \beta mc)$$

or the corresponding equation with the plus sign. The linearized equation (2.12) has the advantage that it is of the first order in $\partial/\partial t$ just as the Schrödinger equation. The derivatives with respect to the space coordinates are of the same order, which is necessary for relativistic covariance.

Dirac has shown that the matrices α_n must have at least four columns in order to satisfy eqn.(2.11). But, even then these matrices are not determined uniquely. Dirac assumed them to be of the following form.

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad , \quad \alpha_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

$$\alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad (2.13)$$

In the presence of an electromagnetic field, eqn (2.12) becomes,

$$H = -C\left[\vec{\alpha}\left(\vec{P} - \frac{\epsilon}{C}\vec{A}\right) + \beta mc\right] + \epsilon V \qquad (2.14)$$

with

$$\vec{\alpha} = \alpha_x \vec{I} + \alpha_y \vec{J} + \alpha_z \vec{K}$$

Thus the Dirac equation in the presence of electromagnetic field is, if one arbitrary chooses the right factor of eqn.(2.10) ,

$$\left[P_o + \alpha_x P_1 + \alpha_y P_2 + \alpha_z P_3 + \beta mc\right] \psi = 0 \qquad (2.15)$$

where ,

$$P_o = \frac{-i\hbar}{c}\frac{\partial}{\partial t} - \frac{\epsilon V}{c} \quad , \quad P_1 = -i\hbar\frac{\partial}{\partial x} - \frac{\epsilon A_x}{c} \quad .etc.$$

Since the expression (2.14) contains the operator α_n whose representatives (2.13) are four row , four column matrices, Dirac assumes that the wave function ψ is determined by the matrix

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \qquad (2.16)$$

According to this theory the electron is determined by four wave function

$\psi_\lambda(x,y,z,t)$, where $(\lambda = 1,2,3,4)$

The probability that an electron will be in a volume element $d\tau$ at time t is

$$\sum_{\lambda=1}^{4} |\psi_\lambda|^2 \, d\tau \qquad (2.17)$$

Eqn. (2.15) represents a system of four simultaneous first order partial differential equation :

$$\begin{aligned}
(P_o + mc)\psi_1 + (P_1 - iP_2)\psi_4 + P_3\psi_3 &= 0 \\
(P_o + mc)\psi_2 + (P_1 + iP_2)\psi_3 - P_3\psi_4 &= 0 \\
(P_o - mc)\psi_3 + (P_1 - iP_2)\psi_2 + P_3\psi_1 &= 0 \\
(P_o - mc)\psi_4 + (P_1 + iP_2)\psi_1 - P_3\psi_2 &= 0
\end{aligned} \qquad (2.18)$$

First, if one wishes to find a periodic solution, P_o must be replaced by $(E-(\epsilon V)/c)$. E being the energy of the electron. Secondly, if we assume that the velocity of the electron is small (V << c) compared with that of light, so that

$$E - mc^2 \ll E + mc^2$$

then one can see that ψ_3 and ψ_4 both satisfy Schödinger's equation. Further more if ψ' is a solution to the Schrödinger's equation, an approximate solution of (2.18) is

$$\begin{aligned}
\psi_3 &= A\psi' \\
\psi_4 &= B\psi' \\
\psi_1 &= -[P_o(P_1 - iP_2) + AP_3]\psi'/2mc \\
\psi_2 &= -[A(P_1 + iP_2) - aP_3]\psi'/2mc
\end{aligned} \qquad (2.19)$$

A and B are arbitrary constants , and P_1 , P_2 , P_3 are operators in eqns. (2.18) and (2.19). The components ψ_1 , ψ_2 are much smaller than ψ_3, ψ_4 and can be neglected in the expression (2.17) for the charge density. Thus if (2.17) is normalized to unity, and if the four functions also to be normalized, one must have this approximation

$$AA^* + BB^* = 1$$

Thus, with this approximation, expression (2.19) becomes

$$\psi = \psi' \begin{pmatrix} 0 \\ 0 \\ A \\ B \end{pmatrix} \qquad (2.20)$$

From here, the spin part of the appropriate eigen function in the rest frame is given by

$$\chi = \begin{pmatrix} 0 \\ 0 \\ A \\ B \end{pmatrix} \qquad (2.21)$$

By referring to the results of sec.1.3 for the two components spinors, the components of the spin function for the direction ϑ, φ which is defined in the rest frame are connected by the relation

$$\frac{B}{A} = \tan\frac{\vartheta}{2}\, e^{i\varphi} \qquad (2.22$$

The exact solution of eqn. (2.18) representing an electron moving in free space (V = 0) with momentum (p_x, p_y, p_z) and energy E has been given by Darwin [19] and is

$$\begin{aligned} \psi_1 &= -[AP_z + B(P_x - iP_y)]S/(mc + E/c) \\ \psi_2 &= -[A(P_x + iP_y) - BP_z]S/(mc + E/c) \\ \psi_3 &= AS \\ \Psi_4 &= BS \end{aligned} \qquad (2.23)$$

where $P_x^2 + P_y^2 + P_z^2 = E^2/c^2 - m^2c^2$.

here S denotes $\exp\{i\,[\,P_x x + P_y y + p_z z - Et\,]/\hbar\}$ and A and B are arbitrary constants.

The wave function describing free electron in the Z - axis of propagation can be taken as

$$\psi_\lambda = a_\lambda\, i\, \exp(Kz - wt)$$

where a_λ is arbtrary constant which must be determined

Substituting $S = \exp i(P_z Z - Et)/\hbar$ into eqn.(2.23) and using the relations $E = \hbar w$ and $p_z = \hbar k$, one obtains by comparison

$$\left.\begin{aligned} a_1 &= -AK\hbar c/(mc^2 + E) \;, \quad a_2 = BK\hbar c/(mc^2+E) \\ a_3 &= A \qquad\qquad\quad , \quad a_4 = B \end{aligned}\right\} \qquad (2.24)$$

From here, one can see that a_λ are not all independent, and from the result of (2.24), the general form of the plane wave is found to be

$$\psi = \left[A \begin{pmatrix} -\dfrac{cP_z}{E+mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix} + B \begin{pmatrix} 0 \\ \dfrac{cP_z}{E+mc^2} \\ 0 \\ 1 \end{pmatrix} \right] e^{i(kz-wt)} \qquad (2.25)$$

This wave function (eqn. (2.28)) is not an eigen function of Σ_x and Σ_y except for the special case $P_z = 0$. On the other hand it is an eigen function $\Sigma_z = h\sigma_z/2$ with the eigen value ($\hbar/2$).

Hence, it can be seen that in the relativistic case, it is only in the rest frame of the electron that one can speak of a transverse spin direction of the plane wave (i.e. spins perpendicular to the direction of propagation). Only in the rest frame can one assign an eigen value to the spin operator in an arbitrary direction ϑ, φ as in eqn.(2.21) [4].

2.2. The Scattering of Electrons by a Central Force

2.2.1. The Differential Cross - Section

The scattering of relativistic electrons with spin by a central field will be consider . The electrons will be taken as an incident plane wave in the Z - direction. In analogy to non - relativistic scattering theory, the solutions to the Dirac equation with the asymptotic form is given by[4,12].

$$\Psi_\lambda \xrightarrow[r\to\infty]{} a_\lambda e^{ikz} + U_\lambda(\theta,\phi)\ e^{ikr}r^{-1} \qquad (2.26)$$

for the four components of the wave function (λ = 1,2,3,4). The first and the second terms of expression (2.26) represent the incident and scattered wave, respectively.

Generalizing the differential elastic scattering cross section obtained from the Schrödinger theory one finds

$$\frac{d\sigma(\theta,\phi)}{d\Omega} = \sigma(\theta,\phi) = \frac{\sum_{\lambda=1}^{4} |U_\lambda(\theta,\phi)|^2}{\sum |a_\lambda(\theta,\phi)|^2} \qquad (2.27)$$

For normalized wave functions , the denominator in(2.27)is 1.

The quantities a_λ are not independent [see solution (2.24)]. This help us to simplify the expression (2.27). Referring from the solution (2.24) for a plane wave with arbitrary spin direction, which shows that

$$m = \frac{a_1}{a_3} = \frac{k\hbar c}{E+mc^2} = \frac{a_2}{a_4} \qquad (2.28$$

The same relation exists between the U_λ for asymptotically scattered wave. Thus eqn. (2.27) becomes

$$\alpha(\theta,\phi) = \frac{|U_3|^2 + |U_4|^2 + |U_3|^2 m^2 + |U_4|^2 m^2}{|a_3|^2 + |a_4|^2 + |a_3|^2 m^2 + |a_4|^2 m^2}$$

$$= \frac{|U_3|^2 + |U_4|^2\,[1+m^2]}{|a_3|^2 + |a_4|^2\,[1+m^2]}$$

$$= \frac{|U_3|^2 + |U_4|^2}{|a_3|^2 + |a_4|^2} \qquad (2.29)$$

In the following, the scattering of electron waves whose spins are in the +Z or -Z direction is considered. If the solution to the scattering problem is known for these two basic states one can construct all other cases from them.

In the case in which the spin of the incident wave in the

+Z direction, its wave function from last section is

$$\begin{bmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{bmatrix} = \begin{bmatrix}\cdot\\ \cdot\\ \cdot\\ 1\\ 0\end{bmatrix} e^{ikz} \qquad (2.30)$$

The small components ψ_1 and ψ_2, due to their dependance on the "large" components ψ_3 and ψ_4 (eqn. 2.28), yield no additional information as is shown clearly by (2.29); they are therefore need not be considered further. To solve the scattering problem for solutions of the Dirac equation with the asymptotic form

$$\begin{bmatrix}\psi_3\\ \psi_4\end{bmatrix} \xrightarrow[r\to\infty]{} \begin{bmatrix}1\\ 0\end{bmatrix} e^{ikz} + \begin{bmatrix}f_1(\theta,\phi)\\ g_1(\theta,\phi)\end{bmatrix} \frac{e^{ikr}}{r} \qquad (2.31)$$

this takes account of the fact that the second component of the wave function is no longer necessarily zero after scattering as the spin may change its direction due to spin-orbit coupling. Thus, g, is called spin -flip amplitude.

Analogously, for the incident wave with the other spin direction (spins anti parallel to the direction of motion), a solution with the asymptotic form is given by

$$\begin{bmatrix}\psi_3\\ \psi_4\end{bmatrix} \xrightarrow[r\to\infty]{} \begin{bmatrix}0\\ 1\end{bmatrix} e^{ikz} + \begin{bmatrix}g_2(\theta.\phi)\\ f_2(\theta,\phi)\end{bmatrix} \frac{e^{ikr}}{r} \qquad (2.32)$$

To obtain the function f_1, f_2 g_1, and g_2 use may be made of the sets of solutions found by Darwin of the equation (2.18) with the scalar scattering potential V a function of r only and the vector potential zero. The groups of solutions are given as [13]

$$\left.\begin{aligned}\Psi_3 &= (l+1)\, G_l(r)\, P_l(\cos\theta) \quad , \quad \Psi_4 = -G_l(r)\, P_l^1(\cos\theta)\, e^{i\phi} \\ \Psi_3 &= l\, G_{-l-1}(r)\, P_l(\cos\theta) \qquad\qquad \Psi_4 = G_{-l-1}(r)\, P_l^1(\cos\theta)\, e^{i\phi}\end{aligned}\right\} (A)$$

$$\left.\begin{aligned}\Psi_3 &= G_l(r)\, P_l^1(\cos\theta)\, e^{-i\phi} \quad , \quad \Psi_4 = (l+1)\, G_l(r)\, P_l(\cos\theta) \\ \Psi_3 &= -G_{-l-1}(r)\, P_l^1(\cos(\theta)\, e^{-i\phi} \qquad \Psi_4 = l G_{-l-1}(r)\, P_l^1(\cos\theta)\end{aligned}\right\} (B) \qquad (2.33)$$

For the two cases, (A) referring to electron with spins parallel and (B) with spins anti parallel to the direction of incidence.

Where P_l and P_l^1 are the Legendre polynomials and associate Legendre functions, respectively , and G_l is a solution of the simultaneous equation

$$\begin{aligned}\frac{1}{\hbar}\left[\frac{E}{c} + \frac{\epsilon V}{c} + mc\right]F_l + \frac{dG_l}{dr} - \frac{1}{r}G_l = 0 \\ -\frac{1}{\hbar}\left[\frac{E}{c} - mc\right]G_l + \frac{dF_l}{dr} + \frac{l+2}{r}F_l = 0\end{aligned} \qquad (2.34)$$

and G_{-l-1} is a solution of a similar pair of equations with -l-1 in place of l.

By eliminating of the function F_l, one obtains

$$\frac{d^2G_l}{dr} + \left(\frac{2}{r} - \frac{\alpha'}{\alpha}\right)\frac{dG_l}{dr} + \left(\alpha\beta - \frac{l(l+1)}{r^2} + \frac{1}{r}\frac{\alpha'}{\alpha}\right)G_l = 0 \qquad (2.35)$$

where, $\alpha = 1/h(E/c + \epsilon v/c + mc)$, $\beta = 1/h\ (E/c + \epsilon v/c - mc)$

$\alpha' = d\alpha/dr$

Substitution of $G_l = \alpha^{1/2} L_l(r)\ r^{-1}$ brings the equation into the Schrödinger form of the radial part

$$d^2L_l/dr^2 + [\ K^2 - (l(l+1))/r^2 - U_l(r)\ ]L_l = 0 \qquad (2.36)$$

with

$$\begin{aligned}-U_l(r) &= \frac{2E\epsilon V}{\hbar^2c^2} + \frac{\epsilon^2V^2}{\hbar^2c^2} + \frac{(l+1)}{r}\frac{\alpha'}{\alpha} - \frac{3\alpha'^2}{4\alpha^2} + \frac{\alpha''}{2\alpha} \quad , \\ K^2 &= (E^2 - m^2c^4)/\hbar^2c^2\end{aligned} \qquad (2.37)$$

A similar result follows for L_{-l-1} with -l-1 in place of l.

Of the terms appearing in the expression (2.37) for $U_l(r)$,

the first two are independent of the electron spin and are typical of the Klein - Gordon equation for a particle without spin. The remaining terms are a consequence of spin-orbit interaction depend, not only on the potential, but also on the force and its radial derivative.

As with the treatment of scattering in the Schrödinger theory, the solution of the radial differential equations for potentials decrease faster than r^{-1} have the asymptotic form

$$G_l(r) \xrightarrow{r\to\infty} (Kr)^{-1} \sin(Kr - (l\pi/2) + \eta_l) \qquad (2.38)$$
$$G_{-l-1} \xrightarrow{r\to\infty} (Kr)^{-1} \sin(Kr - (l\pi/2) + \eta_{-l-1})$$

Since l(l+1) remains fixed as $l \to -l-1$.

