ELECTRON SCATTERING IN GRAPHENE BY NON-SYMMETRIC POTENTIAL WITH MAGNETIC DIPOLE MOMENT IN THE FRAME OF BORN APPROXIMATION

By

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Abstract

The thesis is designed to study the scattering process of electron in graphene by spherically non-symmetric potentials within the Born approximation. The scattering process with electric and magnetic dipoles parallel and transverse to the graphene plane were studied and the obtained numerical result shows the scattering process by electric dipole is dominant in comparison with the magnetic dipole. In addition, we obtained non-zero backscattering for non-symmetric potentials.

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Introduction

The scattering of electrons by different scatterers in graphene has been intensively studied since its experimental discovery [1]. It is known that the backscattering cross section of massless electrons by the impurities with radially symmetric potentials is equal to zero. The electron scattering in graphene has been studied via scattering phases [2] and with the help of 2D Born approximation [3-5]. Graphene is atomically thin two -dimensional film of carbon atoms arranged laterally in honeycomb structure [6-7]. In graphene sheet the conduction and valence bands consisting of π orbitals cross at K and K' points of the Brillouin zone, where the Fermi level is located [8-9]. The main characteristic of graphene is that its electrons and described by the Dirac's like equation for massless particles [10]. The main result of these studies of electrons scattering in graphene through different mechanisms with radially symmetric potentials is the absence of the backscattering. The scattering potential formed by the vector potential of the electric and magnetic dipoles moment is not central symmetric [11]. The calculated scattering 2D cross section is not equal to zero for the back scattering. It is not true for the scattering by electric and magnetic dipoles that possess non-radially symmetric potentials. But only very large nanomagnetic impurities with gigantic magnetic moments can provide the scattering cross section comparable with that one by the electric dipoles. A comparison of the transport cross sections by Coulomb potential and by electric dipoles shows that they could be comparable.

The thesis is designed as follows. In Chapter 1, we discus symmetric potential and non-symmetric potential. In Chapter 2, we present the Born approximation for the scattering problems on the basis of 2D Dirac like equation of massless electron. In Chapter 3, we consider scattering by impurity with magnetic dipole moments. In Chapter 4, we calculate the transport cross sections. In Chapter 5, we conclude the findings of the research work.

Chapter 1

Symmetric and Non-Symmetric Potential

Symmetric potential is a potential that is possible to find exact solution to the eigen-value problem of the Hamiltonian but in the case of non-symmetric potential, it is impossible to find exact solution to the eigen-value problem of the Hamiltonian [12]. In this Chapter we try to develop some basic differences for symmetric and non-symmetric potential.

1.1 Symmetric potential

In physics, a potential may be referred as the scalar potential or the vector potential. In either case, it is a field defined in space, from which many important physical properties may be derived. Leading examples are the magnetic(vector) potential and the electric potential, from which the motion of vector potentials or electrically charged bodies may be obtained. Specific forces have associated potentials, including the Coulomb potential, the Van der Waals Potential and others. The symmetric potential ensures that the solutions can be classified according to their parity and the application of boundary conditions. A symmetric potential depends only on the distance r between the particles and the observation point of the field. It is independent of the polar angles θ and the azmuthal angle ϕ. In the general case, the dynamics of a particle in spherically symmetric potential are governed by a Hamiltonian of the following form [13]

$$\hat{H} = \frac{\hat{p}^2}{2m_o} + \hat{V}(r), \tag{1.1.1}$$

where m_o is the mass of the particle, $\hat{p}$ are the momentum operator, and the potential $\hat{V}(r)$ depends only on r, the modulus of the radius of the radius vector $V(r)$.
The solutions for such potentials are $V(r) = 0$, or solving the vacuum in the basis of spherical harmonics, which serves as the basis for other cases,

$$V(r) = \begin{cases} V_0, & r < r_o, \\ 0, & \text{elsewhere}, \end{cases} \tag{1.1.2}$$

or a particle in the spherical equivalent of the square well, useful to describe scattering and bound states of a nucleus or quantum dots.
Some examples of symmetric potentials are:
(i) The potential of a freely moving particle in a spherical box of radius R, given by

$$V(r) = \begin{cases} 0, & 0 \leq r \leq R, \\ \infty, & r > R, \end{cases} \tag{1.1.3}$$

(ii) The potential of the square well type

$$V(r) = \begin{cases} -V_0, & 0 \leq r \leq R \\ 0, & r > R \end{cases} \tag{1.1.4}$$

(iii) Anisotropic harmonic oscillator potential given by

$$V(r) = \frac{1}{2} m\omega^2 r^2 \tag{1.1.5}$$

(iv) The potential that governs the electrons motion in hydrogen atom is also asymmetric potential. That is,

$$V(r) = \frac{-Ze^2}{r} \tag{1.1.6}$$

The potentials (1.1.3) and (1.1.4) serve as schematic descriptions of quantum particles, for examples, in case of the so-called bag model of hadronic matter.

The potential (1.1.5) describes the motion of a charge in a uniformly charged sphere and can be employed to describe the motion of protons and neutrons in atomic nuclei.

The potential (1.1.6) leads to the stationary electronic states of the hydrogen atom ($Z = 1$). The corresponding wave functions serve as basic functions for multi-electron systems in atoms, molecules and crystals.

1.2 Non-symmetric potential

A Non-symmetric potential is potential that depends on the distance between the particle r and direction (θ, φ) along which is discover [14]. In general case, the scattered wave is not spherically symmetric, its amplitude depends on the direction (θ, φ) and hence

$$\phi_{sc}(\vec{r}) = Af(\theta, \varphi)\frac{e^{\vec{k}.\vec{r}}}{r}, \tag{1.2.1}$$

where $f(\theta, \varphi)$ called the scattering amplitude, $\vec{k}$ is the wave vector associated with the scattered particle, $\vec{k}_0$ is the wave vector associated with the incident particle and θ is the angle between $\vec{k}_0$ and $\vec{k}$. After the scattering has taken place, the total wave consists of a superposition of the incident plane and scattered wave:

$$\psi(\vec{r}) = \phi_{inc}(\vec{r}) + \phi_{sc}(\vec{r}) = A[e^{\vec{k}_0.\vec{r}} + f(\theta, \varphi)\frac{e^{\vec{k}.\vec{r}}}{r}] \tag{1.2.2}$$

where $e^{\vec{k}_0.\vec{r}}$ is the incident plane wave, $f(\theta, \varphi)\frac{e^{\vec{k}.\vec{r}}}{r}$ is the scattered wave and A is a normalization factor.

The Hamiltonian operator in spherical polar coordinates is

$$\frac{-\hbar^2}{2m}\Big[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial^2\phi} - \frac{2m}{\hbar^2}V(\vec{r})\Big]\psi_{\vec{k}_0} = E\psi_{\vec{k}_0}(\vec{r}) \tag{1.2.3}$$

To solve this problem we employe the relation $\hat{\vec{L}} = \frac{(\vec{r}\times\hat{\vec{p}})}{\hbar}$ with its projection, $\hat{L}_z$, along the z-axis. The square of the angular momentum $\hat{\vec{L}}$ and its projection $\hat{L}_z$ are constants of motion (this satisfies the commutation $[\hat{H}, \hat{\vec{L}}^2] = [\hat{H}, \hat{L}_z] = 0$).
Here, $\hat{\vec{p}} = -i\hbar\vec{\nabla}$. Using this relation together with the expression of the cartesian coordinates, (x, y, z) interms of polar coordinates (r, θ, φ), one can show that

$$\hat{\vec{L}}^2 = -\hbar^2[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}]. \tag{1.2.4}$$

Since $\hat{\vec{L}}^2$ commutes with its components, $[\hat{\vec{L}}^2, \hat{L}_i] = 0$, $i = x, y, z$, it can be diagonalized simultaneously with any one of these components by the same set of eigenfunctions. Choosing the component that lie along the z-axis, the corresponding eigenfunctions are the spherical harmonics [15-16], $Y_{lm}(\theta, \varphi)$, such that

$$\hat{\vec{L}}^2 Y_{lm}(\theta, \phi) = \hbar^2 l(l+1) Y_{lm}(\theta, \varphi) \tag{1.2.5}$$

and

$$\hat{L}_z Y_{lm}(\theta, \varphi) = \hbar_m Y_{lm}(\theta, \varphi) \tag{1.2.6}$$

The subscript l and m in (1.2.5) and (1.2.6) are orbital angular momentum quantum number and the magnetic or azimuthal quantum number, respectively. Therefore, Eqs.(1.2.4), (1.2.5) and (1.2.6) are some examples of non-symmetric, because its angular momentum depends on the angle θ and φ.

Chapter 2

Born Approximation

The Born approximation is the most commonly used approximation, which directly employes the incident field as the total field inside the scatterer. In this Chapter, we discuss theory of Born approximation and the Hamiltonian of 2D motion of the massless electron in graphene in an external field.

2.1 Theory of Born approximation

In scattering theory and, in particular in quantum mechanics, the Born approximation consists of taking the incident field in place of the total field as the driving field at each point in the scattered in coming plane. The Born approximation is named after Max Born who proposed this approximation in early days of quantum theory development [17]. The Born approximation is used in quite different physical contexts. In neutron scattering, the firstorder Born approximation is almost adequate, except for neutron optical phenomena like internal total reflection in a neutron guide, or grazing-incidence small-angle scattering [18]. It is the perturbation method applied to scattering by an extended body. It is accurate if the scattered field is small, compared to the incident field, in the scattered in coming plane. For example, the radar scattering of radio waves by a light styrofoam column can be approximated by assuming that each part of the plastic is polarized by the same electric field that would be present at that point without the column, and then calculating the scattering as a radiation integral over that polarization distribution. Born approximation is widely used in (inverse) scattering problems [19-20] to alleviate the computional diffculity, but its validity and applicability are not well defined. Among the approximation methods, the Born approximation is the most commonly used one, which directly employs the incident field as the total field inside the scatterer [21]. However, its applicability at high frequencies is belived to be unsatisfactory. Some criteria have been developed in the past decades to identify the validity of this approximation and they can generally be classified into the following three categories [22-24].

The first one is like

$$\triangle\varepsilon_r kL \ll 1, \tag{2.1.1}$$

where L is stands for the scale of the scatterer and $\triangle\varepsilon_r$ stands for relative dielectric of scatterer and k stands for wave vector variable of scatterer. This kind of criterion is generally concluded from some special numerical experiments where even scatterers are considered, so its rigour is limited.

The second one is the extension of the previous one. It follows

$$\triangle\varepsilon_r\{1, kL, (kL)^2\} \ll 1, \tag{2.1.2}$$

The third one is like

$$k^2\triangle\varepsilon_r\frac{V}{4\pi r} \ll 1 \tag{2.1.3}$$

where V is the volume of the scatterer and r is the detection distance. This criterion is derived from the receiver is much smaller than the incident field. However, this comparsion should actually be made in the scatterer, so the generality of this criterion is not satisfactory.

2.2 The Hamiltonian of 2D motion of the massless electron in graphene in the external field

The Hamiltonian of 2D motion of the massless electron in graphene in the electron-magnetic dipole iteraction U can be written as [1]

$$\hat{H} = v_F \hat{\sigma}.\left(\hat{p} - \frac{e\vec{A}}{c}\right) + U, \tag{2.2.1}$$

where v_F is the Fermi velocity, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ are the pauil matrices, e and c are the electron charge and speed of light in vacuum, respectively; $\hat{p}$ is the 2D momentum operator, $\mathbf{A}$ is the vector potential. The Schrodinger equation corresponding to the Hamiltonian (2.2.1) is

$$\hat{H}\Psi = E\Psi, \tag{2.2.2}$$

with $\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}$ can be presented as a system of coupled equations.
From Eqs. (2.2.1) and (2.2.2)

$$v_F(\sigma_x + \sigma_y)(\hat{p} - \tfrac{eA}{c}) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = (E - U) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix},$$

$$v_F(\sigma_x(\hat{p} - \tfrac{eA}{c}) + \sigma_y(\hat{p} - \tfrac{eA}{c})) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = (E - U) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix},$$

$$v_F \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} (\hat{p}_x - \tfrac{eA_x}{c}) + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} (\hat{p}_y - \tfrac{eA_y}{c}) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = (E - U) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix},$$

$$v_F \begin{pmatrix} 0 & \hat{p}_x - \frac{eA_x}{c} \\ \hat{p}_x - \frac{eA_x}{c} & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i(\hat{p}_y - \frac{eA_y}{c}) \\ i(\hat{p}_y - \frac{eA_y}{c}) & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} =$$
$$(E - U) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix},$$

$$v_F \begin{pmatrix} 0 & \hat{p}_x - i\hat{p}_y - \frac{eA_x}{c} + i\frac{eA_y}{c} \\ \hat{p}_x + i\hat{p}_y - \frac{eA_x}{c} - i\frac{eA_y}{c} & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = (E-U) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix},$$

$$v_F \begin{pmatrix} 0 & \hat{p}_x - i\hat{p}_y - \frac{e}{c}(A_x - iA_y) \\ \hat{p}_x + i\hat{p}_y - \frac{e}{c}(A_x + iA_y) & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = (E-U) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix},$$

$$v_F \begin{pmatrix} 0 & \hat{p}_- - \frac{eA_-}{c} \\ \hat{p}_+ - \frac{eA_+}{c} & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = (E-U) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix},$$

$$v_F(\hat{p}_- - \frac{eA_-}{c})\psi_2 = (E-U)\psi_1, \tag{2.2.3}$$

$$v_F(\hat{p}_+ - \frac{eA_+}{c})\psi_1 = (E-U)\psi_2, \tag{2.2.4}$$

$$v_F\hat{\pi}_-\psi_2 = (E-U)\psi_1, \tag{2.2.5}$$

$$v_F\hat{\pi}_+\psi_1 = (E-U)\psi_2, \tag{2.2.6}$$

where ψ_1, ψ_2 are the wave functions, $\hat{\pi}_\pm = \hat{p}_\pm - \frac{eA_\pm}{c}$, $\hat{p}_\pm = \hat{p}_x \pm i\hat{p}_y$, $A_\pm = A_x \pm iA_y$ with $\hat{p}_x, \hat{p}_y$ and A_x, A_y being the components of the momentum operator and the vector potential, respectively. Substitution of ψ_1 from equation (2.2.5) into (2.2.6) and vice versa allows one to decouple the system equations. Thus,

$$\psi_1 = \tfrac{v_F\hat{\pi}_-\psi_2}{E-U} = \tfrac{v_F\hat{\pi}_-}{E-U} \cdot \tfrac{v_F\hat{\pi}_+\psi_1}{E-U},$$

$$(E-U)^2\psi_1 = v_F^2(\hat{\pi}_-\hat{\pi}_+)\psi_1,$$

$$\hat{\pi}_-\frac{1}{(E-U)}\hat{\pi}_+\psi_1 = \frac{E-U}{v_F^2}\psi_1, \tag{2.2.7}$$

$$\psi_2 = \tfrac{v_F\hat{\pi}_+\psi_1}{E-U} = \tfrac{v_F\hat{\pi}_+}{E-U} \cdot \tfrac{v_F\hat{\pi}_-\psi_2}{E-U},$$

$$(E-U)^2\psi_2 = v_F^2(\hat{\pi}_+\hat{\pi}_-)\psi_2,$$

$$\hat{\pi}_+ \frac{1}{(E-U)} \hat{\pi}_- \psi_2 = \frac{E-U}{v_F^2} \psi_2. \tag{2.2.8}$$