Let us construct from the particular solutions (2.33A), (partial waves), a solution which has the required form (2.31). This can be done if they are combined as follows [13]

$$\psi_3 = \sum_{l=0}^{\infty} \left((l+1)e^{i\eta_l}G_l + l e^{i\eta_{-l-1}}G_{-l-1}\right) i^l P_l(\cos\theta)$$

$$\psi_4 = \sum_{l=1}^{\infty} \left(-e^{i\eta_l}G_l + e^{i\eta_{-l-1}}G_{-l-1}\right) i^l P_l^1(\cos\theta)\, e^{i\phi} \qquad (2.39)$$

From these and previous results one can obtain

$$f_1(\theta,\phi) = \frac{1}{2ik}\sum_{l=0}^{\infty}\left[(l+1)(e^{2i\eta_l} - 1) + l(e^{2i\eta_{-l-1}} - 1\right] P_l(\cos\theta) \qquad (2.40)$$

$$g_1(\theta,\phi) = \frac{1}{2ik}\sum_{l=1}^{\infty}\left[e^{-2i\eta_l} + e^{2i\eta_{-l-1}}\right]P_l^1(\cos\theta)\, e^{i\phi}$$

The solution of the scattering problem is thus reduced to a calculation of the scattering phase η_l. These depend, as in the non-relativistic case, on the energy of the incident electrons and on the scattering potential (scattering substance). Hence the scattering amplitudes $f_1(\theta,\phi)$ and $g_1(\theta,\phi)$, apart from

depending on the scattering angle, also depend on these two variables.

For the case (2.32) of anti parallel spin, one finds, by a similar procedure, that

$$f_2(\theta,\phi) = f_1(\theta,\phi) = f(\theta) \ ,$$

and that

$$g_2(\theta,\phi) = - g(\theta)\ e^{-i\phi} \qquad (2.41)$$

where, $g_1(\theta,\phi) = g(\theta)\ e^{i\phi}$

The physical quantities which can be measured in a scattering experiment are determined by a scattering amplitude $f(\theta)$ and $g(\theta)$, where $f(\theta)$ is analogous to the scattering amplitudes known from the scattering theory based on Schrödinger's equation, and $g(\theta)$ describes the change of spin direction during the scattering process.

Now the general case of arbitrary initial spin direction is treated in which the incident wave is given by

$$A\begin{bmatrix}1\\0\end{bmatrix}e^{ikz} + B\begin{bmatrix}0\\1\end{bmatrix}e^{ikz} = \begin{bmatrix}A\\B\end{bmatrix}e^{ikz} = \begin{bmatrix}a_3\\a_4\end{bmatrix}e^{ikz} \qquad (2.42)$$

Where A and B, according to eqn. (2.22), specify the spin direction in the rest frame. Using eqns. (2.31), (2.32), (2.41) and (2.42), one obtains by coherent superposition for the asymptotic form of the scattered wave as

$$\begin{bmatrix}U_3\\U_4\end{bmatrix}\frac{e^{ikr}}{r} = A\begin{bmatrix}f_1\\g_1\end{bmatrix}\frac{e^{ikr}}{r} + B\begin{bmatrix}g_2\\f_2\end{bmatrix}\frac{e^{ikr}}{r} = \begin{bmatrix}Af - Bge^{-i\phi}\\Bf + Age^{i\phi}\end{bmatrix}\frac{e^{ikr}}{r} \qquad (2.43)$$

Thus, from (2.29) the differential cross section is given by

$$\sigma(\theta,\phi) = \frac{|U_3|^2 + |U_4|^2}{|A|^2 + |B|^2}$$

$$= |f|^2 + |g|^2 + (fg^* - gf^*)\left(\frac{-AB^*e^{i\phi} + A^*Be^{-i\phi}}{|A|^2 + |B|^2}\right) \qquad (2.44)$$

Eqn. (2.44) shows that the scattering intensity generally depends on ϕ, illustrated in Fig. (2.1) for $s(\theta) > 0$, and A = B = 1. For this condition the differential cross section is

$\sigma(\theta,\phi) = (|f|^2 + |g|^2)\ (1 - S(\theta)\sin\phi\ )$

Eqn. (2.44) can be re-written as

$$\sigma(\theta,\phi) = (|f|^2 + |g|^2)\left[1 + S(\theta)\,\frac{(A^*Be^{-i\phi} - AB^*e^{i\phi})}{i(|A|^2 + |B|^2)}\right] \qquad (2.45)$$

where

$$S(\theta) = \frac{i(fg^* - f^*g)}{|f|^2 + |g|^2} \qquad (2.45^*$$

Known as Sherman function

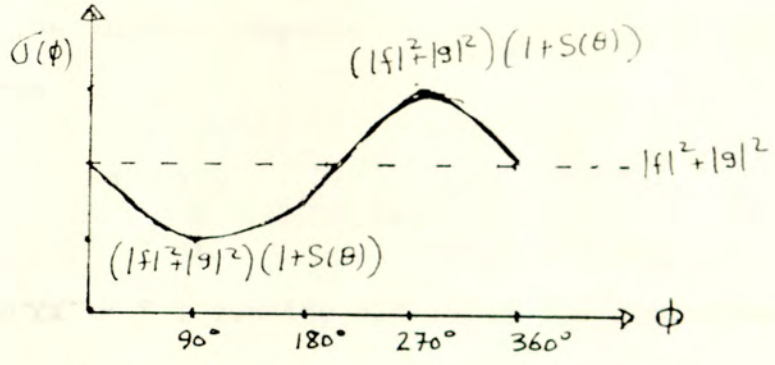


Fig. (2.1) Dependance of the differential cross section on the azimuthal angle ϕ. (for $s(\theta) > 0$ and A= B = 1)

2.2.2 Dependance of Differential Cross Section on Polarization.

The change of the density matrix due to a collision process is considered. The effect of collisions on a spin wave function such as eqn. (2.42) is to change A and B to new values U_3 and U_4 of eqn. (2.43), respectively. This may be represented as a transformation of χ to χ' spinor.

$\chi = \begin{vmatrix} a \\ b \end{vmatrix}$ of a pure initial state spinor, and

$$\chi' = \begin{bmatrix} U_3 \\ U_4 \end{bmatrix} = \begin{bmatrix} Af - Bge^{-i\phi} \\ Bf + Age^{i\phi} \end{bmatrix} \quad \textit{of the final state spinor.}$$

This can be represented mathematically as, transformation

$$\chi' = \begin{bmatrix} f & -ge^{-i\phi} \\ ge^{i\phi} & f \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = S\chi \qquad (2.46)$$

S is defined as the spin scattering matrix so that

$$S = \begin{bmatrix} f & -ge^{-i\phi} \\ ge^{i\phi} & f \end{bmatrix} \quad \textit{apart from normalization factor}$$

It is a function of the scattering angle θ,ϕ as well as the electron energy.

The density matrix of the scattered beam may now be written

$$\begin{aligned} \rho' &= \chi' \chi'^{*} \\ &= S\chi' (S\chi')^{*} = S\chi'\chi'^{*}S^{*} \\ &= S\rho S^{*} \end{aligned}$$

since $\chi\chi^{+} = \rho$ (density matrix of the unscattered state) , it follows that

$$\rho' = S\rho S^{*} = \tfrac{1}{2}S(I + \vec{P}.\vec{\sigma})S^{*}\, tr(\rho) \qquad (2.47)$$

Eqn. (2.47) can be used to directly write the dependance of the differential cross section on the polarization $\vec{P}$ of the incident beam. It is clearly seen that $tr(\rho') = |U_3|^2 + |U_4|^2$ and $tr(\rho) = |A|^2 + |B|^2$. Taking the ratio of the two and comparing with eqn.(2.29) one has

$$\sigma(\theta,\phi) = \frac{tr(\rho')}{tr(\rho)} \qquad (2.48)$$

Therefore with (2.47) the dependence of the differential cross

section on the polarization of the primary beam is

$$\sigma(\theta,\phi) = \tfrac{1}{2}tr[S(I + \vec{P}.\vec{\sigma})S^{*}] \qquad (2.49)$$

To evaluate this one must form the trace of the product

$$\begin{pmatrix} f & -ge^{-i\phi} \\ ge^{i\phi} & f \end{pmatrix}\begin{pmatrix} 1+P_z & P_x-iP_y \\ P_x+iP_y & 1-P_z \end{pmatrix}\begin{pmatrix} f^{*} & g^{*}e^{-i\phi} \\ -g^{*}e^{i\phi} & f^{*} \end{pmatrix}$$

The calculation yields

$$\sigma(\theta,\phi) = (|f|^2+|g|^2)\left(1-\frac{S(\theta)}{2i}[e^{i\phi}(P_x-iP_y)-e^{-i\phi}(P_x+iP_y)]\right) \qquad (2.50$$

The differential cross section is thus independent of the longitudinal polarization component P_z.

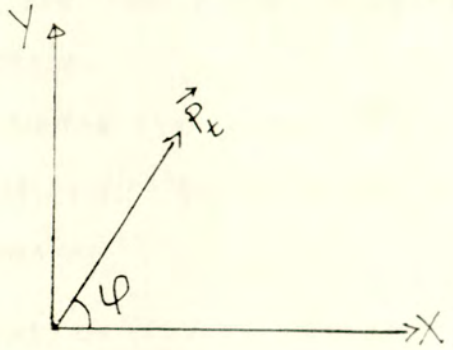


Fig. 2.2 Transverse polarization component

With $P_t \exp(\pm i\varphi) = P_x \pm iP_y$, where P_t is the magnitude of the transverse polarization $\vec{P}_t$ (See Fig.(2.2)). Thus,

$$\sigma(\theta,\phi) = I(\theta)\left(1 - \frac{S(\theta)}{2i}P_t[e^{i(\phi-\varphi)} - e^{-i(\phi-\varphi)}]\right)$$
$$= I(\theta)(1 - P_t S(\theta)\,Sin(\phi-\varphi)) \qquad (2.51)$$

This shows that for an electron beam which has no transverse polarization the differential cross section is independent of the azimuthal angle ϕ, and simply has the value $I(\theta) = |f(\theta)|^2 + |g(\theta)|^2$.

Eqn.(2.51) can be further simplified if one defines the

direction of the transverse polarization component in the X-direction (see Fig. 2.3a). Then it follows that the differential cross section for a primary beam with arbitrary polarization is

$$\sigma(\theta,\phi) = I(\theta)\ [1 - P_t S(\theta)\sin\phi] \qquad (2.52$$

If we take a unit vector $\vec{n}$ perpendicular to the scattering plane

$$\vec{n} = \frac{\vec{K} \times \vec{K'}}{|\vec{K} \times \vec{K'}|}$$

where $\vec{K}$ & $\vec{K'}$ are the plane containing the incident and scattered direction.

According to the Fig.(2.3a) , $\vec{K}$ = (0,0,1), $\vec{K'}$ = (cosϕ , sinϕ ,0) , $\vec{P}$ = (P_x,0,P_z), $P_x = P_t$. From these conditions the unit vector $\vec{n}$ is given by

$$\vec{n} = (-\sin\phi,\ \cos\phi,\ 0) \qquad (2.53)$$

so that

$$-P_t\sin\phi = \vec{P}.\vec{n}$$

and thus from (2.52)

$$\sigma(\theta,\phi) = I(\theta)(1 + S(\theta)\vec{P}.\vec{n}) \qquad (2.54)$$

This formula is independant of the choice of coordinate system as the scalar product is invarient under coordinate transformation.This is the basic equation for the measurement of electron polarization by " Mott scattering" [4]. Mott scattering is a scattering process which used to determine the polarization of the electron beam [see Fig. (2.3b)].

N_L and N_r are the number of electrons scattered to the left and right by the target, respectively, having primary incident polarization $\vec{P}_o$.

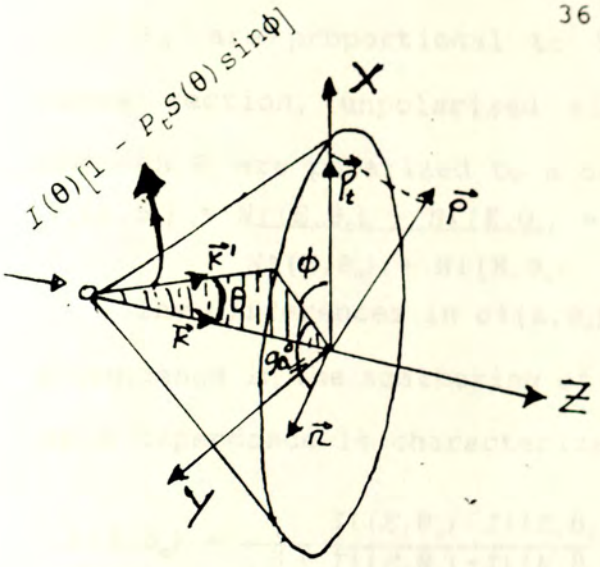


Fig. 2.3a Scattering of polarized beam

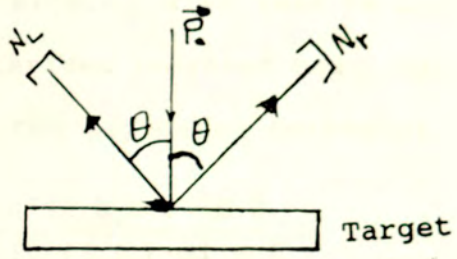


Fig 2.3b Mott Scattering

2.3. Spin Orbit Elastic Scattering

The physical basis of spin - dependece in elastic scattering can most easily be visualized for the case of electron scattering from a free atom. For motion in a central potential V(r), the spin orbit term in the interaction Hamiltonian from solution (1.47) is given by

$$V_{so} = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dv(r)}{dr}\vec{S}.\vec{L}$$

if one consider an unpolarized incident beem of energy E as consisting of equal numbers of electrons with " spin - up" (e↑) and "spin - down" (e↓) relative to the scattering plane, these electrons experience different potentials as a consequence of V_{so}. Thus, the number of spin - up ($N\uparrow(\theta_o,E)$ and spin - down $N\downarrow(\theta_o,E)$ electrons scattered in a particular direction θ_o relative to the incident beem, will in general not be the same, i.e. the corresponding differential scattering cross section $\sigma\uparrow(E,\theta_o)$ and $\sigma\downarrow(E,\theta_o)$ are different. Since $N\uparrow(E,\theta_o)$ and

$N\downarrow(E,\theta_o)$ are proportional to the corresponding differential cross section, unpolarized electrons elastically scattered through θ_o are polarized to a degree

$$P_u(E,\theta_o) = \frac{N\uparrow(E,\theta_o) - N\downarrow(E,\theta_o)}{N\uparrow(E,\theta_o) + N\downarrow(E,\theta_o)} = \frac{\sigma\uparrow(E,\theta_o) - \sigma\downarrow(E,\theta_o)}{\sigma\uparrow(E,\theta_o) + \sigma\downarrow(E,\theta_o)} \quad (2.55)$$

The differences in $\sigma\uparrow(E,\theta_o)$ and $\sigma\downarrow(E,\theta_o)$ also lead to spin dependence in the scattering of a polarized incident beam. This spin dependance is characterized by the asymmetry parameter

$$A(E,\theta_o) = \frac{1}{|\vec{P}_o|}\frac{I\uparrow(E,\theta_o) - I\downarrow(E,\theta_o)}{I\uparrow(E,\theta_o) + I\downarrow(E,\theta_o)} = \frac{\sigma\uparrow(E,\theta_o) - \sigma\downarrow(E,\theta_o)}{|\vec{P}_o|(E,\theta_o) + \sigma\downarrow(E,\theta_o)} \quad (2.56)$$

where $I\uparrow(E,\theta_o)$ and $I\downarrow(E,\theta_o)$ are the scattered electron currents at angle θ_o for incident electrons with the spin - up and spin - down, respectively, and $\vec{P}_o$ is the polarization of primary beam. $1/|\vec{P}_o|$ is a normallization factor accounting for beam polarization $|\vec{P}_o|$ is in general less than unity. In the case of atomic scattering, $S(\theta_o,E) = A(E,\theta_o) = P_u(E,\theta_o)$.

An interseting aspect of $P_u$and A is that large polarization features occur in atomic scattering only near cross - section minima, because only in such regions are there sizable differences in the relative magnitudes of $\sigma\uparrow$ and $\sigma\downarrow$ [4,7]

2.4. Polarization of an Electron Beam by Scattering

The density - matrix formalism readily produces the remarkable fact that an initially unpolarized electron beam is polarized by the scattering process. From (1.24) one has

$$\vec{P}' = tr(\rho'\vec{\sigma})/tr(\rho')$$

If the primary beam is unpolarized one obtains from (2.47), with $\vec{P}$ =0,

$$\rho'_u = \tfrac{1}{2}S(I + \vec{P}.\vec{\sigma})\ S^{*}tr(\rho) = \tfrac{1}{2}SS^{*}tr(\rho) \qquad (2.57$$

so that the polarization of the scattered beam is

$$\vec{P}'_u = \frac{tr(SS^{*}\vec{\sigma})\,tr(\rho)}{2tr(\rho'_u)} \qquad (2.58)$$

From expressions (2.48) and (2.50) one has $tr(\varrho')/tr(\varrho) = \sigma(\theta,\phi) = |f(\theta)|^2 + |g(\theta)|^2$, where (2.50) has been applied in the special case of an unpolarized primary beam. Furthermore, with $\vec{\sigma} = \Sigma\vec{e}_i\sigma_i$ where $\vec{e}_i$ are unit vectors along x,y,z direction and σ_i are defined by (1.6) one has

$$\tfrac{1}{2}tr(SS^{*}\vec{\sigma}) = \tfrac{1}{2}tr\begin{pmatrix} f^2 + g^2 & fg^{*}e^{-i\phi} - f^{*}ge^{-i\phi} \\ f^{*}ge^{i\phi} - fg^{*}e^{i\phi} & f^2 + g^2 \end{pmatrix}\begin{pmatrix} \vec{e}_z & \vec{e}_x - i\vec{e}_y \\ \vec{e}_x + i\vec{e}_y & -\vec{e}_z \end{pmatrix}$$

upon evaluating the matrix product, one may obtain

$$\tfrac{1}{2}tr(SS^{*}\ \vec{\sigma}) = i(fg^{*} - f^{*}g)\ (-\sin\phi e_x + \cos\phi e_y)$$

Since from (2.53), $\vec{n}$ = (- sinφ , cosφ ,o), one finally obtains,

$$\vec{P}'_u = S(\theta)\ \vec{n} \qquad (2.59)$$

where $\vec{P}_u$ is the polarization obtained by scattering of an unpolarized electron beam, and S(θ) is the Sherman function.

This happens because different scattering potentials results in different scattering cross sections one obtains different number of e↑ and e↓ in the scattered beam. In other words: The scattering beam is polarized even though the incident beam is an unpolarized, and acquires a polarization of magnitude S(θ) perpendicular to the scattering plane. This together with the result of the last section, shows that the Sherman function describes two important features : The extent

of the left - right asymmetry in the scatering of a polarized beam and the amount of polarization produced by scattering of an unpolarized beam [3,4,13].

2.5. Behaviour of Polarization in Scattering.

It hs been considered in the preceding section that polarization of the scattered beam from an unpolarized incident beam from an unpolarized incident beam was $S(\theta)\vec{n}$. Now, given an incident electron beam with arbitrary polarization $\vec{P}_o$, the Polarization $\vec{P}'$ after scattering from eqn. (1.24) is

$$\vec{P}' = \frac{tr(\rho'\vec{\sigma})}{tr(\rho')} = \frac{\frac{1}{2}tr\left[(I + \vec{P}_o.\vec{\sigma})S^*\vec{\sigma}\right]}{\frac{1}{2}tr\left[(I + \vec{P}_o.\vec{\sigma})S^*\right]} \qquad (2.60)$$

where $\vec{P}_o$ is the primary polarization.

The denominator has already been evaluated (see solution (2.49) to (2.54)) with the result $(|f(\theta)|^2+|g(\theta)|^2)$ $(1+ S(\theta)$ $\vec{P}_o.\vec{n})$. The numerator can be evaluated similarly. As a result, one obtains for the polarization after scattering

$$\vec{P}' = \frac{(\vec{P}_o.\vec{n} + S(\theta))\vec{n}+T(\theta)(\vec{P}_o-(\vec{P}_o.\vec{n})\vec{n})+U(\theta)(\vec{n}x\vec{P}_o)}{1+\vec{P}_o.\vec{n}\,S(\theta)} \qquad (2.61)$$

with,

$$S(\theta) = \frac{i(fg^*-f^*g)}{f^2+g^2}\,,\quad T(\theta) = \frac{f^2-g^2}{f^2+g^2}\,,\quad U(\theta) = \frac{fg^*+f^*g}{f^2+g^2} \qquad (2.62)$$

If one resolves the polarization vector into components P_{op} parallel to the scatering plane and P_{on} perpendicular to it (i.e., parallel to $\vec{n}$, see Fig.(2.4)) one has $\vec{P}_o = \vec{P}_{on} + \vec{P}_{op}$. As $(\vec{P}_o.\vec{n})\vec{n} = \vec{P}_{on}$ and $\vec{n} \times \vec{P}_{on} = 0$ or $\vec{n} \times \vec{P}_o = \vec{n} \times \vec{P}_{op}$. Eqn.(2.61) can also be written in the form

$$\vec{P}' = \frac{(P_{on} + S(\theta))\vec{n} + T(\theta)\vec{P}_{op} + U(\theta)(\vec{n}x\vec{P}_{op})}{1+P_{on}\,S(\theta)} \qquad (2.63)$$

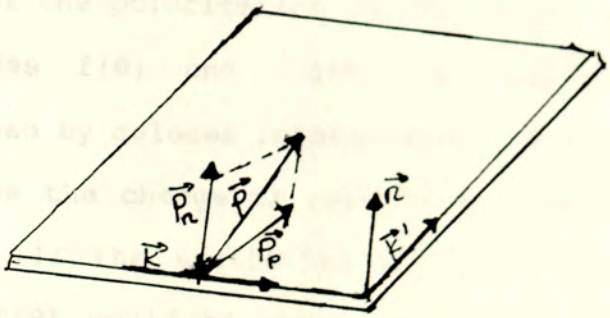


Fig. 2.4 Decomposition of arbitrary initial polarization $\vec{P}_o$. $\vec{K}$ and $\vec{K}'$ are the elctron wave vectors before and after scattering.

In the formula only the essential components of the initial polarization appear. The expression (2.60) may be written again in another form, taking into account vector identity,

$$\vec{a}x(\vec{b}x\vec{c}) = (\vec{a}.\vec{c})\vec{b} - (\vec{a}.\vec{b})\vec{c} \ ,$$

which in our case

$$\vec{n}x(\vec{P}_o x\vec{n}) = \vec{P}_o - (\vec{P}_o.\vec{n})\vec{n} = \vec{P}_{op}$$

Then,

$$\vec{P}' = \frac{[\vec{P}_o.\vec{n}+S(\theta)]\vec{n} + T(\theta)\vec{n}\ x\ [\vec{p}_o x\vec{n}] + U(\theta)(\vec{n}x\vec{P}_o)}{1 + \vec{P}_o\vec{n}S(\theta)} \qquad (2.64)$$

The terms T(θ) and U(θ) describes the change of the polarization vector during the scattering process. If $U(\theta) \neq 0$, there is a component of the polarization P′ perpendicular to the plane ($\vec{n}$, $\vec{P}_{op}$) which is identical to the plane ($\vec{P}_{on}$, $\vec{P}_{op}$), i.e. U(θ) describes the rotation of the initial plane. T(θ) is seen from expression (2.63) to describe the change of the

polarization component parallel to the scattering plane. The change of the polarization vector is due to the two scattering amplitudes f(θ) and g(θ). An amplitude f(θ) which is determined by coloumb interaction, and an amplitude g(θ) which describes the change of spin direction during the scattering process. If the scattering amplitudes g(θ) were zero, eqn. (2.62) T(θ) would be equal to 1 while S(θ) & U(θ) would be zero, thus, according to eqn.(2.63), there would be no change of the polarization during the scattering process [3,4].

The angle α, through which the polarization componenet P_{op} in the scattering plane is rotated, is given by (see Fig.(2.5))

$$\tan\alpha = \frac{U(\theta)\ |\vec{n}\ \vec{P}_{op}}{T(\theta)\ |\vec{P}_{op}} = \frac{U(\theta)}{T} \qquad (2.65$$

Also, from (2.64), it can be shown that the angle α_2 between the vector $\vec{n}$ & $\vec{p}'$ is given by the following simple equation

$$\tan\alpha_2 = \frac{\vec{P}_o \times \vec{n}\ (1 - s^2)^{1/2}}{S(\theta) + \vec{P}_o \cdot \vec{n}} = \frac{P_o \sin\alpha_1 (1 - s^2)^{1/2}}{S(\theta) + P_o \cos\alpha_1} \qquad (2.66$$

Where α_1 is the angle between $\vec{n}$ and $\vec{P}_o$.

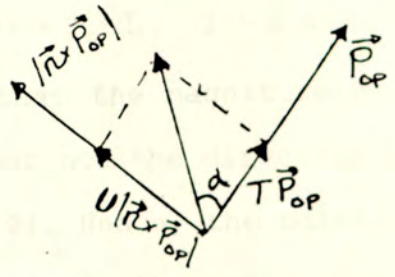


Fig. 2.5 Angle of rotation of the polarization component $\vec{P}_{op}$

It is useful for polarization measurments to express $\vec{P}'$ in the form of three orthogonal components with directions given by the unit vectors $\vec{n}$, $\vec{K}$ and $\vec{K} \times \vec{n}$ or $\vec{n}$, $\vec{K}'$, and $\vec{K}' \times \vec{n}$. The

following expression is given for the case that the unit vectors for the components of $\vec{P}'$ are given by $\vec{n}$, $\vec{K}'$ and $\vec{K}' \times \vec{n}$, and the unit vectors for the components of $\vec{P}_o$ are given by $\vec{n}$, $\vec{K}$, and $\vec{K} \times \vec{n}$. Then eqn.(2.64) may be written in the form [17,18]

$$\vec{P}' = \frac{(S(\theta) + \vec{P}_o . \vec{n})\vec{n} + [L\vec{P}_o . \vec{K} + R\vec{P}_o . (\vec{K} \times \vec{n})]\vec{K}' + [L\vec{P}_o . (\vec{K} \times \vec{n}) - R\vec{P}_o . \vec{K}](\vec{K}' \times \vec{n})}{1 + \vec{P}_o . \vec{n} S(\theta)} \quad (2.67)$$

where, $L(\theta) = U(\theta) \sin\theta + T(\theta) \cos\theta$

$R(\theta) = U(\theta) \sin\theta - T(\theta) \cos\theta$, and θ is the angle between $\vec{K}$ & $\vec{K}'$

The results given here show that the scattering amplitudes $f(\theta)$ and $g(\theta)$ provide a complete description of the intensity distribution and the behaviour of the polarization in the scattering process.

The following special cases are readily derived from the general case given by (2.67).

1. Initial beam is only polarized in the transverse direction such that $\vec{P}_o . \vec{n} = P_o$, $\vec{P}_o . \vec{K} = 0$ and $\vec{P}_o . (\vec{K} \times \vec{n}) = 0$, then eqn. (2.67) reduces to

$$\vec{P}' = [(S(\theta) + P_o)\vec{n}] / (1 + S(\theta) P_o) \quad (2.68a)$$

it shows that the magnitude of the polarization vector only changes, but not the direction of the polarization vector $\vec{P}_o$ (i.e. $P_{op} = 0$). Hence, the polarization conserves its direction perpendicular to the scattering plane. If the initial beam is completely polarized in the transverse direction such that $\vec{P}_o . \vec{n} = 1$, $\vec{P}_o . \vec{K} = 0$ and $\vec{P}_o . (\vec{K} \times \vec{n}) = 0$, then eqn. (2.67) reduces to

$$\vec{P}' = \vec{n}$$

2. Initial beam is completely polarized in the

longitudinal direction such that $\vec{P}_o.\vec{n} = 0$, $\vec{P}_o.(\vec{k} \times \vec{n}) = 0$ and $\vec{P}_o.\vec{K} = 1$, then eqn. (2.67) reduces to

$$\vec{P}' = S(\theta)\vec{n} + L\vec{K}' - R(\vec{K}' \times \vec{n}) \qquad (2.68b)$$

3. Initial beam is unpolarized such that $\vec{P}_o = 0$

$$\vec{P}' = S(\theta)\,\vec{n} \qquad (2.68c)$$

In general, scattering changes not only the direction but also the magnitude of the polarization vector as shown in the above cases.

From (2.63), it can be shown that the magnitude of $\vec{P}'$ can be expressed simply in terms of $S(\theta)$ and $\vec{P}_o$. Using the relation $S^2(\theta) + T^2(\theta) + U^2(\theta) = 1$, which follows immediately from the definition (2.62),

$$\vec{P}'^2 = \frac{(P_{on} + S(\theta))^2 + T^2 P_{op}^2 + U^2 P_{op}^2}{(1 + P_{on}S(\theta))^2}$$

with $P_o^2 - P_{on}^2 = P_{op}^2$ one has

$$\begin{aligned}\vec{P}'^2 &= \frac{(P_{on} + S)^2 + (1 - S^2)(P_o^2 - P_{on}^2)}{(1 + P_{on}S)^2} \\ &= \frac{(1 + P_{on}S)^2 - [1 - P_o^2 - S^2 + P_o^2 S^2]}{(1 + P_{on}S)^2} \\ &= 1 - \frac{[(1 - P_o^2)(1 - S^2)]}{(1 + \vec{P}_o.\vec{n}S(\theta))^2}\end{aligned} \qquad (2.69)$$

Eqn. (2.69) demobstrate the following facts:

a) For a completely polarized beam, $|\vec{P}_o| = 1$, the magnitude of the polarization remains constant (i.e. $|\vec{P}'| = 1$).

b) For $S(\theta) = 0$, the magnitude of the scattered polarization remains constant (i.e. $|\vec{P}'| = 1$), but the direction of the scattered polarization depends on the direction of the initial beam polarization.

2.6. Equality of Polarizing and Analyzing Power

The connection between the following two facts is given now which are proved in the previous sections.

1) Scattering as a polarizer : a beam that is originally unpolarized acquires the polarization $\vec{P} = S(\theta)\vec{n}$ from scattering, i.e., the polarization is determined by the Sherman function.

2) Scattering as an analyzer : the left - right asymmetry observed with the scattering of a beam that is polarized perpendicular to the scattering plane is also determined by $S(\theta)$. For a completely polarized beam ($|\vec{P}_o| = 1$) one has

$$A = \frac{N_l - N_r}{N_l + N_r} = \frac{1 + S(\theta) - (1 - S(\theta))}{1 + S(\theta) + 1 - S(\theta)} = S(\theta)$$

(N_l, N_r = number of electrons scattered to left and right, respectively).