Now, we focus on the solution of (2.2.7) and (2.2.8) for the case r is much large (far from the scattering center); that is when $\frac{\bar{U}}{E} < 1$. It is to mean that the energy of the incident electron is much greater than the average potential. Using Eqns. (2.2.7) and (2.2.8), we obtain the following relations:-

$$\frac{1}{E}[\hat{\pi}_- \{1 - \tfrac{U}{E}(-1) + \left(\tfrac{U}{E} \right)^2 \tfrac{(-1)(-1-1)}{2!} + ...\}]\hat{\pi}_+ \psi_1 = (\tfrac{E-U}{v_F^2})\psi_1,$$

$$\tfrac{1}{E}[\hat{\pi}_- \{1 + \tfrac{U}{E} + \tfrac{U^2}{E^2} + ...\}]\hat{\pi}_+ \psi_1 = \tfrac{E}{v_F^2}(1 - \tfrac{U}{E})\psi_1,$$

$$\hat{\pi}_- \{1 + \frac{U}{E} + \frac{U^2}{E^2} + ...\}\hat{\pi}_+ \psi_1 = \frac{E^2}{v_F^2}(1 - \frac{U}{E})\psi_1. \tag{2.2.9}$$

Similarly,

$$\frac{1}{E}[\hat{\pi}_+ \{1 - \tfrac{U}{E}(-1) + \left(\tfrac{U}{E} \right)^2 \tfrac{(-1)(-1-1)}{2!} + ...\}]\hat{\pi}_- \psi_2 = (\tfrac{E-U}{v_F^2})\psi_2,$$

$$\tfrac{1}{E}[\hat{\pi}_+ \{1 + \tfrac{U}{E} + \tfrac{U^2}{E^2} + ...\}]\hat{\pi}_- \psi_2 = \tfrac{E}{v_F^2}(1 - \tfrac{U}{E})\psi_2,$$

$$\hat{\pi}_+ \{1 + \frac{U}{E} + \frac{U^2}{E^2} + ...\}\hat{\pi}_- \psi_2 = \frac{E^2}{v_F^2}(1 - \frac{U}{E})\psi_2. \tag{2.2.10}$$

Taking into account the explicit expressions of π_+ and $A_\pm$ (see their definitions after system (2.2.5) and (2.2.6)), one can show that

$$\hat{\pi}_- \hat{\pi}_+ = (\hat{p}_- - \tfrac{eA_-}{c})(\hat{p}_+ - \tfrac{eA_+}{c}),$$

$$= [(\hat{p}_x - i\hat{p}_y) - \tfrac{e}{c}(A_x - iA_y)][(\hat{p}_x + i\hat{p}_y) - \tfrac{e}{c}(A_x + iA_y)],$$

$$= \{[\hat{p}_x - i\hat{p}_y - \tfrac{e}{c}A_x + \tfrac{e}{c}iA_y][\hat{p}_x + i\hat{p}_y - \tfrac{e}{c}A_x - \tfrac{e}{c}iA_y]\},$$

$$= \{\hat{p}_x^2 + i\hat{p}_x\hat{p}_y - \tfrac{e}{c}\hat{p}_x A_x - \tfrac{e}{c}i\hat{p}_x A_y - i\hat{p}_y\hat{p}_x + \hat{p}_y^2$$

$$+\tfrac{e}{c}i\hat{p}_yA_x - \tfrac{e}{c}\hat{p}_yA_y - \tfrac{e}{c}A_x\hat{p}_x - \tfrac{e}{c}iA_x\hat{p}_y,$$

$$+\tfrac{e^2}{c^2}A_x^2 + \tfrac{e^2}{c^2}iA_xA_y + \tfrac{e}{c}iA_y\hat{p}_x - \tfrac{e}{c}A_y\hat{p}_y - \tfrac{e^2}{c^2}iA_yA_x + \tfrac{e^2}{c^2}A_y^2\},$$

$$= (\hat{p}_x^2 + \hat{p}_y^2) + \tfrac{e^2}{c^2}(A_x^2 + A_y^2) - \tfrac{e}{c}[2A_x\hat{p}_x + 2A_y\hat{p}_y] - \tfrac{e}{c}i[\hat{p}_xA_y + \hat{p}_yA_x],$$

$$= \hat{p}^2 + \tfrac{e^2}{c^2}\vec{A}^2 - \tfrac{e}{c}[2\vec{A}.\hat{p}] - \tfrac{e}{c}i[-i\hbar\tfrac{\partial}{\partial x}A_y - i\hbar\tfrac{\partial}{\partial y}A_x],$$

$$= \hat{p}^2 + \tfrac{e^2}{c^2}\vec{A}^2 - \tfrac{e}{c}[2\vec{A}.\hat{p}] - \tfrac{e}{c}i(-i\hbar)[\tfrac{\partial}{\partial x}A_y - \tfrac{\partial}{\partial y}A_x],$$

$$= \hat{p}^2 + \tfrac{e^2}{c^2}\vec{A}^2 - \tfrac{e}{c}[2\vec{A}.\hat{p}] - \tfrac{e}{c}\hbar B_z,$$

$$= \hat{p}^2 + \frac{e^2}{c^2}\vec{A}^2 - \frac{e}{c}[2\vec{A}.\hat{p} + \hbar B_z]. \qquad (2.2.11)$$

Similarly,

$$\hat{\pi}_+\hat{\pi}_- = (\hat{p}_+ - \tfrac{eA_+}{c})(\hat{p}_- - \tfrac{eA_-}{c}),$$

$$= [(\hat{p}_x + i\hat{p}_y) - \tfrac{e}{c}(A_x + iA_y)][(\hat{p}_x - i\hat{p}_y) - \tfrac{e}{c}(A_x - iA_y)],$$

$$= \{[\hat{p}_x + i\hat{p}_y - \tfrac{e}{c}A_x - \tfrac{e}{c}iA_y][\hat{p}_x - i\hat{p}_y - \tfrac{e}{c}A_x + \tfrac{e}{c}iA_y]\},$$

$$= \{\hat{p}_x^2 - i\hat{p}_x\hat{p}_y - \tfrac{e}{c}\hat{p}_xA_x + \tfrac{e}{c}i\hat{p}_xA_y + i\hat{p}_y\hat{p}_x + \hat{p}_y^2$$

$$-i\tfrac{e}{c}\hat{p}_yA_x - \tfrac{e}{c}\hat{p}_yA_y - \tfrac{e}{c}A_x\hat{p}_x + \tfrac{e}{c}iA_x\hat{p}_y$$

$$+\tfrac{e^2}{c^2}A_x^2 - \tfrac{e^2}{c^2}iA_xA_y - \tfrac{e}{c}iA_y\hat{p}_x - \tfrac{e}{c}A_y\hat{p}_y - \tfrac{e^2}{c^2}iA_yA_x + \tfrac{e^2}{c^2}A_y^2\},$$

$$= (\hat{p}_x^2 + \hat{p}_y^2) + \tfrac{e^2}{c^2}(A_x^2 + A_y^2) - \tfrac{e}{c}[2A_x\hat{p}_x + 2A_y\hat{p}_y] + \tfrac{e}{c}i[\hat{p}_xA_y - \hat{p}_yA_x],$$

$$= \hat{p}^2 + \tfrac{e^2}{c^2}\vec{A}^2 - \tfrac{e}{c}[2\vec{A}.\hat{p}] + \tfrac{e}{c}i[-i\hbar\tfrac{\partial}{\partial x}A_y + i\hbar\tfrac{\partial}{\partial y}A_x],$$

$$= \hat{p}^2 + \tfrac{e^2}{c^2}\vec{A}^2 - \tfrac{e}{c}[2\vec{A}.\hat{p}] - \tfrac{e}{c}i(-i\hbar)[\tfrac{\partial}{\partial x}A_y - \tfrac{\partial}{\partial y}A_x],$$

$$= \hat{p}^2 + \tfrac{e^2}{c^2}\vec{A}^2 - \tfrac{e}{c}[2\vec{A}.\hat{p}] + \tfrac{e}{c}\hbar B_z,$$

$$= \hat{p}^2 + \frac{e^2}{c^2}\vec{A}^2 - \frac{e}{c}[2\vec{A}.\hat{p} - \hbar B_z]. \tag{2.2.12}$$

$$[\hat{\pi}_+, \hat{\pi}_-] = \hat{\pi}_+\hat{\pi}_- - \hat{\pi}_-\hat{\pi}_+,$$