From 1 and 2 above, one can easily see that polarizer and analyzer are characterize by one and the same function $S(\theta)$.

Considering the incident unpolarized beam to be a mixture of equal numbers of electrons polarized in the opposite direction, one half are totally polarized in the direction ↑ perpendicular to the scattering plane; the other half are totally polarized in the opposite direction (see Fig. 2.6). From (2.54), it follows from this for the e↑ beam that the scattering intensities to the left is propertional to $1+S(\theta)$ $\vec{P}.\vec{n} = 1 + S(\theta)$, whereas the intensities to the right is proportional to $1 - S(\theta)$ due to the opposite vector $\vec{n}$. For the e↓ beam the corresponding intensities proportional to $1 - S(\theta)$ and $1 + S(\theta)$ to the right and left, respectively. In both cases the polarization vectors remain unchanged, since they are

perpendicular to the scattering plane and have the magnitude 1.

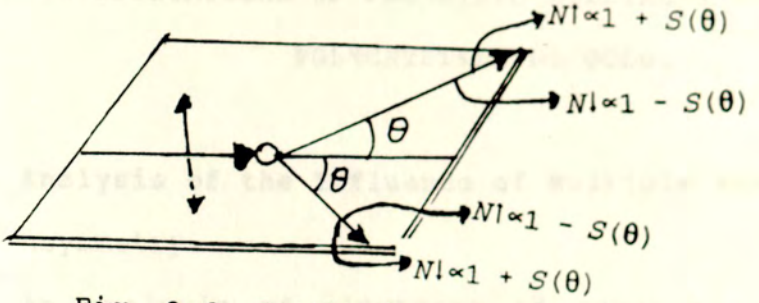


Fig. 2.6 Scattering of an unpolarized beam

The fact that there are different numbers of e↑ and e↓ in the scattered beam means that the beam is polarized. Fig. 2.6 illustrates that for scattering to the left the degree of polarization is

$$P = \frac{N\uparrow - N\downarrow}{N\uparrow + N\downarrow} = \frac{1 + S - (1 - S)}{1 + S + 1 - S} = S(\theta)$$

Similarly, for scattering to the right the polarization P = $-S(\Theta)$. Thus, polarization after the scattering of an unpolarized beam to the right and left, both quantities are described by the same function $S(\Theta)$ [4.7].

CHAPTER III

3. INVESTIGATIONS OF POLARIZED ELECTRONS SCATTERING BY POLYCRYSTALLINE GOLD.

3.1. Analysis of the Influence of Multiple Scattering on the Asymmetry.

An analysis of electrons of moderate energies by the surface of solid could not be done without allowance for the multiple scattering of electrons on target atoms [20]. Several models have been suggested to allow for multiple scattering for the intensity of elastically scattered electrons [21,22].

Calculations of asymmetry were made using the scheme proposed [21] to determine the intensity of elastically scattered electrons.

The following assumptions were made.

1) Elastic scattering of electrons on single atoms represents independent events and the differential cross sections for single scattering are the same for atoms in isolated and aggregate atoms. In view of the absence of experimental results, theoretical values of the differential cross sections and asymmetries of elastic scattering by free atoms [23,24] were used. From eqns. (2.55) and (2.56) in the case of single collision $P_u = A = S(\Theta)$.

2) The intensity of a beam of electrons that have not lost the primary energy E_p in the course of motion in matter decreases continuously and is governed by an attenuation coefficient μ. Where, $\mu = d(Q_{in} + Q_{el})$ and Q_{el} and Q_{in} are the integral cross sections for elastic and inelastic processes, d is the atomic density.

3) It was considered that there are no interaction between the incident and reflected electrons, and the observed effects are not modulated by diffraction as in crystalline solids.

The following comments should be made about these assumptions. The use of the differential scattering cross sections of isolated atoms in the calculation of the intensity of a single interaction of electrons with ionic cores in a solid is fully justified [21]. Scattering through a large angle (backward scattering) is characterized by a small impact parameter, i.e., it occurs at distance close to the center of an atom. Naturally, the values of the potentials of free atom and an ionic core in a solid should be similar at such distances [25]. Nevertheless, this assumption is not well satisfied when the differential cross sections represent the scattering through small angles which occur in the expression for calculating the intensity in the case of multiple interactions. However, the calculated intensities of elastically and multiply scattered electrons are not very sensitive to details of the dependence of the low angle scattering cross sections because of dominant contribution of single scattering [21].

Assumption 2 is based on the good agreement between the experimental and the theoretical values of the intensity of elastically scattered electrons [21] which lead to the conclusion that the main mechanism governing the scattering process are included in the adapted model.

Assumption 3 is based on the experimental work [9]. Before the experimental measurements were carried out, it was cheked that the sample didn't show any diffraction pattern. In

accordance with this fact is, that in the calculation of the asymmetry diffraction condition was not taken into account.

The asymmetry of the elastic scattering (through an angle θ) of polarized electrons parallel to the normal of scattering plane of the beam can generally be found from the expression

$$A(\theta) = \frac{\sum_{n=1}^{N} A_n(\theta)\, I_n(\theta)}{\sum_{n=1}^{N} I_n(\theta)} \qquad (3.1)$$

where A_n is the asymmetry of n-fold scattering of polarized electrons and I_n is the intensity of n-fold scattered electrons. In the case of single scattering, $A_1(\theta)$ is the asymmetry for the scattering by a single atom. According to eqn. (2.56), $A_1(\theta) = S(\theta)$.

To calculate the intensity of n-fold scattered electrons, a proposed model [21] was applied. Therefore, the intensity of electrons which have been elastically scattered once and only once is

$$I_1(\theta) = I_o d \int_0^{\infty} \exp\left(\frac{-z\mu}{\cos\alpha}\right) \frac{dz}{\cos\alpha}\, \sigma(\theta) \exp\left(\frac{-z\mu}{\cos\gamma}\right) = \frac{d I_o \sigma(\theta)}{\mu\left(1 + \frac{\cos\alpha}{\cos\gamma}\right)} \qquad (3.2)$$

where I_o is the intensity of the primary beam, and α, γ are the angles of incidence and reflection measured from the normal to the target surface; $\sigma(\theta)$ is the differential scattering cross section, and z is running coordinate directed along the normal to the surface of the target.

It is shown in the case of double interaction [21] the intensity obtained in the approximation of small angles

scattering is

$$I_2(\theta_3) \approx \frac{I_o d^2}{2\mu^2(1+\frac{\cos\alpha}{\cos\gamma})}\int \sigma(\theta_1)\,\sigma(\theta_2)\,d\Omega_2 \qquad (3.3$$

where θ_3 is the angle between the direction of the incident and scattered beams, whereas θ_1 and θ_2 are the large and small intermediate scattering angles [see Fig. (3.1)].

A similar calculation of the n - fold scattering gives

$$I_n(\theta_3) = I_o \frac{d^n}{n[1+\frac{\cos\alpha}{\cos\gamma}]\mu^n}\int_{\Omega_2}\cdots\int_{\Omega_n}\sigma(\theta_1)\ldots\sigma(\theta_n)\,d\Omega_2\ldots d\Omega_n \qquad (3.4$$

To evaluate the convolution integral in eqn.(3.4) would require a considerable computations. Instead of such calculations the following approximation is made [21]. Recognizing that $\sigma(\theta)$ is strongly peaked in a forward direction, the main contribution to the convolution comes from multiple scattering events in which all but one of the scattering is near forward. In this approximation the convolution integral for n multiple scattering process is

$$\int_{\Omega_2}\cdots\int_{\Omega_n}\sigma(\theta_1)\ldots\sigma(\theta_n)\,d\Omega_2\ldots d\Omega_n \approx n\langle\sigma(\theta_3)\rangle(Q_{el}^f)^{n-1} \qquad (3.5)$$

where Q_{el}^f is the total cross sections for elastic scattering into the forward direction and $\langle\sigma(\theta_3)\rangle$ is the average differential cross section taken over an angular range centered at θ_3.

The small angle approximation is justified because the differential cross section for the scattering through the angles less than 30° exceeds considerably the cross section for the scattering for the other angles more than 10^2 times [23].

Fig. 3.1 shows schematically double scattering for a fixed

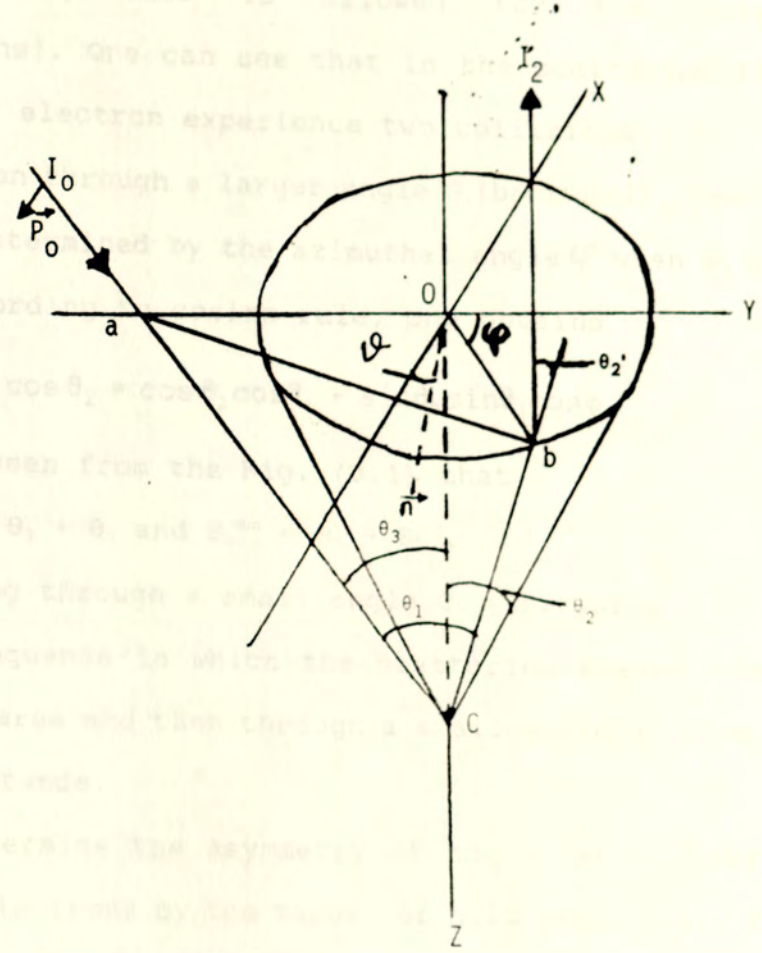


Fig. 3.1. Schematic representation of double scattering of a beam of polarized electrons.

value of a small angle θ_2. In this figure the angles θ_1 and θ_3 are shown for the backward scattering and θ_2 is the forward scattering. [This is allowed for the programs of calculations]. One can see that in the scattering through an angle θ_3 an electron experience two collisions.

1)reflection through a larger angle θ_1(backward), the values of which is determined by the azimuthal angle φ when θ_3 and θ_2 are fixed. According to cosine rule, one obtains

$$\cos\theta_1 = \cos\theta_2\cos\theta_3 + \sin\theta_2\sin\theta_3\cos\varphi \qquad (3.6)$$

and it is seen from the Fig. (3.1) that

$\theta_1^{max} = \theta_3 + \theta_2$ and $\theta_1^{min} = \theta_3 - \theta_2$.

2)Scattering through a small angle θ_2 (forward)

The sequence in which the scattering events occur first through a large and then through a small angle or vice versa is of no importance.

To determine the asymmetry of the elastic scattering of polarized electrons by the target of gold (eqn. 3.1), first the intensity $I_n(\theta_3)$ and asymmetry $A_n(\theta_3)$ for multiple scattering should be calculated. To do so $I_n(\theta_3)$ and $A_n(\theta_3)$ were calculated using the following methods.

1) The value of $\sigma_n(\theta_3)$ of the scattering through an angle θ_3 in interaction of different scattering multiplicity was calculated. In the case of double scattering from eqn. (3.5) this quantity is given by

$$\int_{\Omega_2}\sigma_1(\theta_1)\,\sigma_1(\theta_2)\,d\Omega_2 = 2\langle\sigma(\theta_3)\rangle\int_{\Omega_2}\sigma_1(\theta_2)\,d\Omega_2$$
$$= \sigma_1(\theta_3)\int_{\Omega_2}\sigma_1(\theta_2)\,d\Omega_2$$

and then,

$$\sigma_2(\theta_3) = \frac{\int_{\Omega_2} \sigma_1(\theta_1)\,\sigma_1(\theta_2)\,d\Omega_2}{\int_{\Omega_2} \sigma_1(\theta_1)\,d\Omega_2} \qquad (3.7)$$

where $\sigma_1(\theta_1)$ and $\sigma_1(\theta_2)$ are the theoretical differential cross sections for a large angle (θ_1) and a small angle (θ_2) of scattering.

To calculate the differential cross sections for triple, quadruple, etc. scattering process, we substituted in eqn. (4.7) not the tabulated (theoretical) differential cross section for a single scattering $\sigma(\theta_1)$ but the calculated values of $\sigma_2(\theta_3)$, $\sigma_3(\theta_3)$, etc., respectively. This is due to the small - angle approximation. Following the same procedure, the following general formula was used to calculate for n - multiple scattering (n > 2)

$$\sigma_n(\theta_3) = \frac{\int \sigma_{n-1}(\theta_3)\,\sigma_1(\theta_2)\,d\Omega_2}{\int \sigma_1(\theta_2)\,d\Omega_2} \qquad \text{where } n = 3,4,\ldots \qquad (3.8$$

The cross section for the scattering through a small angle $\sigma_1(\theta_2)$ was taken constant in calculations of interactions of any multiplicity.

In this case the expression for the intensity of n - fold scattered beam of eqn.(3.4) written as

$$I_n(\theta_3) = \frac{I_o d^n}{n(1 + \frac{\cos\alpha}{\cos\gamma})\mu^n}\sigma^n(\theta_3)\,(Q_{e^-}^{f})^{n-1} \qquad (3.9)$$

2) The expression of the asymmetry $A_n(\theta_3)$ for n - multiple interactions could be obtained using the following method. A primary polarized beam with polarization P_o was used. The

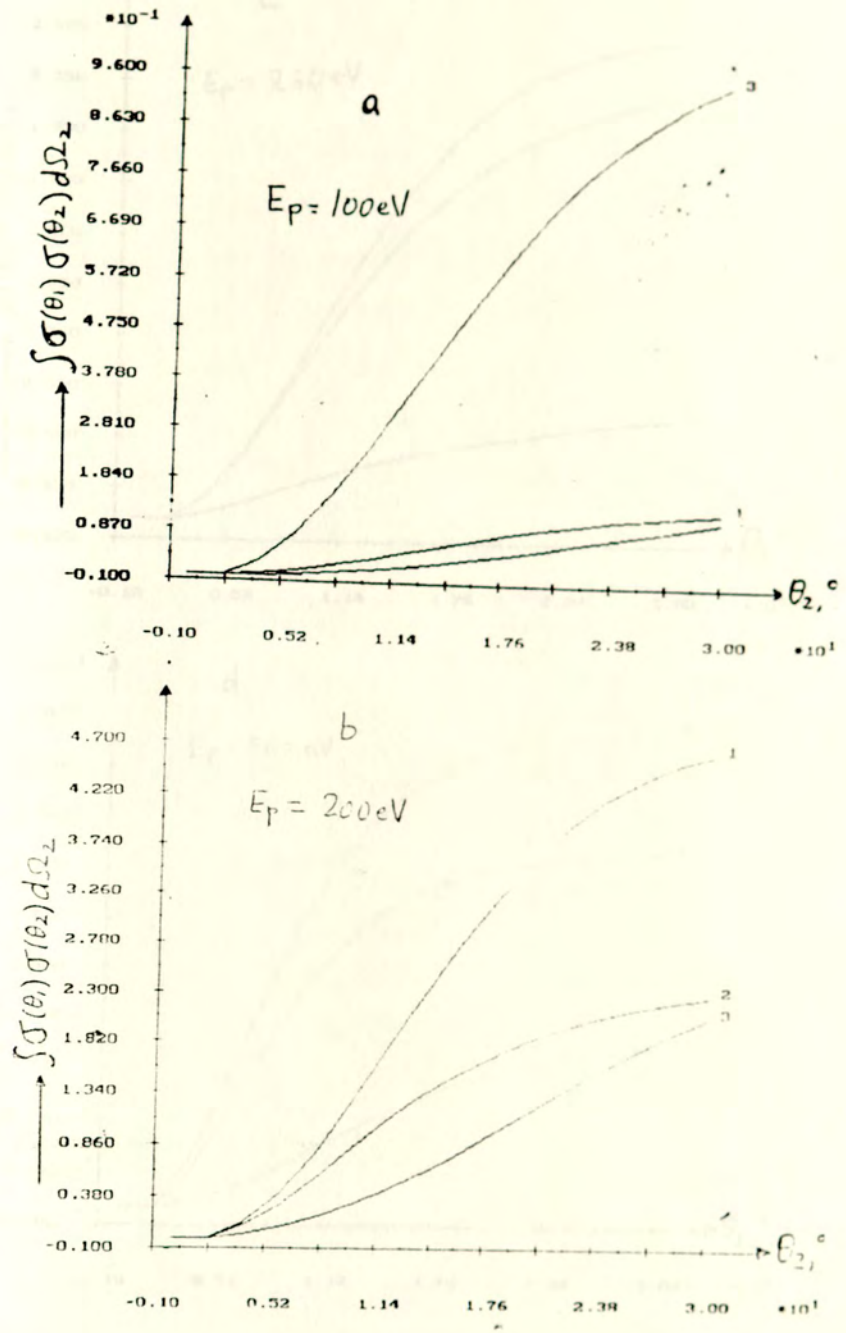


Fig 3.2 Dependence of $\int\sigma(\theta_1)\sigma(\theta_2)d\Omega_2$ on the small angle θ_2 for electron energy a) E_p = 100 , b) 200 eV. The numbers 1,2 and 3 along side the curve give the scattering angle θ_3 = 22°, 44° and 90°, respectively.

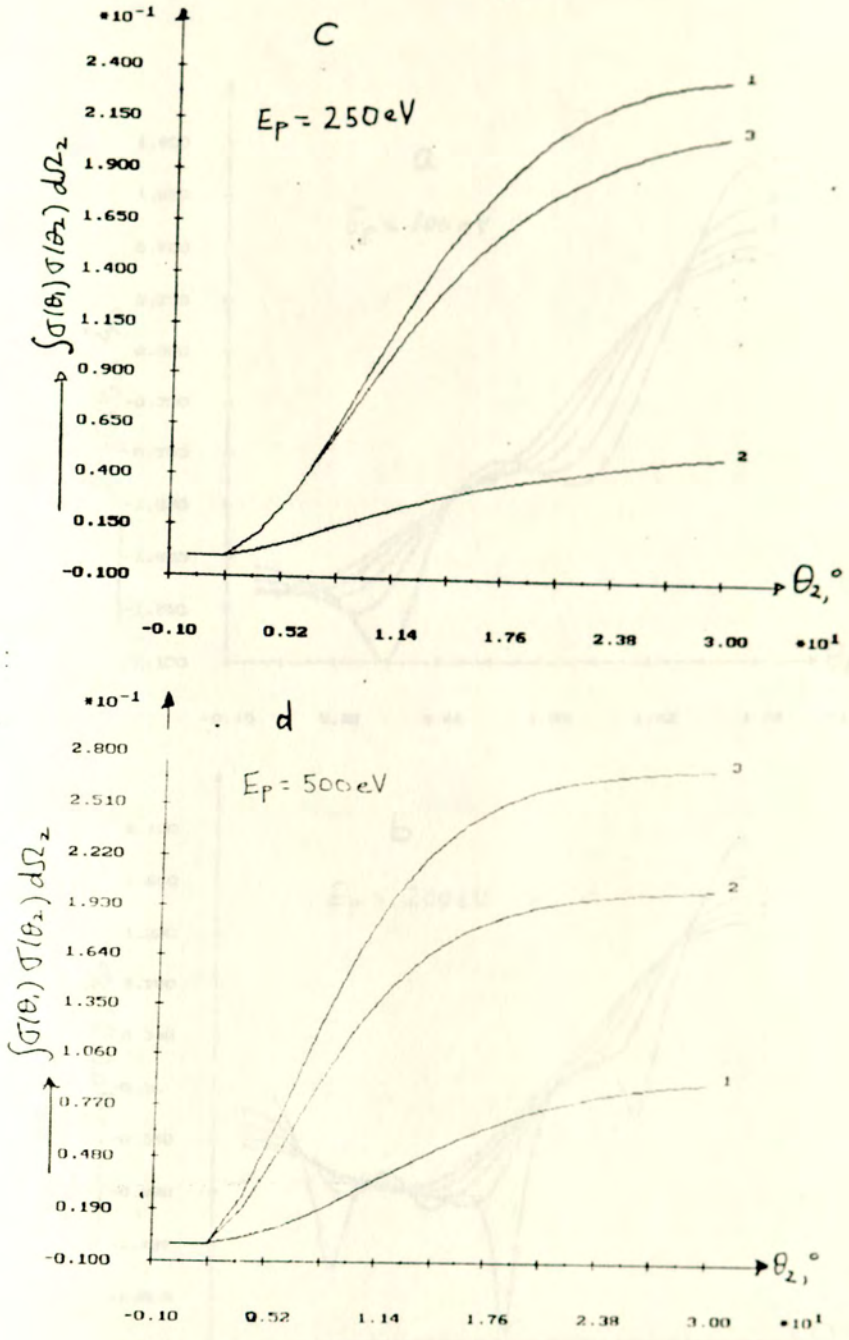


Fig 3.2 Dependence of $\int\sigma(\theta_1)\sigma(\theta_2)d\Omega_2$ on the small angle θ_2 for electron energy c) E_p = 250 , d) 500 eV.
The numbers 1,2 and 3 along side the curve give the scattering angle θ_3 = 22°, 44° and 90°, respectively.

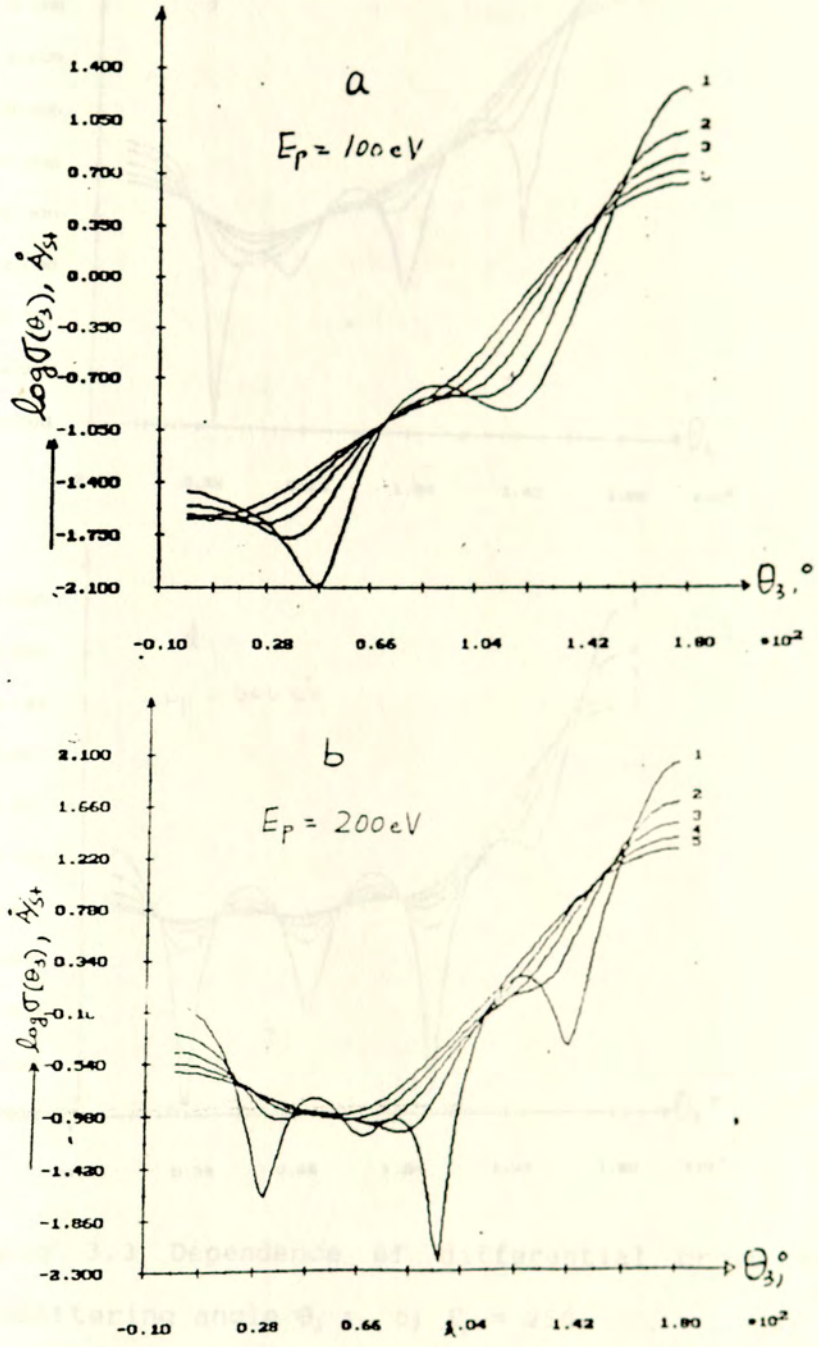


Fig 3.3 Dependence of differential cross section on the scattering angle θ_3 : a) E_p = 100 , b) 200 eV
The numbers alongside the curve give the scattering multiplicity

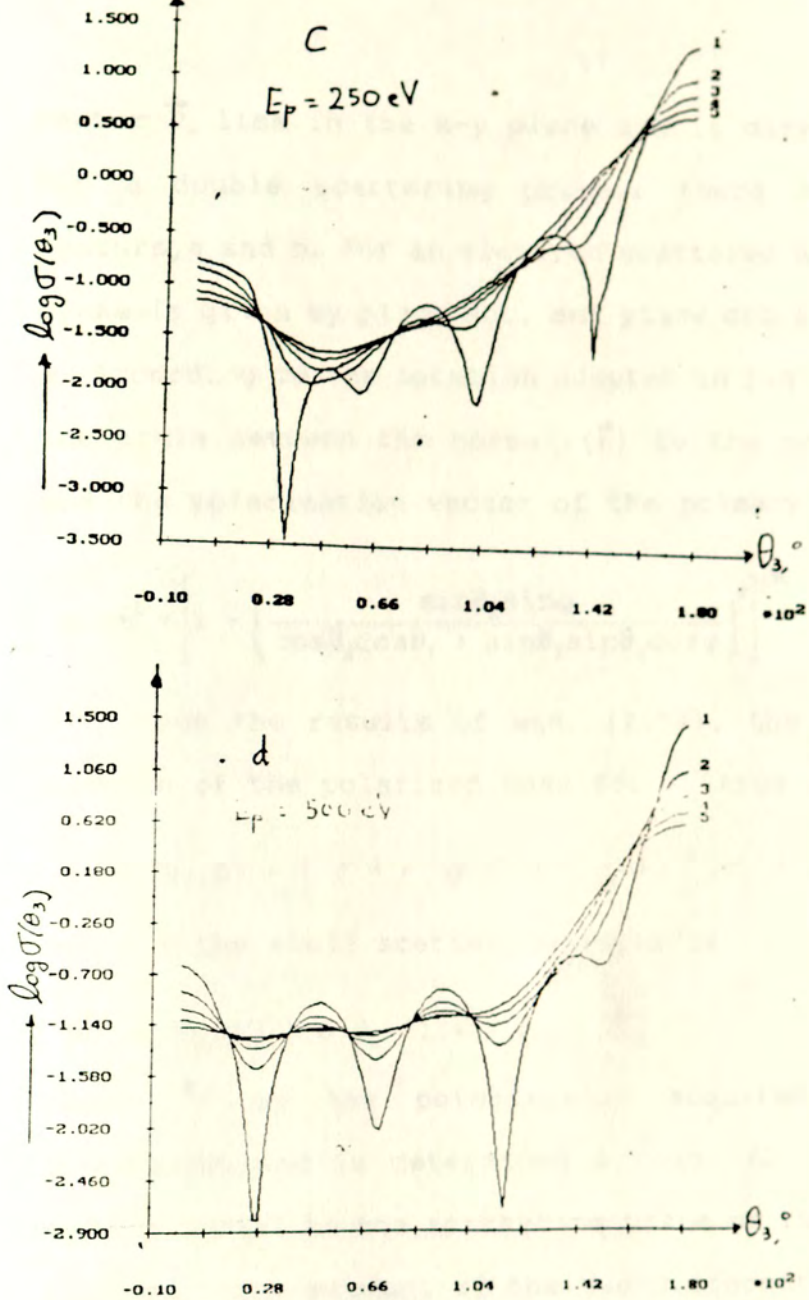


Fig 3.3 Dependence of differential cross section on the scattering angle θ_3 : c) E_p = 250 , d) 500 eV
The numbers alongside the curve give the scattering multiplicity

vector $\vec{P}_o$ lies in the x-y plane and is directed along x-axis. For a double scattering process there are two scattering centers, a and b. For an electron scattered at a, the scattering plane is given by plane abc, and plane cob is for scattering at b. According to the notation adopted in Fig. 3.1, the cosine of the angle between the normal ($\vec{n}$) to the scattering plane abc and the polarization vector of the primary beam is given by

$$\cos\psi = \left[1 + \left(\frac{\sin\theta_2 \sin\varphi}{\cos\theta_2\cos\theta_3 + \sin\theta_2\sin\theta_3\cos\varphi}\right)^2\right]^{-1/2} \qquad (3.10)$$

From the results of eqn. (2.54), the differential cross section of the polarized beam for a large angle Θ_1 is

$$A)\ \sigma_1(\theta_1,\phi) = [\,f^2 + g^2][1 + S(\theta_1)\vec{P}_o.\vec{n}] = \sigma(\theta_1)[1 + S(\theta_1)\vec{P}_o.\vec{n}]$$

and for the small scattering angle is

$$B)\ \sigma_1(\theta_2,\phi') = \sigma(\theta_2)[1 + S(\theta_2)\vec{P}'.\vec{n}']$$

where $\vec{P}'$ is the polarization acquired after the first scattering and is determined by eqn. (2.61); $\vec{n}'$ is the unit vector normal to the scattering plane of the second scattering process. The product of the two differential cross sections, A and B, above gives

$$\sigma_1(\theta_1,\phi)\,\sigma_1(\theta_2,\phi) = \sigma_1(\theta_1)\,\sigma_1(\theta_2)[1 + \vec{P}_o.\vec{n}S(\theta_1) + \vec{P}.\vec{n}S(\theta_2) + (\vec{P}_o.\vec{n})(\vec{P}'.\vec{n})S(\theta_1)S(\theta_2)] \qquad (3.11)$$

To get a convenient expression for asymmetry calculation, the following approximations were made.