$$\Rightarrow [\hat{\pi}_+, \hat{\pi}_-] = \hat{p}^2 + \tfrac{e^2}{c^2}\vec{A}^2 - \tfrac{e}{c}2\vec{A}.\hat{p} + \tfrac{e}{c}\hbar B_z - \hat{p}^2 - \tfrac{e^2}{c^2}\vec{A}^2 + \tfrac{e}{c}2\vec{A}.\hat{p} + \tfrac{e}{c}\hbar B_z,$$

$$= 2\frac{e}{c}\hbar B_z. \tag{2.2.13}$$

where $B_z = (\nabla \times \mathbf{A})_z$ is the z component of the magnetic field and $[\hat{\pi}_+, \hat{\pi}_-]$ denotes a commutator. Here, we chose the Coulomb gauge

$$\nabla.A = 0 \tag{2.2.14}$$

In the scattering problems, the terms containing the vector potential $\mathbf{A}$ and U are being small compared to the energy of electron E. We put them in the right- hand side of equations (2.2.9) and (2.2.10) keeping only terms linear on $\frac{U}{E}$ one obtains the following equation for functions $\psi_{1,2}$:

$$(\nabla^2 + k^2)\psi_{1,2} = \hat{V}_{1,2}\psi_{1,2}. \tag{2.2.15}$$

where $\psi_{1,2}$ can be defined as the functions ψ_1 and ψ_1 describe the electron in states related to the two sublattices of graphene.

Here we introduced the wave vector $k = \frac{E}{\hbar\nu_F}$ and operater,

$$\hat{V}_{1,2} = \frac{1}{\hbar^2}\{\frac{e^2}{c^2}A^2 - \frac{e}{c}[2\vec{A}.\hat{p} \pm \hbar B_z] + \frac{EU}{\nu_F^2} + \hat{\pi}_\mp\frac{U}{E}\hat{\pi}_\pm\}. \tag{2.2.16}$$

It consists of two parts: terms associated with the vector potential $\mathbf{A}$ and the corresponding component of magnetic field B_Z transversal to the graphene plane, and terms associated with the potential energy of electron U. It is worth noting that this part of $V_{1,2}$ contains the space derivatives of U. The two Eqs, in (2.2.15) are independent and specify the wave functions $\psi_{1,2}$ of electrons belonging to different sub lattices of graphene.

2.3 Scattering amplitude For 3D geometry

Scattering can be broadly defined as the redirection of radiation out of the original direction of propagation, usually due to interactions with molecules and particles.
Reflection, refraction, diffraction etc. are actually all just forms of scattering. In many situations, light interacts with inhomogeneous systems, in which case the generic light-matter interaction process is referred to as scattering.
If an electromagnetic wave falls on a system of charges, then under its action the charges are set in motion. This motion in turn produces radiation in all directions; there occurs, we say, a scattering of the original wave.
The scattering is most conveniently characterized by the ratio of the amount of energy emitted by the scattering system in a given direction per unit, to the energy flux density of the incident radiation. This ratio clearly has dimensions of area, and is called the effective scattering cross-section (or simply the cross section). Let dI be the energy radiated by the system into solid angle $d\Omega$ per second for an incident wave with poynting vector $\mathbf{S}$. Then the effective cross-section for scattering (into the solid angle $d\Omega$)is

$$d\sigma = \frac{dI}{\mathbf{S}}. \tag{2.3.1}$$

The scattered particles are described, at a great distance from the scattering center (for potentials that vanish faster than r^{-1} as $r \to \infty$) by an out going spherical wave of the form $f(\theta)e^{i\vec{k}\cdot\vec{r}}/r$ [11,15], where $f(\theta)$ is some function of the scattering angle θ (the angle between the z-axis and the direction of the scattered particle). This function is called the scattering amplitude, a quantity of central importance in scattering theory. Thus the exact wave function, which is a solution of Schrödinger's equation with potential energy $V(r)$, must have at large distances the asymptotic form

$$\psi \approx e^{ik_0 z} + f(\theta)\frac{e^{i\vec{k}.\vec{r}}}{r}. \tag{2.3.2}$$

The probability per unit time that the scattered particle will pass through a surface element $dS = r^2 d\Omega$ (where $d\Omega = 2\pi \sin\theta d\theta$ is an element of solid angle) is $(v/r^2) \mid f(\theta) \mid^2 dS = v \mid f(\theta) \mid^2 d\Omega$. Its ratio to the current density in the incident wave is

$$d\sigma = \mid f(\theta) \mid^2 d\Omega = 2\pi \sin\theta \mid f(\theta) \mid^2 d\theta, \tag{2.3.3}$$

Here, $d\sigma$ is called the cross-section and have a unit of area. The field scattered in the far zone has the general form of a perturbed spherical wave,

$$U_s(\mathbf{r}) = U_0 \cdot \frac{e^{ikr}}{r} \cdot f(\mathbf{K}_s, \mathbf{K}_i), \tag{2.3.4}$$

where $U_s(\mathbf{r})$ is the scattered field at position $\mathbf{r}$, $r = \mid \mathbf{r} \mid$, and $f(\mathbf{K}_s, \mathbf{K}_i)$ defines the scattering amplitude, U_0 is the incident field. The differential cross-section associated with the particle is defined as

$$\sigma_d(\mathbf{K}_s, \mathbf{K}_i) = \lim_{r\to\infty} r^2 \mid \frac{\mathbf{S}_s}{\mathbf{S}_i} \mid, \tag{2.3.5}$$

where $\mathbf{S}_s$ and $\mathbf{S}_i$ are the poynting vectors associated along the scattered and initial direction, respectively, with moduli $\mid \mathbf{S}_{i,s} \mid = \frac{1}{2\eta} \mid U_{i,s} \mid^2$

Note that, according to eqn. (2.3.5), σ_d is defined in the far-zone. It follows immediately that the differential cross-section equals the modulus squared of the scattering amplitude,

$$\sigma_d(\mathbf{K}_s, \mathbf{K}_i) = \mid f(\mathbf{K}_s, \mathbf{K}_i) \mid^2 . \tag{2.3.6}$$

for backscattering, $\mathbf{K}_s = -\mathbf{K}_i$

$$\sigma_b = \sigma_d(-\mathbf{K}_i, \mathbf{K}_i), \tag{2.3.7}$$

where σ_b is referred to as the backscattering cross section.

The normalized version of σ_d defines the so-called differential cross-section ,

$$p(\mathbf{K}_s, \mathbf{K}_i) = 4\pi \frac{\sigma_d(\mathbf{K}_s, \mathbf{K}_i)}{\int_{4\pi} \sigma_d(K_s, K_i) d\Omega} \tag{2.3.8}$$

The phase function p defines the angular probability density associated with the scattered light. The integral in the denominator of eqn. (2.3.8) defines the scattering cross section

$$\sigma_s = \int_{4\pi} \sigma_d(\mathbf{K}_s, \mathbf{K}_i) d\Omega \tag{2.3.9}$$

Thus, the unit of the scattering cross section is $[\sigma_s]= m^2$.

In general, if the particle also absorbs light, we can define an analogous absorption cross section, such that the attenuation due to the combined effect is governed by a total cross section,

$$\sigma = \sigma_a + \sigma_s \tag{2.3.10}$$

For particles of arbitrary shapes, sizes, and refractive indices, deriving expression for differential cross-section (σ_d) and the scattering cross sections (σ_s), is very difficult. However, if simplifying assumptions can be made, the problem becomes tractable.

Chapter 3

Scattering by Impurity with Magnetic Dipole Moment

Scattering by impurity with magnetic dipole moment is important for an electron moving in the magnetic field **B** of the magnetic impurity described by the vector potential is subjected to the Lorentz force acting on its charge.
In this Chapter, we discuss theory of the scattering by impurity with magnetic dipole moment transversal to the graphene plane and differential cross-section of electron scattering in graphene by impurities with non-symmetric scattering potential.