1) As shown in eqn. (2.61), when a beam with initial polarization $\vec{P}_o$ is scattered, the magnitude and the new direction of polarization $\vec{P}'$ after a collision depends on the ratio of the amplitudes of the forward scattered f(Θ) and the

scattering accompanied by spin flip $g(\theta)$. For the region of electron energies ($E_p \leq 500$ eV), $f(\theta) \approx 10^2 g(\theta)$ for small angles, and $f(\theta) \approx 10 g(\theta)$ for large angles of scattering [23,24]. Thus, it is possible to approximate eqn. (2.54) as $\vec{P}_o = \vec{P}'$.

2) In the case of single scattering, if the direction of the polarization beam is parallel to the normal of scattering plane, the asymmetry of the scattering is related by $A_1(\theta) = S(\theta)$. Since the asymmetry in the scattering of polarized electrons through small angle is much smaller than the scattering through large angles [23,24], the contribution of $A_1(\Theta_2) = S(\Theta_2)$ in eqn.(3.11) can be ignored.

From the above two considerations, eqn. (3.11) is approximated as

$$\sigma_1(\theta_1,\phi)\sigma_1(\theta_2,\phi') = \sigma_1(\theta_1)\sigma_1(\theta_2)[1 + P_o\cos\vartheta A_1(\theta_1)] \qquad (3.12)$$

Multiplying both sides by $d\Omega_2$ gives

$$\int_{\Omega_2}\sigma_1(\theta_1,\phi)\sigma_1(\theta_2,\phi')d\Omega_2 = \int_{\Omega_2}\sigma(\theta_1)\sigma(\theta_2)[1 + P_o\cos\vartheta A_1(\theta_1)]d\Omega_2 \qquad (3.13)$$

This is proportional to the intensity of double scattered electrons in the direction of Θ_3.

Substituting eqn.(3.13) into eqn. (2.56), tha asymmetry in the course of double scattering was calculated from

$$A_2(\theta_3) = \frac{\int_{\Omega_2}\sigma_1(\theta_1)\sigma_1(\theta_2)A_1(\theta_1)\cos\vartheta d\Omega_2}{\int_{\Omega_2}\sigma_1(\theta_1)\sigma_1(\theta_2)d\Omega_2} \qquad (3.14)$$

Following the procedure as in the calculation of n - multiple differential cross section, the asymmetries were calculated using

$$A_n(\theta_3) = \frac{\int_{\Omega_2} \sigma_{n-1}(\theta_3)\,\sigma_1(\theta_2)\,A_{n-1}(\theta_3)\cos\vartheta\, d\Omega_2}{\int_{\sigma_2} \sigma_{n-1}(\theta_3)\,\sigma_1(\theta_2)\, d\Omega_2} \qquad (3.15)$$

where n= 3,4,...

Before calculations of the scattering differential cross sections and asymmetries the range of integration is selected after an analysis of the dependence of the integral in the numerator of eqn.(3.7) on the angle of the cone representing scattering through a small angle θ_2. The angle of the onset of saturation of this dependence governs the range of the angle θ_2. This can be seen in Fig. 3.2 for different energies. In these calculations the range of small angles up to 30° was used.

Calculations of $\sigma_n(\theta_3)$ and $A_n(\theta_3)$ were made by standard method of numerical integration of eqns.(3.8) and (3.15) on a computer for double scattering and for scattering of higher multiplicity of E_p = 100, 200, 250, and 500 eV electron energies and the results are presented in Fig. 3.3 and Fig. 3.4, respectively.

Typical results of the calculations presented in Fig.3.3 shows that an increase in scattering multiplicity results in rapid smooth out of all the singularities typical of the differential cross section for single scattering. For n>3 and relatively for large values of θ the angular distributions become nearly isotropic. In the case of scattering asymmetry Fig. 3.4, inspite of the fact that the singularities of the

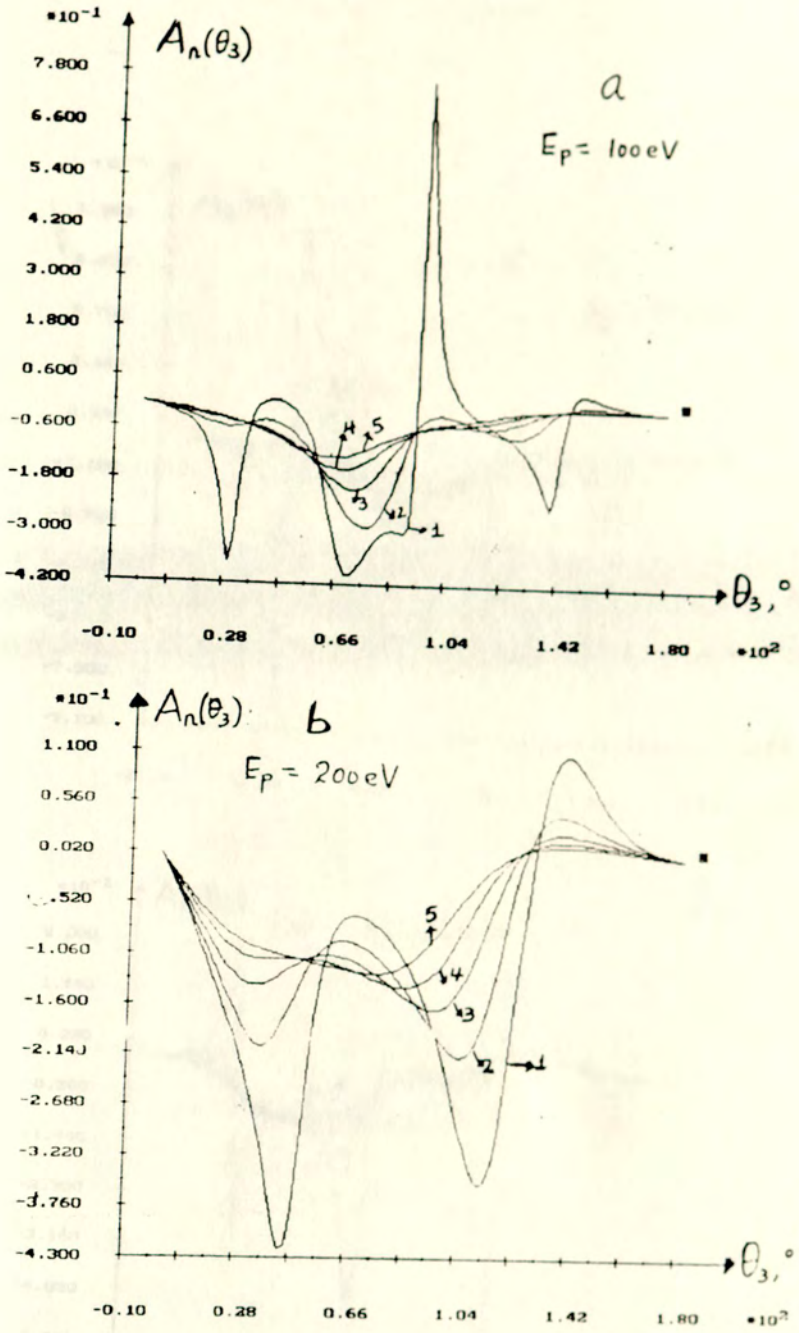
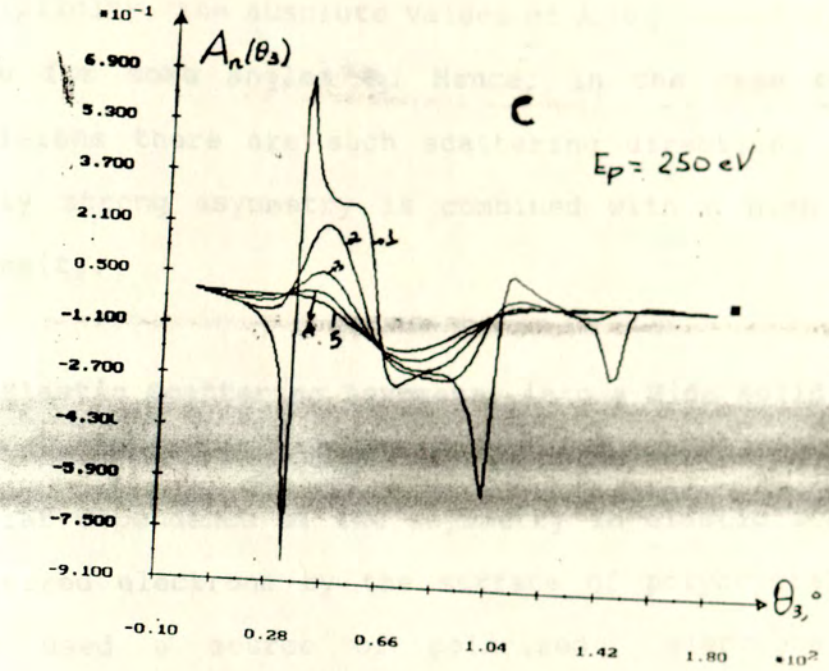


Fig 3.4 Dependence of asymmetry on the scattering angle θ_3:

a) E_p = 100 , b) 200 eV

The numbers along side the curve give the scattering multiplicity.



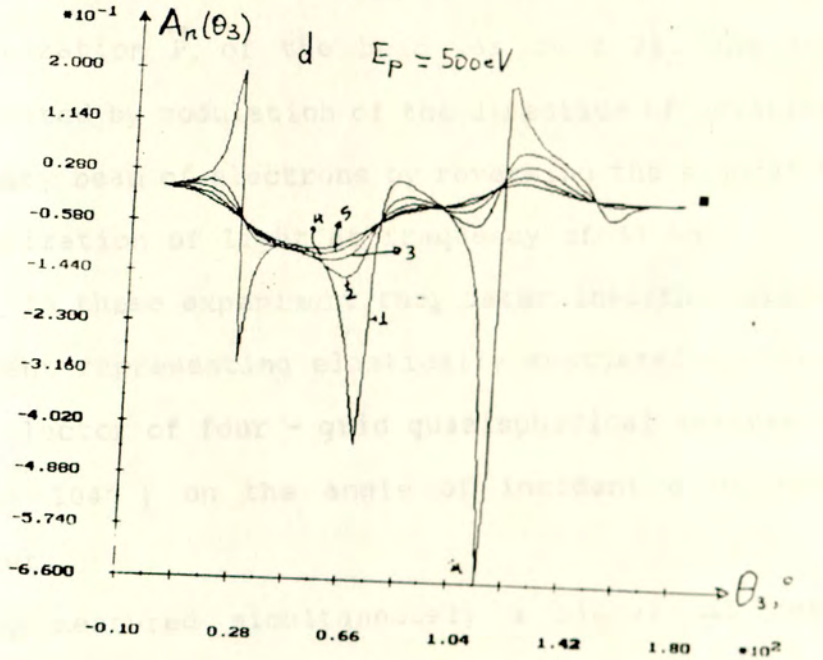


Fig 3.4 Dependence of asymmetry on the scattering angle θ_3:
c) E_p = 250 , d) 500 eV
The numbers along side the curve give the scattering multiplicity.

dependence $A_n(\theta_3)$ are also smoothed out on increase in the multiplicity, the absolute values of $A_n(\theta_3)$ remain sufficiently large for some angles θ_3. Hence, in the case of multiple collisions there are such scattering directions in which a fairly strong asymmetry is combined with a high scattering intensity.

3.2 Elastic Scattering Asymmetry into a Wide Solid Angle

Petrove et al. [9] investigated experimentally the angular dependence of the asymmetry in elastic scattering of polarized electrons by the surface of polycrystalline gold. They used a source of polarized electrons based on photoemission from $GaAs_{0.64}P_{0.36}$ solid solutions [26,27]. The polarization $\vec{P}_0$ of the beam was 35 ± 2%. The asymmetry was separated by modulation of the direction of polarization of the primary beam of electrons by reversing the sign of the circular polarization of light at frequency of 31 kHz.

In these experiment they determined the dependence of the current representing elastically scattered electrons reaching a collector of four - grid quasispherical analyzer (collection angle 104°) on the angle of incident α of the beam on a target.

They measured simultaneously a signal ΔI resulting from reversal of the direction of polarization of the incident beam. [The same symbol I is used for the current as for the intensity of the electron beam]. The asymmetry resulting from

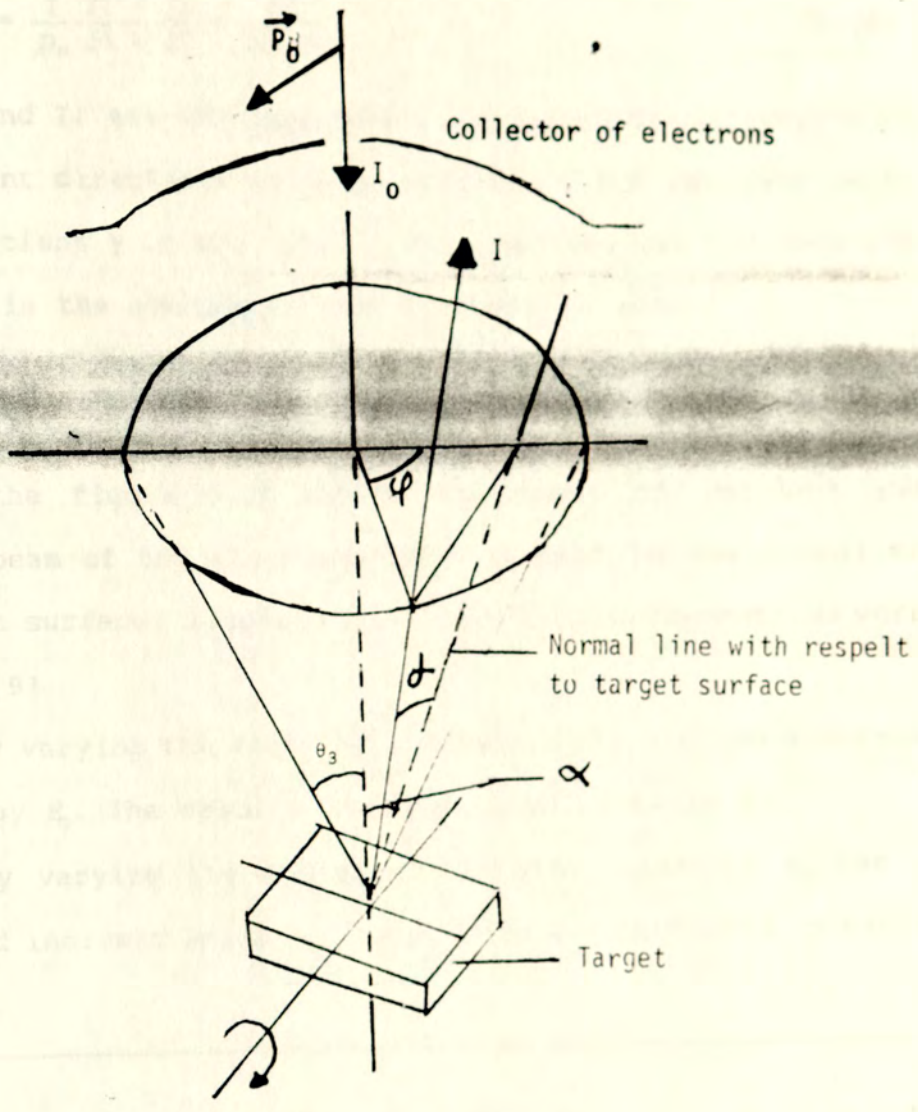


Fig. 3.5. Schematic representation of the scattering of polarized electrons along the direction of collector

such scattering was found from

$$A = \frac{1}{P_o}\frac{I\uparrow - I\downarrow}{I\uparrow + I\downarrow} = \frac{\Delta I}{2P_o I} \qquad (3.16)$$

where I↑ and I↓ are the currents to a collector corresponding to different directions of polarization of the incident beam. The coefficient ½ in eqn. (3.16) was used because the measured current I is the average of the currents I↑ and I↓.