3.1 Magnetic dipole moment

We define the magnetic dipole moment to be a vector pointing out of the current loop and with a magnitude equal to the product of the current and loop area.

$$\vec{\mu} = I\vec{A} \tag{3.1.1}$$

If the dipole moment in every unit cell was the same, there would be no scattering of electrons since the dipole potential would then be periodic. Dipole scattering is an important phenomenon in electromagnetic theory; the color of the sky is believed to be due to dipole scattering of the light wave by molecules in the atmosphere.Such scattering of electron waves in solids is a much less explored phenomenon. Dipole scattering in highly compensated semiconductors such as Si, Ge and $GaAs$ had been studied a long time ago by [25-27] to acceptor pairs. The form of the dipole scattering originates due to fundamentally different origin-due to the material in homogeneity, even in the absence of any impurities carries moving in alloys composed of *highily* polar materials will experience scattering due to the spatially varying polarization coupled with the alloy disorder. The effect of dipole scattering on the mobility of a quantum confined two-dimensional electron gas at $AlGaN$ or GaN interface due to the varying dipole moment in $Al_xGa_{1-x}N$ barrier was *recently* investigated [28].

3.2 Vector potential of the dipole magnetic field

The divergence of the vector potential vanishes for static field.The vector potential of the magnetic dipole is given by [29].

$$\vec{A}_{md} = \frac{\mu_0}{4\pi}\frac{\vec{m}\times\vec{r}}{r^3}, \tag{3.2.1}$$

where $\vec{A}_{md}$ is represents the vector potential of the magnetic dipole.
Taking the curl gives the dipole magnetic field

$$\vec{B}_{md} = \vec{\nabla}\times\vec{A}_{md}, \tag{3.2.2}$$

$$\vec{B}_{md} = \frac{\mu_0}{4\pi}\vec{\nabla}\times\frac{\vec{m}\times\vec{r}}{r^3}. \tag{3.2.3}$$

In the same way as the electric potential, we can write the magnetic potential as a multipole expansion. Because the magnetic potential is a vector, the expansion is a series of vector integrals. The most general form of the vector potential is

$$\vec{A}(r) = \frac{\mu_0}{4\pi}I\oint\frac{dl'}{|\vec{r}-\vec{r'}|} \tag{3.2.4}$$

We can expand the integrand in terms of Legendre Polynomials as

$$\frac{1}{|\vec{r}-\vec{r'}|} = \frac{1}{\sqrt{r^2+r'^2-2rr'\cos\theta}} = \frac{1}{r}\frac{1}{\sqrt{1+\frac{r'^2}{r^2}-\frac{2r'}{r}\cos\theta'}}$$
$$= \frac{1}{r}\sum_{n=0}^{\infty} P_n(\cos\theta')(\frac{r'}{r})^n, \tag{3.2.5}$$

where P_n are the Legendre Polynomials.

The potential becomes

$$\vec{A}(\vec{r}) = \frac{\mu_0}{4\pi} I \sum_{n=0}^{\infty} P_n \frac{1}{r^{n+1}} \oint P_n(\cos\theta')(\frac{r'}{r})^n \tag{3.2.6}$$

The first three terms in this sums are called the monopole, dipole and quadrupole terms.

The monopole term is

$$\vec{A}_0 = \frac{\mu_0}{4\pi} I \oint dl' = 0. \tag{3.2.7}$$

Integration of the vector line element around any closed loop is zero. For the dipole

$$\vec{A}_1 = \frac{\mu_0}{4\pi r^2} I \oint r' \cos\theta' dl', \tag{3.2.8}$$

θ' is the angle between r'and r, we can write this as

$$\vec{A}_1 = \frac{\mu_0}{4\pi r^2} I \oint \vec{r'} \cdot \hat{r} dl', \tag{3.2.9}$$

Here $\hat{r}$ is a constant as far as the integral is concerned, we can write the integral in term of the vector area a enclosed by the loop.

$$\vec{A}_1 = \frac{\mu_0}{4\pi r^2} I \vec{a} \times \hat{r} \tag{3.2.10}$$

The quantity

$$\vec{m} \equiv I\vec{a} \tag{3.2.11}$$

is defined as the magnetic dipole moment of the current loop, so the dipole potential is

$$\vec{A}_1 = \frac{\mu_0}{4\pi r^2} \vec{m} \times \hat{r} \tag{3.2.12}$$

The magnetic field due to a dipole is

$$\vec{B}_1 = \vec{\nabla} \times \vec{A}_1$$
$$= \frac{\mu_0}{4\pi}\vec{\nabla} \times (\vec{m} \times \frac{\hat{r}}{r^2}). \quad (3.2.13)$$

We can use a vector identity to expand the curl, and use the fact that $\vec{m}$ is a constant for a given current loop; so its derivatives are all zero. We get

$$\vec{B}_1 = \frac{\mu_0}{4\pi}[\vec{m}(\vec{\nabla}.\frac{\hat{r}}{r^2}) - (\vec{m}.\vec{\nabla})\frac{\hat{r}}{r^2}]. \quad (3.2.14)$$

We can now use

$$\hat{r} = \tfrac{1}{r}(x\hat{x} + y\hat{y} + z\hat{z})$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

Therefore,

$$(\vec{m}.\vec{\nabla})\tfrac{\hat{r}}{r^2} = (m_x\tfrac{\partial}{\partial x} + m_y\tfrac{\partial}{\partial y} + m_z\tfrac{\partial}{\partial z})\tfrac{\hat{r}}{r^2},$$

$$= (m_x\tfrac{\partial}{\partial x} + m_y\tfrac{\partial}{\partial y} + m_z\tfrac{\partial}{\partial z})(\tfrac{x+y+z}{r^3}),$$

$$= m_x\tfrac{\partial}{\partial x}(\tfrac{x}{r^3}) + m_y\tfrac{\partial}{\partial y}(\tfrac{y}{r^3}) + m_z\tfrac{\partial}{\partial z}(\tfrac{z}{r^3}),$$

$$= m_x\tfrac{\partial}{\partial x}(\tfrac{x}{(x^2+y^2+z^2)^{\frac{3}{2}}}) + m_y\tfrac{\partial}{\partial y}(\tfrac{y}{(x^2+y^2+z^2)^{\frac{3}{2}}}) + m_z\tfrac{\partial}{\partial z}(\tfrac{z}{(x^2+y^2+z^2)^{\frac{3}{2}}}),$$

$$= \tfrac{m_x}{r^3} - \tfrac{3x^2m_x}{r^5} + \tfrac{m_y}{r^3} - \tfrac{3y^2m_y}{r^5} + \tfrac{m_z}{r^3} - \tfrac{3z^2m_z}{r^5},$$

$$= \tfrac{m_x}{r^3} + \tfrac{m_y}{r^3} + \tfrac{m_z}{r^3} - \tfrac{3}{r^5}(x^2m_x + y^2m_y + z^2m_z),$$

$$= \tfrac{1}{r^3}[m_x + m_y + m_z] - \tfrac{3}{r^5}[x^2m_x + y^2m_y + z^2m_z],$$

$$= \frac{1}{r^3}\vec{m} - \frac{3}{r^3}(\vec{m}.\hat{r})\hat{r}. \quad (3.2.15)$$

Putting this all together, we get

$$\vec{B}_1 = \frac{\mu_0}{4\pi r^3}[3(\vec{m}.\hat{r})\hat{r} - \vec{m}]. \quad (3.2.16)$$