Schematic representation of the scattering of polarized electrons along the direction of a collector is shown in Fig. 3.5. In the figure α, γ denote the angle of incident and emergent beam of the electrons with respect to the normal to the target surface, respectively. Scattering asymmetries were obtained [9]

1) By varying the angle of incident α for a fixed electron energy E_p. The results are tabulated in table 3.1.

2) By varying the energy of incident electron E_p for a fixed incident angle α. The results are tabulated in table 3.2.

α,°	0	2	6	10	12	16	20	22	26	28	32
-A(α),%	0	0.3	0.6	1.0	1.3	1.8	2.3	2.9	3.7	4.0	5.0

Table 3.1 E_p = 100 eV

E, eV	100	200	250	500
-A(E),%	5.0	0.7	-0.3	1.85

Table 3.2 α = 32°

Absolute experimental error ≈ 0.4 %

To compare the calculated and experimental results, it has

been found first the asymmetry of the scattering of polarized electrons by a solid in a wide angle equals to the angle of collector. According to Fig. 3.5, the actual angle γ of emergence of electrons depend on azimuthal angle φ related as

$$\cos\gamma = \cos\theta_3\cos\alpha + \sin\theta_3\sin\alpha\cos\varphi$$

In the case of such scattering the quantity $A(\alpha)$ can be found from the relation

$$\frac{\sum_{n=1}^{N}\int A_n(\theta_3)\cos\varphi\, I_n(\theta_3)\, d\Omega}{\sum_{n=1}^{N}\int I_n(\theta_3)\, d\Omega} \qquad (3.17)$$

where I_n and A_n are the current and the asymmetry of the scattering into an element $d\Omega$ of a wide solid angle. The factor $\cos\varphi$ allows for the scattering of electrons not parallel to the normal of the scattering plane.

An analysis of the expression for the intensity in the case of multiple scattering of electrons (eqn. 3.9) made it possible to simplify the procedure of calculation of the quantity $A(\alpha)$ in eqn. (3.17). Eqn. (3.9) can be considered as consisting of two factors. One of which $\{ (Q_{el}^{-1})^{n-1}(d^n)/(n\mu^n) \}$ is independent of the angles α and θ_3, whereas the second $\{(1+\cos\alpha/\cos\gamma)^{-1}\ \sigma_n(\theta_3)\}$ is dependent of the angles α and θ_3.

The total probability of energy losses when an electron crosses the target - vacuum interface also applied. The dependence of the probability of the surface energy loss on the angle of incidence or emergence for gold is given by [22]

$$P(E_p,\alpha) = 2.7 \,/\, (E_p^{1/2}\cos\alpha)$$

where E is an eV. This loss of energy reduces the intensity of the elastically scattered electron beam, so that the elastic

scattered electrons of eqn. (3.9) must be multiplied by the factor $(1 - P(E_p,\alpha))$ for the incident and $(1 - P(E_p,\gamma))$ for the scattered beam.

Therefore, the final expression for the scattering asymmetry of polarized electrons of different multiplicity in a wide solid angle is

$$A_n(\alpha) = \frac{\int A_n(\theta_3)\cos\varphi\,(1-P(E_p,\gamma))\left(1+\frac{\cos\alpha}{\cos\gamma}\right)^{-1}\sigma_n(\theta_3)\,d\Omega}{\int (1-P(E_p,\gamma))\left(1+\frac{\cos\alpha}{\cos\gamma}\right)^{-1}\sigma_n(\theta_3)\,d\Omega} \qquad (3.18)$$

The calculations were carried out by standard method of numerically integration on a computer in the range of angles θ_3 from 0° to 52°. The language used for the calculation was Turbo Pascal, and the programmes were created by Dr. S. Kotelinkove and Dr. A.N. Mishin. Use was made of the values of $\sigma_n(\theta_3)$ and $A_n(\theta_3)$ shown in Fig. 3.3 and Fig. 3.4, respectively.

The results of the calculations of $A_n(\alpha)$ for four electron energies E_p are presented in Fig. 3.6. It can be seen that the asymmetry of the scattering of polarized electrons rises monotonically on increase in the angle of incidence of electrons on the target and there is a tendency to reduce the difference between A_n and A_{n-1} asymmetries with increasing n [n- number of scattering multiplicity].

Fig. 3.6c of electron energy 250 eV shows a different behaviour than the other three electron energies of Fig. (3.6c,b,d). This different arises dueto the behaviour of the asymmetry of the single and multiple scattering for 250 eV in the region of scattering angle between θ_3 = 0° to 52°. $A_n(\alpha)$ depends on the behaviour of $A_n(\theta_3)$ and $\sigma_n(\theta_3)$ due to an integration of $A_n(\theta_3)\ \sigma_n(\theta_3)$ of eqn. (3.18). According to Fig.

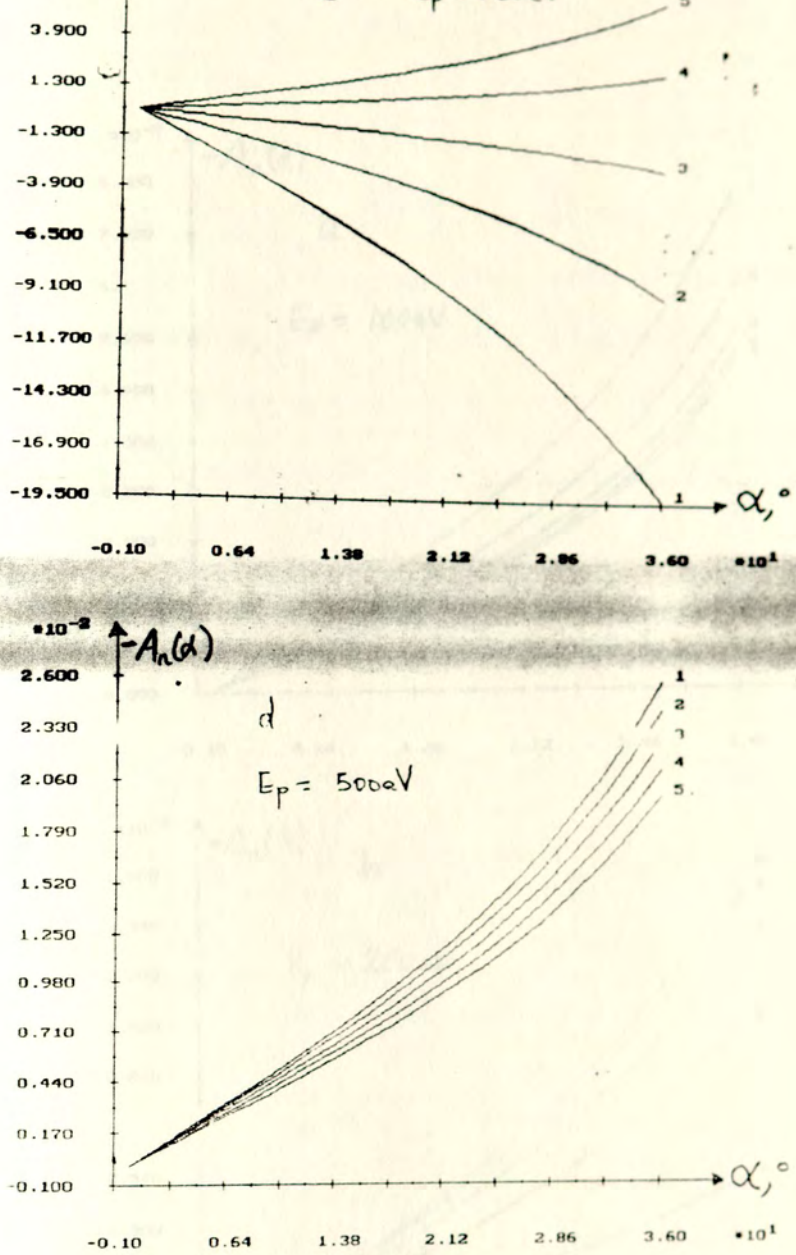


Fig 3.6 Dependence of asymmetry on the angle of incidence α for different multiplicity of the scattering electrons into a collector: c) E_p = 250 , d) 500 eV
The numbers along side the curve give the scattering multiplicity.

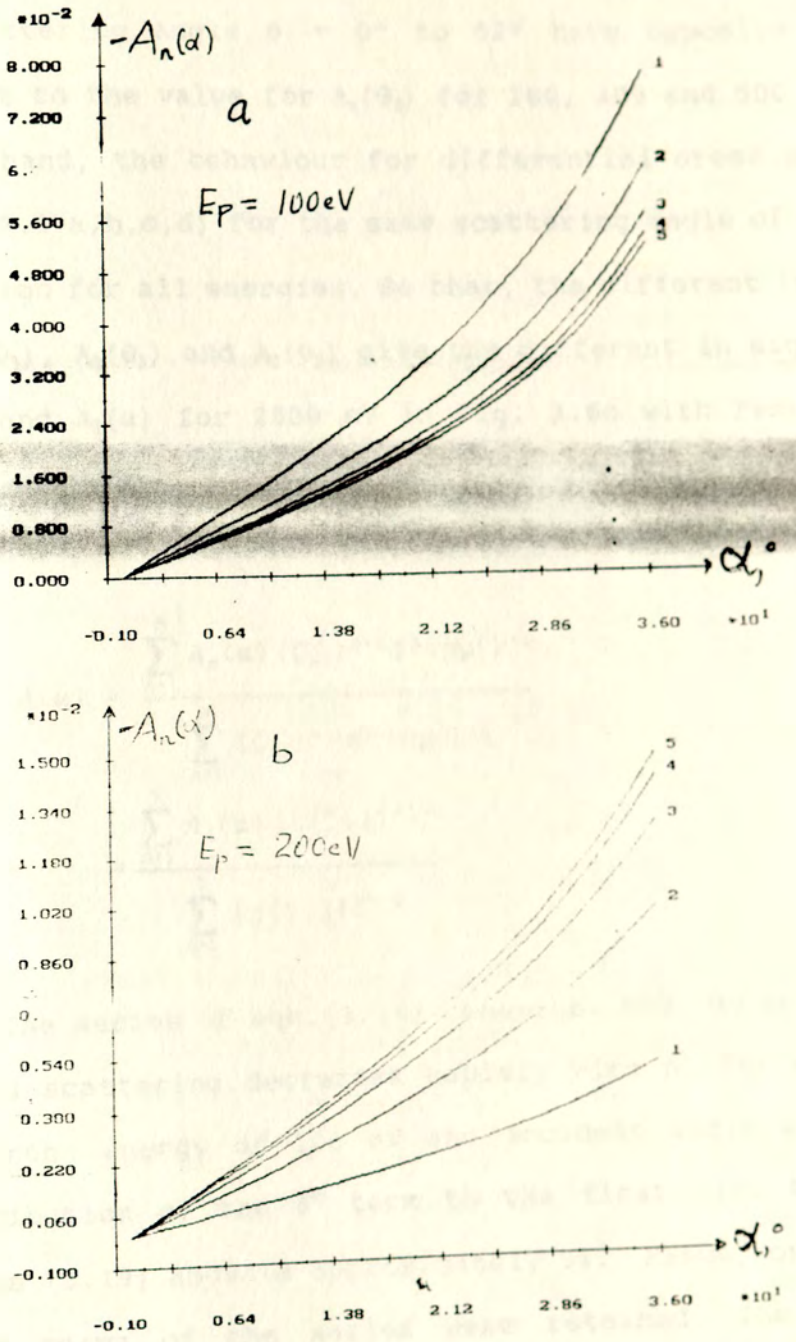


Fig 3.6 Dependence of asymmetry on the angle of incidence α for different multiplicity of the scattering electrons into a collector: a) E_p = 100 , b) 200 eV

The numbers along side the curve give the scattering multiplicity.

3.4c the average value for $A_1(\theta_3)$, $A_2(\theta_3)$ and $A_3(\theta_3)$ in the region of scattering angle θ_3 = 0° to 52° have opposite sign with respect to the value for $A_n(\theta_3)$ for 100, 200 and 500 eV. On the other hand, the behaviour for differential cross sections of Fig. (3.3 a,b,c,d) for the same scattering angle of θ_3 have the same sign for all energies. So that, the different in behaviour of $A_1(\theta_3)$, $A_2(\theta_3)$ and $A_3(\theta_3)$ give the different in sign of $A_1(\alpha)$, $A_2(\alpha)$ and $A_3(\alpha)$ for 2500 eV in Fig. 3.6c with respect to the other energies.

The final calculation of $A(\alpha)$ was made using

$$A(\alpha) = \frac{\sum_{n=1}^{N} A_n(\alpha)\,(Q_{el}^{f})^{n-1} d^{n} (n\mu^{n})^{-1}}{\sum_{n=1}^{N} (Q_{el}^{f})^{n-1} d^{n} (n\mu^{n})^{-1}} = \frac{\sum_{n=1}^{5} A_n(\alpha)\,[n(1.2)^{n}]^{-1}}{\sum_{n=1}^{5} [n(1.2)^{n}]^{-1}} \qquad (3.19)$$

The series of eqn.(3.19) converges and the probability of n-fold scattering decreases rapidly with n. For example, for electron energy of 100 eV and incident angle α = 36° the contribution of the 6th term to the first five terms of the series (3.19) amounts approximately 3%. Hence, only the first five terms of the series were retained. The attenuation coefficient depends on the electron energy, and its exact value is unknown. In these calculations, for all electron energies, $Q_{in} = 0.2Q_{el}^{f}$ was used, so that $\mu = 1.2Q_{el}^{f}d$.