3.3 The vector potential of the magnetic dipole moment transversal to the graphene plane

The transversal conductivity of the magnetic dipole of the graphene was studied in the case of weak non-quantizing and quantizing magnetic field [30]. In the case of non- quantizing magnetic field expression of the current density was derived from the Boltzmann equation and at high temperatures:

$$e\hbar v_F^2 H/\triangle c \ll \theta$$

where θ is the electron gas temperature in energy units and $\triangle c$ is change of speed of light in a vacuum. In the case of quantizing magnetic field expression for the graphene transversal magnetic conductivity taking in to account the scattering on the acoustic phonons was derived in the Born approximation and at low temperatures:

$$e\hbar v_F^2 H/\triangle c \gg \theta$$

The vector potential of the magnetic dipole transversal to the graphene plane has two components

$$A_x = -\frac{d_m}{a^2 m}\frac{y}{r^3}, A_y = \frac{d_m}{a^2 m}\frac{x}{r^3} \tag{3.3.1}$$

where a_m is magnetic impurity by a sphere of radius, d_m is the dipole moment. The magnetic field of the dipole $\vec{B} = \vec{\nabla} \times \bar{A}$ has only one nonzero component

$$B_z = -\frac{d_m}{a_m^2 r^3}, \tag{3.3.2}$$

3.4 The differential cross-section of electron scattering in graphene by impurities with non symmetric potential

At large distances from the scattering center due to the smallness defined by (2.2.16), the functions $\psi_{1,2}$ can be presented as

$$\psi_{1,2} = \psi^0_{1,2} + \psi^1_{1,2}, \tag{3.4.1}$$

where $\psi^1_{1,2}$ are the small corrections to the functions $\psi^{(0)}_{1,2}$, which satisfy the two Eqs.in (2.2.15) with the zeroth hand side. If the beam of incident electrons propagates along the x-axis, then $\psi^0_{1,2} = \frac{1}{\sqrt{2}} \exp(ikr)$. The incident wave function can be written as:

$$\Psi_{inc}(x) = \begin{pmatrix} \Psi^0_1 \\ \Psi^0_2 \end{pmatrix},$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \exp(ikr). \tag{3.4.2}$$

The factor $\frac{1}{\sqrt{2}}$ provides the normalization of the wave function (3.4.2) to unity. The wave functions $\Psi^1_{1,2}$ satisfy the equation

$$(\nabla^2 + k^2)\Psi^1_{1,2} = \hat{V}_{1,2}\Psi^0_{1,2}. \tag{3.4.3}$$

At large distances from the scattering center, $\Psi^1_{1,2}$ have the form

$$\Psi_{sc} = \frac{\exp(ikx)}{\sqrt{r}} \begin{pmatrix} f_1(\varphi) \\ f_2(\varphi) \end{pmatrix}. \tag{3.4.4}$$

The functions $f_{1,2}(\varphi)$ are analogous to the scattering amplitudes with the scattering angle φ. They have dimension of the square root in 2D and are controlled by the scattering mechanism. The 2D differential cross or the differential length is a ratio of the scattered current J_{sc} through the elementary length dl (transversal to the radius vector $\mathbf{r}$) and the incident current J_{inc}.

$$d\sigma(\varphi) = \frac{J_{sc}}{J_{inc}} dl. \tag{3.4.5}$$

The incident current is directed along the x-axis and equal to

$$\begin{aligned} J_{inc} &= \nu_F \Psi^*_{inc} \hat{\sigma}_x \Psi_{inc} \\ &= \nu_F \tfrac{e^{-ikr}}{\sqrt{2}} (1,1) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tfrac{e^{ikr}}{\sqrt{2}}, \\ &= \tfrac{\nu_F}{2} [1,1] \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \\ &= \nu_F. \end{aligned} \tag{3.4.6}$$

The scattered current can be calculated as

$$J_{sc} = \sqrt{J_x^2 + J_y^2}, \tag{3.4.7}$$

where J_x and J_y are the components of the scattered current given by

$$\begin{aligned} J_x &= \nu_F \psi^*_{sc} \hat{\sigma}_x \psi_{sc}, \\ &= \nu_F Re \tfrac{e^{-ikr}}{\sqrt{r}} (f_1^*(\varphi), f_2^*(\varphi)) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} f_1(\varphi) \\ f_2(\varphi) \end{pmatrix} \tfrac{e^{ikr}}{\sqrt{r}} \\ &= \tfrac{\nu_F}{r} Re(f_2^*(\varphi), f_1^*(\varphi)) \begin{pmatrix} f_1(\varphi) \\ f_2(\varphi) \end{pmatrix}, \\ &= \tfrac{\nu_F}{r} Re[2 f_1^*(\varphi) f_2(\varphi)], \\ &= 2\frac{\nu_F}{r} R_e[f_1^*(\varphi) f_2(\varphi)]. \end{aligned} \tag{3.4.8}$$

$$J_y = \nu_F \psi^*_{sc} \hat{\sigma}_y \psi_{sc},$$

$$= \nu_F I_m \tfrac{e^{-ikr}}{\sqrt{r}} (f_1^*(\varphi), f_2^*(\varphi)) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} f_1(\varphi) \\ f_2(\varphi) \end{pmatrix} \tfrac{e^{ikr}}{\sqrt{r}},$$

$$= \tfrac{\nu_F}{r} I_m (f_2^*(\varphi), f_1^*(\varphi)) \begin{pmatrix} f_1(\varphi) \\ f_2(\varphi) \end{pmatrix},$$

$$= \tfrac{\nu_F}{r} I_m [2 f_1^*(\varphi) f_2(\varphi)],$$

$$= 2\frac{\nu_F}{r} I_m [f_1^*(\varphi) f_2(\varphi)]. \tag{3.4.9}$$

The differential cross section (3.4.5) with account of Eqs.(3.4.7), (3.4.8) and (3.4.9) can be presented as

$$d\sigma(\varphi) = \tfrac{J_{sc}}{J_{inc}} dl,$$

$$= \tfrac{\sqrt{(J_x^2 + J_y^2)}}{\nu_F} dl,$$

$$= \tfrac{\sqrt{\frac{4\nu_F^2}{r^2}[R_e(f_1^*(\varphi)f_2(\varphi))^2 + I_m(f_1^*(\varphi)f_2(\varphi))^2]dl}}{\nu_F},$$

$$= \tfrac{2\nu_F}{\nu_F r} |f_1^*(\varphi) f_2(\varphi)|.dl, \text{ but } dl = r d\varphi$$

$$= \tfrac{2}{r} |f_1^*(\varphi) f_2(\varphi)| d\varphi.r,$$

$$= 2 |f_1^*(\varphi) f_2(\varphi)| d\varphi,$$

$$\frac{d\sigma(\varphi)}{d\varphi} = 2 |f_1^*(\varphi) f_2(\varphi)|. \tag{3.4.10}$$

This formula will be used below for obtaining the cross-section of electron scattering in graphene by impurities with non symmetrical scattering potential.

3.5 Scattering by impurity with radially symmetric electrostatic potential

We calculate the electron scattering cross-section by a nonmagnetic impurity with the radially symmetric electrostatic potential U(r). In this case, operator (2.2.16) with account of $\vec{A} = 0 \Rightarrow B_Z = 0$, $\vec{A}\pm = 0$, $B_Z = \vec{\nabla} \times \vec{A}$, $\nu_F = \frac{E}{k\hbar}$, $\hat{\pi}_\pm = \hat{p}_\pm - \frac{e\vec{A}_\pm}{c}$, $\hat{\pi}_\mp = \hat{p}_\mp - \frac{e\vec{A}_\mp}{c}$ takes the form

$$\hat{V}_{1,2} = \tfrac{1}{\hbar^2}\{\tfrac{EU}{\nu_F^2} + \hat{\pi}_\mp \tfrac{U}{E} \hat{\pi}_\pm\},$$

$$= \tfrac{1}{\hbar^2}\{\tfrac{EU}{(\frac{E}{k\hbar})^2} + \hat{\pi}_\mp \tfrac{U}{E} \hat{\pi}_\pm\},$$

$$= \tfrac{1}{\hbar^2}\{\tfrac{EUk^2\hbar^2}{E^2} + (\hat{p}_\mp - \tfrac{e\vec{A}_\mp}{c})\tfrac{U}{E}(\hat{p}_\pm - \tfrac{e\vec{A}_\pm}{c})\},$$

$$= (\frac{U}{E}k^2 + \frac{1}{\hbar^2}\hat{p}_\mp \frac{U}{E}\hat{p}_\pm). \tag{3.5.1}$$

It is convenient to use the rectangular coordinate system with the x-axis along the incident electron beam. With account of the Explicit form of $\psi^0_{1,2}$(3.4.2),Eq.(3.4.3), can be written as

$$\{\nabla^2 + k^2\}\psi^1_{1,2} = V_{1,2}(\mathbf{r})\frac{1}{\sqrt{2}}\exp[ikx] \tag{3.5.2}$$

where

$$V_{1,2}(\mathbf{r}) = \frac{k}{E}[2k + (-i\frac{\partial}{\partial x} \mp \frac{\partial}{\partial y})]U(r), \tag{3.5.3}$$

$U(r)$ is Coulomb Scattering potential.

Now we can use the results [11] of 2D scattering problem and write down $f_{1,2}(\varphi)$ in the form:

$$f_{1,2}(\varphi) = -\frac{1}{4\sqrt{\pi k}}\int \exp(-i\mathbf{q}.\mathbf{r}')V_{1,2}(\mathbf{r}')d^2r' \tag{3.5.4}$$

where $\hbar\mathbf{q}$ is a transferred momentum under scattering and $V_{1,2}$ is given by Eq.(3.5.3). Integral (3.5.4) can be done presenting U(r) in the form of 2D Fourier transform:

$$U(r) = \frac{1}{(2\pi)^2}\int U(\mathbf{g})\exp(i\mathbf{g}.\mathbf{r})d^2g, \tag{3.5.5}$$

Substituting Eq. (3.5.5) in Eq. (3.5.3) and performing integration in Eq.(3.5.4) over d^2r, we get $\delta(\mathbf{q}\text{-}\mathbf{g})$. Subsequent integration over d^2g gives

$$V_{1,2}(\mathbf{r}) = \tfrac{k}{E}[2k + (-i\tfrac{\partial}{\partial x} \mp \tfrac{\partial}{\partial y})]U(r),$$

$$= \tfrac{k}{E}[2k + (-i\tfrac{\partial}{\partial x} \mp \tfrac{\partial}{\partial y})]\tfrac{1}{4\pi^2}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g,$$

$$= \frac{1}{4\pi^2}\frac{k}{E}2k\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g + \frac{1}{4\pi^2}\frac{k}{E}(-i\frac{\partial}{\partial x}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g \mp \frac{1}{4\pi^2}\frac{k}{E}\frac{\partial}{\partial y}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g, \tag{3.5.6}$$

$$f_{1,2}(\varphi) = -\tfrac{1}{4\sqrt{\pi k}}\int \exp(-i\mathbf{q}.\mathbf{r}')[\tfrac{1}{4\pi^2}\tfrac{k}{E}2k\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g +$$

$$\tfrac{1}{4\pi^2}\tfrac{k}{E}(-i\tfrac{\partial}{\partial x}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g \mp \tfrac{1}{4\pi^2}\tfrac{k}{E}\tfrac{\partial}{\partial y}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g]d^2r',$$

$$= -\tfrac{1}{4\sqrt{\pi k}}\int \exp(-i\mathbf{q}.\mathbf{r}')[\tfrac{1}{(2\pi)^2}\tfrac{k}{k\hbar\nu_F}2k\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g +$$

$$\tfrac{1}{(2\pi)^2}\tfrac{k}{k\hbar\nu_F}(-i\tfrac{\partial}{\partial x}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g \mp \tfrac{1}{(2\pi)^2}\tfrac{k}{k\hbar\nu_F}\tfrac{\partial}{\partial y}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g]d^2r',$$

$$= -\tfrac{1}{4\sqrt{\pi k}}\int \exp(-i\mathbf{q}.\mathbf{r}')[\tfrac{1}{(2\pi)^2}\tfrac{1}{\hbar\nu_F}2k\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g$$

$$+\tfrac{1}{(2\pi)^2}\tfrac{1}{\hbar\nu_F}(-i\tfrac{\partial}{\partial x}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g \mp \tfrac{1}{(2\pi)^2}\tfrac{1}{\hbar\nu_F}\tfrac{\partial}{\partial y}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g]d^2r',$$

$$= -\tfrac{1}{4\sqrt{\pi k}}.\tfrac{1}{\hbar\nu_F}[2k + (-i\tfrac{\partial}{\partial x} \mp \tfrac{\partial}{\partial y}]d^2r'\int \exp(-i\mathbf{q}.\mathbf{r}')\tfrac{1}{(2\pi)^2}\int U(g)\exp(i\mathbf{g}.\mathbf{r})d^2g,$$

$$\Rightarrow V_{1,2}(\vec{r}) = -\frac{U(\mathbf{q})}{4\hbar\nu_F\sqrt{\pi k}}[2k + q_x \mp iq_y]. \tag{3.5.7}$$

Here $U(\mathbf{q})$ is the Fourier transform of $U(r)$ according to Eq.(3.5.5). In the coordinate system with the x-axis along the wave vector $\mathbf{k}$ of the incident electrons $q_x = -q\sin\frac{\varphi}{2}$, $q_y = q\cos\frac{\varphi}{2}$ (See. Fig.3.1). With the help of $q = 2k\sin\frac{\varphi}{2}$, we obtain

$$f_{1,2}(\varphi) = -\tfrac{U(\mathbf{q})}{4\hbar\nu_F\sqrt{\pi k}}[2k - q\sin\varphi/2 \mp iq\cos\varphi/2],$$

$$= -\tfrac{U(\mathbf{q})}{4\hbar\nu_F\sqrt{\pi k}}[2k - 2k\sin^2\varphi/2 \mp i2k\sin\varphi/2\cos\varphi/2],$$

$$= -\tfrac{U(\mathbf{q})}{4\hbar\nu_F\sqrt{\pi k}}[2k(1-\sin^2\varphi/2 \mp i\sin\varphi/2\cos\varphi/2)],$$

$$= -\tfrac{U(\mathbf{q})}{4\hbar\nu_F\sqrt{\pi k}}[2k(1-\tfrac{1}{2}(1-\cos\varphi) \mp \tfrac{i}{2}\sin\varphi)],$$

$$= -\tfrac{U(\mathbf{q})}{4\hbar\nu_F\sqrt{\pi k}}[k(2-1+\cos\varphi) \mp i\sin\varphi)],$$

$$= -\tfrac{U(\mathbf{q})}{4\hbar\nu_F\sqrt{\pi k}}[k(1+\cos\varphi \mp i\sin\varphi)],$$

$$\Rightarrow f_{1,2}(\varphi) = -\frac{U(\mathbf{q})}{4\hbar\nu_F}\sqrt{\frac{k}{\pi}}(1+\exp(\mp i\varphi)) \tag{3.5.8}$$

The differential cross section of the electron scattering by the radially symmetric potential U(r) according to Eqs. (3.4.10) and (3.5.8) takes the form

$$\tfrac{d\sigma(\varphi)}{d\varphi} = 2|f_1(\varphi)^\star f_2(\varphi)|,$$

$$= 2| -\tfrac{U(\mathbf{q})}{4\hbar\nu_F}\sqrt{\tfrac{k}{\pi}}(1+\exp(-i\varphi)). -\tfrac{U(\mathbf{q})}{4\hbar\nu_F}\sqrt{\tfrac{k}{\pi}}(1+\exp(i\varphi))|,$$

$$= 2| -\tfrac{U(\mathbf{q})}{4\hbar\nu_F}\sqrt{\tfrac{k}{\pi}}|^2[(1+\exp(-i\varphi)).(1+\exp(i\varphi))],$$

$$= 2\tfrac{|U(\mathbf{q})|^2}{(4\hbar\nu_F)^2}\tfrac{k}{\pi}[1+\exp(i\varphi)+\exp(-i\varphi)+1],$$

$$= 2\tfrac{|U(\mathbf{q})|^2}{(4\hbar\nu_F)^2}\tfrac{k}{\pi}[2+\exp(i\varphi)+\exp(-i\varphi)],$$

$$= 2\tfrac{|U(\mathbf{q})|^2}{(4\hbar\nu_F)^2}\tfrac{k}{\pi}[2+\cos\varphi+i\sin\varphi+\cos\varphi-i\sin\varphi],$$

$$= 2\tfrac{|U(\mathbf{q})|^2}{(4\hbar\nu_F)^2}\tfrac{k}{\pi}[2+2\cos\varphi],$$

$$= 2\tfrac{|U(\mathbf{q})|^2}{(4\hbar\nu_F)^2}\tfrac{k}{\pi}2[1+\cos\varphi],$$

$$= 2\tfrac{|U(\mathbf{q})|^2}{(4\hbar\nu_F)^2}\tfrac{k}{\pi}2[2\cos^2\varphi/2],$$

$$= 2\tfrac{|U(\mathbf{q})|^2}{(4\hbar\nu_F)^2}\tfrac{k}{\pi}4[\cos^2\varphi/2],$$

$$= \frac{k|U(\mathbf{q})|^2}{2\pi\hbar^2\nu_F^2}\cos^2\varphi/2. \tag{3.5.9}$$

It coincides with corresponding result [2] obtained in a different way. It is clear that the cross section (3.5.9) is equal to zero for the backscattering $\frac{d\sigma(\varphi)}{|d\varphi|_{\varphi=\pi}} = 0$. The electron scattering in graphene by the impurities with non-radially symmetric potentials will be discussed in the following section.