From eqn.(3.19) it is possible to estimate the contribution of n-fold scattering to the total scattering asymmetry. For example, the result of this calculation shows that the contribution of single interaction to the total

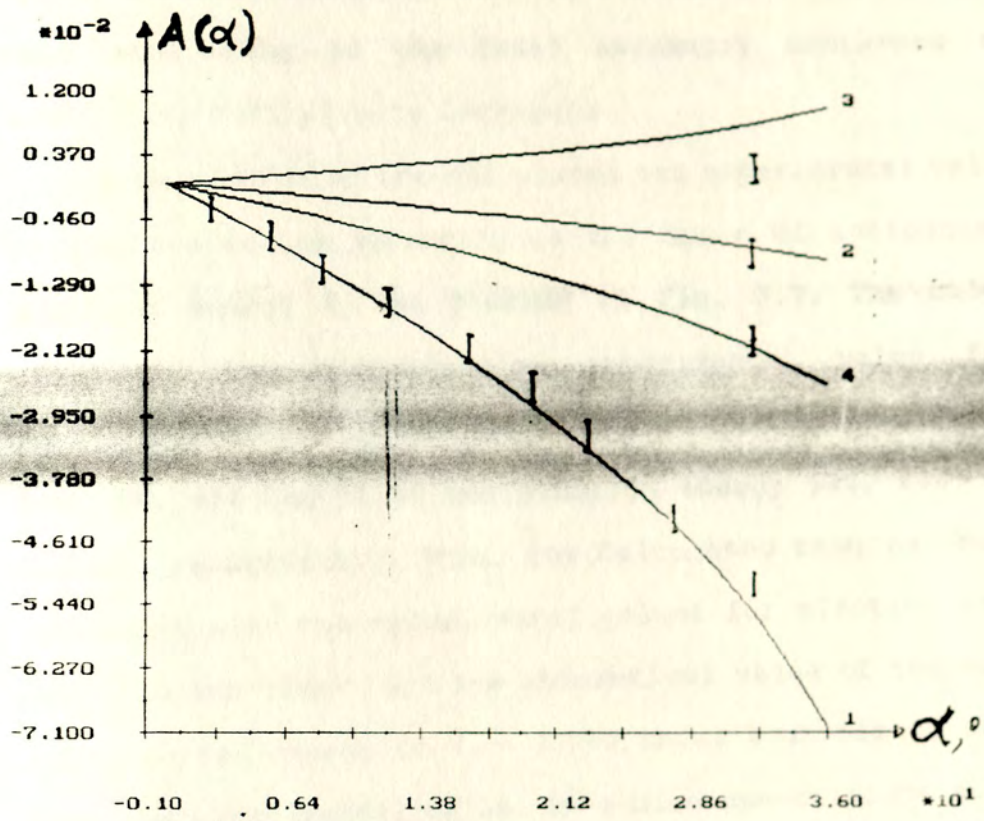


Fig 3.7 Dependence of the scattering asymmetry of the polarized electrons on the angle of incidence α on the surface of polycrystalline gold. The numbers along side the curve give the incident energy of polarized electrons E_p 100 , 200, 250 and 500 eV, respectively.

Calculated (⌒) and experimental (I)[9] values of the scattering asymmetry.

scattering asymmetry depends very weakly on the electron energy E_p and amounts approximately 60%. The contribution of the n-fold scattering to the total asymmetry decreases as the scattering multiplicity increases.

A dependence of the calculated and experimental values [9] of the scattering asymmetry on the angle of incidence α for electron energy E_p was plotted in Fig. 3.7. The calculated error to the corresopnding experimental value for the particular angle of incidence $\alpha = 32°$ amounts approximately 10%, 5%, 43% and 7% of the electron energy 100, 200, 250 and 500 eV, respectively. Thus, the Calculated results shows good agreement with the experimental values for electron energy of 100, 200 and 500eV. But the theoretical value of the asymmetry for electron energy of E_p = 250eV shows significant deviation from the experimental value. This discrepancy might appear due to

1) Approximation $Q_m \approx 0.2\ Q_t'$ for this energy might not be good.

2) Maybe the experimental error is high for this energy.

Generally, the calculated results agreed satisfactorily with the experimental values.

CHAPTER IV

4.1 CONCLUSIONS

Owing to spin-orbit coupling in elastic scattering, the scattering of electrons by a polycrystalline gold target depends on their relative spin orientation. According to the results of the calculations, the total asymmetry depends strongly on the asymmetry of the single scattering process. It has been found that the asymmetry of polarized electrons rises monotonically on increase in the angle of incidence of electrons on the target.

The asymmetry due to interaction of polarized electrons with a polycrystalline solid is due to the scattering by an atomic-like potential of ionic cores in the target. The specific influence of a solid reduces to the following.

1) In view of the high atomic density the elastically scattered electrons experience not only single but multiple scattering by ionic cores in a solid and this changes the asymmetry.

2) When an electron crosses the target - vacuum interface, it loses energy and this reduces the intensity of a beam of elastically scattered electrons which in its turn affects the asymmetry of the scattering in a wide solid angle.

APPENDIX

1. All attached programs contain unit "dr2d". This unit is only to out put graphics on the screen. The procedure to output graphics is called plot 2d.

2. The program "krat" was used for the calculations of the differential scattering cross section and the asymmetry for n-multiple scattering simulation. The file "...\const200.dat" contains the data for the scattering of an electron by the small angles that have not varied. The number 200 in the title of the file "...\const200.dat" indicates that the energy of the incident beam is 200 eV. The input file for the calculation of the n+1- multiple scattering process is the file obtained by the calculation on the n- multiple scattering simulation.

3. The program "polar 1" integrate the asymmetry for the n-multiple scattering simulation in the aperture of the collector, for the various values of the angle between the direction of the incident beam and the normal to the surface of the target.

4. The program"Total-as" calculate the total asymmetry for the scattered beam as a sum of n- multiple asymmetry for each value of the energy.

```
Program Krat;
{$E+}
Uses crt, dr2d;
Var
Sig    :array[1..107] of real;
As     :array[1..107] of real;
Pops   :array[1..91] of real;
Assim :array [1..91] of real;
Ug:array[1..91] of integer;
T3 :array[1..91] of real;
A,B    :real;
T2     :array[1..20] of real;
E:real;
I1,I2,J1,J2,K2,PPI,FiL,N:integer;
i,j,k:integer;
XYZ,DU,B2D:real;
X,Y, RST   :real;
Fi, CosG   :real;
T, D, Z, Z1, T1     :real;
L:integer;
CH:real;
CosEPS,ZP:real;
ArrayNumPoints:TNNumPoints;
G                  :TNmatrix;
outfile:text;
Procedure InputDate;
```

```
Var X     :integer;
    infile:text;
    i     :integer;
begin

assign(infile,'C:\tp60\kotel\scat200\cons200.dat');
reset(infile);
for i:=1 to 16 do readLN(infile,X,X,Sig[i],AS[i];
close(infile);

assign(infile,'C:\tp60\kotel\scat200\sc4_200.dat');
reset(infile);
for i:=1 to 91 do readLN(infile,X,X,Sig[i+16],As[i+16]);
close(infile);
clrscr;
WriteLN('E   I1    I2    J1    J2    K2    PRI    FIL    N')
E:=250; I1:=1; I2:=91; J1:=1; J2:=16; K2:=18; PRI:=1; Fil:=1;
N:=1;
 ( readLn( E ,   I1 ,    I2,    J1 , J2   ,   K2 ,    PRI   ,
  FIL,    N) ; )
WriteL(E:8,'    ',I1,'   ',I2,'    ',J1,'    ',J2,'    ',K2,'
       ',PRI,'    ',FIL,')
end; (-Procedure InputDate -)
```

```
begin
InputDate;
assign(outfile,'C:\tp60\Kotel\scat200\sc5_200dat');
rewrite(outfile);
for i:=I1 to I2 do begin
  XYZ:=0; QU:=; BZD:=0;
  Ug[i]:=(i-1)*2;    T3[i]:=Ug[i]*Pi/180;
  A:=cos(T3[i];       B:=sin(T3[i]);
  for j:=J1 to J2 do begin
     T2[j]:=(j-1)*2*Pi/180;
     X:=cos(T2[j]); Y:=sin(T2[j];
  () RST:=Sig[j]*Y*2*360/K2*sqr(Pi/180);
     for K:=1 to K2 do begin
        F1:=(K-1)*360/K2*Pi/180;
        CosG:=A*X+B*Y*cos(F1);
        if CosG)=1 then CosG:=1;
        if CosG(=-1 then CosG:=1;
        if Cosg=0 then T:=Pi/2 else T:=arctan(sqrt
        (1- sqr(CosG)) /CosG;
        D:T*180/Pi;
        if D(0 then D:=D+180;
        Z:=int(D);
        Z1:=Z;
        while (Z1)2) do Z1:=Z1-2;
       if Z1(2 then T1:=Z+1;
```

```
        if Z1=2 then T1:=Z;
        L:=round(T1/2)+1+16;
        XYZ:=XYZ+Sig[L]*RST;
        QU:=QU+RST;
        CH:= B*X - A*Y*cos(Fi);
        if CH<0 then begin ZP:=-1;  CosEps:=1/sqrt
        (1+sqr (Y*sin(Fi) /CH)) end;
        if CH>0 then begin ZP:=1; CosEps :=1/sqrt
        (1+sqr (Y*sin(Fi) /CH)) end;
              if CH=0 then begin ZP:=1;  CosEps:=0 end;
        BZD:=BZD + Sig[L]*As[L]*RST*CosEps*ZP;
    end; {-for k-}
end; {-for j-}

Pops[i]:=XYZ/QU; Assim[i]:=BZD/XYZ;
WritenLN(i,' Ug[',i,']=',Ug[i],' pops[',i,']= ',Pops[i]:12,'
Assim[',i,']=',Assim[i]:12);
WritenLn(outfile,i,'  ',Ug[i],'    ',Pops[i]:12,'
 ',Assim[i]:12);
G[i,0]:=Ug[i]; G[i,1]:=Pops[i];
end; {-for i-}

close(outfile);
ArrayNumPoints[1]:=60;
 Plot2d(1,ArrayNumPoints,1,1,G);
end.
```

```
Program polar1;
{$E+}
Uses crt, dr2d;
const
Title:array[1..5] of string[3]=('sc1', 'sc2,',  'sc3', 'sc4',
'sc5');
Title1:array[1..5] of string[4]=('As11', 'As12', 'As13', 'As14',
'As15');
Energy:array[1..4] of integer=(100,200,250,500);
N=18;

Var
Z:   array [1..27] of integer
C:   array [1..19] of integer;
I,J,K,L,M: integer;
P: array [1..27] of real
SIG: array [1..27] of real;
POL: array [1..19] of real;
F1:array[1..N] of real;
TOK,POTOK,A,B: real
X,Y,CosG,CH2,T,PT: real;
Ang,Angi:real;
ArrayNumPoints:TNNumPoints;
G              :TNmatrix;
outfile: text;
Procedure InputDate(n,j:integer);
```

```
Var X          : real;
    infile     : text;
    i          : integer
    FileTitle: string;
begin (-Procedure InputDate-)

    FileTitle:='A:\scat'+Energy[n]+'\'+Title[j]+'_'Energy[n]+'
    .dat';
    assing(infile,FileTitle);
    reset(infile);
for i:=1 to 27 do readLn(infile,X,X,Sig[28-i],P[28-i]);
    close (infile);
end; (-Procedure InputDate-)
begin      (-MAIN-)
for i:=1 to 27 do Z[i]:=54-i*2;
for i:=1 to 19 do C[i]:=38-i*2;
for i:=1 to 4 do
 for m:=1 to 5 do
 begin
InputDate(1,m);
assign (outfile,'A:\scat'+Energy[1]+'\'+Title1[m]+'_'+Energy
[1]+'.dat');
rewrite (outfile);
for K:=1 to N do Fi[k]:=cos((K-1)*(2/N)*Pi);
for j:=1 to 19 do begin
TOK:=0; POTOK:=0
Ang:= C[j]*Pi/180;
```

```
A:=cos(Ang);
B:=sin(Ang);
  for i:1 to 27 do begin
Angi:=Z[i]*Pi/180;
X:=A*cos(Angi); Y:=B*sin(Angi);
  for K:=1 to N do begin
   cosG:=X+Y*Fi[K];
   CH2:=(1-2.7/sqrt(E[1])/CosG);
   T:=SIG[1]*(sin(Z[i])*Pi/180)/(1+A/CosG)*CH2;
   PT:=P[1]*Fi[K]*T;
   TOK:=TOK + T;
   POTOK:=POTOK + PT;
  end; (-for K-)
 end; (-for i-)
POL[20-j]:=POTOK/TOK;
Write (j);
end; (-for j-)
for j:=1 to 19 do begin
    writeLn(outfile,C[20-j],'    ',POL[j]);
    writeLn(C[20-j],'    ',POL[j]);
    readLn
    G[j,0]:=C[20-j]; G[j,1]:=-POL[j];
  end
ArrayNumPoints[1]:=19;
Plot2D(1,ArrayNumPoints,1,1,G);
end; (-for m-)
end.
```

```
Program totalas;
{$E+}
uses crt,dr2d;
const
Title:array[1..5] of string [3]=('As1','As2','As3','As4','As5');
Energy:array[1..4] of string[3]=('100', '200', '250', '500');
Var
FileTitle:string;
Atotal:array[1..19,1..4] of real;
A      :array[1..5,1..19,1..4] of real
Angle  :array[1..19] of integer;
Norm   :real;
i,j,n  :integer;
infile,outfile:text;
G:TNmatrix;
ArrayNumPoints:TNnumpoints;
begin  { Main }
clrscr;
Norm:=0;
for j:=1 to 5 do Norm:=Norm + 1/(j*exp(j*ln(1.2)));
for n:=1 to 4 do begin
   for j:=1 to 5 do begin
    FileTitle:='A\scat'+Energy[n]+'\'+Title[j]+'_'+Energy[n]+'
    .dat';
    assign(infile,FileTitle);
```

```
      reset(infile);
      for i:=1 to 19 do readLn(infile,Angle[i],A[j,i,n]);
      close(infile);
     end; (-for j-)
  end; (-for n-)
  for n:=1 to 4 do begin
    for i:=1 to 19 do begin
     Atotal[i,n]:=0;
       for j:=1 to 5 do Atotal[i,n]:=Atotal[i,n]+A[j,i,n]/
       (j*exp(j*ln(1.2)));
        Atotal[i,n]:=Atotal[i,n]/Norm;
       end; (-for j-)
  end; (-for n-)
  assign(outfile,'A:\astot12.dat');
  rewrite(outfile);
  for i=1 to 19 do begin
  writeLn(2*(i-1),'    ',Atotal[i,1]:10,'    ',Atotal[i,2]:10,
  ',Atotal[i,r]:10);
  writeLn(outfile,2*(i-1),'    ',Atotal[i,1]:10,'    ',Atotal[i,2]:
  10,'    ',Atotal[i,:10,'    ',Atotal[i,4]:10);
  end;
  close(outfile);
  for n:=0 to 3 do begin
  for i:1 to 19 do begin
     G[i,2*n]:+Angle[i];  G[i,2*n+1]:Atotal[i,n+1);
   end;
  ArrayNumPoints[n+1]:=19;
```

```
end; (-for-)

readLn;

Plot2d(4,ArrayNumPoints,1,1,G);
end.
```

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DECLARATION

I, the undersigned, declare that this thesis is my work and that all sources of material used for the thesis have been duly acknowledged.

Bereket Neway

Signature -