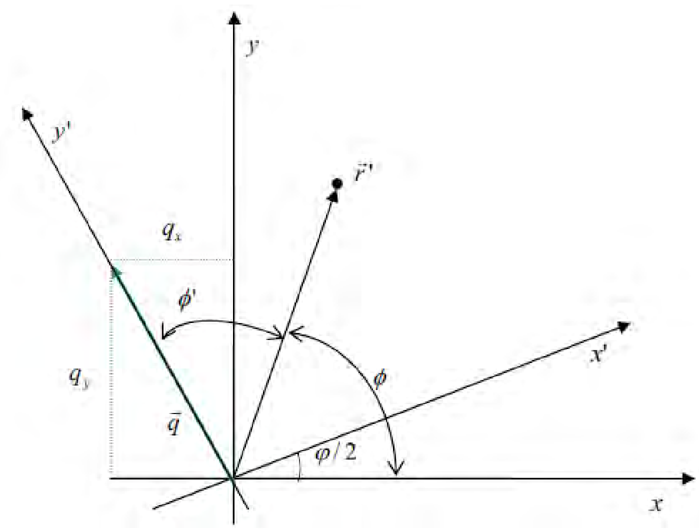

Figure 3.1: The coordinate system x, y (the x-axis is along the beam of incident electrons) and the coordinate system x', y' (the y'-axis is along the vector **q**). The projections **q** on axes x and y are $q_x = -q \sin\varphi/2$ and $q_y = q\cos\varphi/2$ respectively. The vector **r** in the coordinate system x-y is vector **r'** in the system x', y'. It is seen that ϕ' + ϕ - $\varphi/2 = \pi/2$

3.6 Scattering by impurity with electric dipole moment

An impurity breaks the symmetry of the lattice and causes scattering. If the impurity is neutral, the scattering rates are usually negligible. Charged impurities, however, represent screened Coulomb scatterers, with peak potentials that can become comparable to the Fermi energy. Clearly, an electron with a larger kinetic energy will get deflected by a smaller angle as it gets scattered, and we can expect that the mobility increases as the temperature, and with it the average electron kinetic energy, increases. Electron phonon scattering can be divided into deformation potential scattering and scattering of electrons by the corresponding electric fields. By deformation potential scattering, we mean scattering at the lattice deformations caused by the phonons. Here, scattering at acoustic phonons is the most important mechanism. Since the energy transfers are small in electron acoustic phonon scattering, it can be treated as quasi-elastic. Here we consider an impurity possessing an electron dipole moment is modeled by a sphere of radius a_e with a built in point dipole d_e. The potential of the electron-dipole interaction in the coordinate system with the x-axis along the incident beam of electrons is given by [31]

$$U = \frac{ed_e}{\rho^3}[x\cos\alpha + y\sin\alpha] = \frac{ed_e}{\rho^2}\cos(\phi - \alpha), \tag{3.6.1}$$

where $\rho = \sqrt{x^2 + y^2}$ is the radius vector of electron, α and ϕ are the angles between the x-axis and dipole moment and vector ρ, respectively. Further, it will be convenient to use the dimensionless coordinates $r = \frac{\rho}{a_e}$. In this case, we again have to solve Eq. (3.5.2) but $V_{1,2}$ in its left hand side given by the expression

$$V_{1,2} = i\frac{\bar{k}_e U_0}{2\sqrt{2E}}\{-4\bar{k}_e r\cos(\phi - \alpha) + \exp(\mp i\alpha) + 3\exp(\mp i(2\phi - \alpha))\}\frac{1}{r^3}, \tag{3.6.2}$$

where $U_0 = \frac{ed_e}{a_e^2}$ and $\bar{k}_e = ka_e$. This result is obtained with the help of Eq. (3.5.3) with the account of Eq. (3.6.2). The quantities $f_{1,2}$ are given by Eq. (3.5.4). The integration in Eq. (3.5.4) is convenient to perform in a new coordinate system with the y'-axis along the vector $\mathbf{q}$. It is obtained by anticlockwise rotation of the initial coordinate system x, y by the angle $\frac{\varphi}{2}$. In this system the dot product in the exponent of Eq. (3.5.4) becomes $\bar{l}qr'\cos\phi'$, where $\phi' = \frac{\pi}{2} - (\phi - \frac{\varphi}{2})$(see fig 3.1). Here $\bar{q} = qa_e$. The integration over ϕ' in Eq. (3.5.4) is carried out with the help of the relation [32]

$$J_n(Z) = \frac{i^{-n}}{2\pi}\int_0^{2\pi} d\phi' \exp[i(z\cos\phi' + n\phi')], \tag{3.6.3}$$

where $J_n(Z)$ is the first kind Bessel function with an integer n. The subsequent integration over dr' gives the generalized hypergeometric functions. The final result can be written as

$$f_{1,2}(\varphi) = -i\lambda_e\sqrt{\frac{a_e}{\bar{k}}}\{\exp(\mp i\alpha)I_0(\bar{q}) + 4\bar{k}\sin(\frac{\varphi}{2}-\alpha)I_1(\bar{q}) + 3\exp[\pm i(\alpha-\varphi)]I_2(\bar{q})\} \tag{3.6.4}$$

where $\lambda_e = \frac{ed_e\sqrt{\pi}}{(4\hbar\nu_F a_e)}$ is dimensionless. The differential cross section of the scattering by electric dipole (3.4.10) with account of Eq. (3.6.4) takes the form

$$\tfrac{d\sigma(\varphi)}{d\varphi} = 2|f_1^*(\varphi)f_2(\varphi)|$$

$$= 2|i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}\exp(i\alpha)I_0 + i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)I_1 + i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}3\exp(i(\alpha-\varphi)I_2)\times$$

$$(-i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}\exp(-i\alpha)I_0 - i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)I_1 - i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}3\exp(-i(\alpha-\varphi)I_2)|,$$

$$= 2|i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}\exp(i\alpha)I_0[(-i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}\exp(-i\alpha)I_0 - i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)I_1$$

$$-i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}3\exp(-i(\alpha-\varphi)I_2)] + i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)I_1[(-i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}\exp(-i\alpha)$$

$$I_0 - i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)I_1 - i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}3\exp(-i(\alpha-\varphi)I_2)] + i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}3\exp(i(\alpha-\varphi)I_2)$$

$$[(-i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}\exp(-i\alpha)I_0 - i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)I_1 - i\lambda_e\sqrt{\tfrac{a_e}{\bar{k}}}3\exp(-i(\alpha-\varphi)I_2)]|,$$

$$= 2|\lambda_e^2\tfrac{a_e}{k}I_0^2 + \lambda_e^2\tfrac{a_e}{k}4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)I_0I_1 + \lambda_e^2\tfrac{a_e}{k}I_0^2 + \lambda_e^2\tfrac{a_e}{k}3\exp(i\varphi)I_0I_2$$

$$+\lambda_e^2\tfrac{a_e}{k}4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)\exp(-i\alpha)I_0I_1 + \lambda_e^2\tfrac{a_e}{k}16k^2\sin^2(\tfrac{\varphi}{2}-\alpha)I_1^2 + \lambda_e^2\tfrac{a_e}{1}2k\sin(\tfrac{\varphi}{2}-\alpha)$$

$$\exp(-i(\alpha-\varphi))I_1I_2 + \lambda_e^2\tfrac{a_e}{k}3\exp(-i\varphi)I_0I_2 + \lambda_e^2\tfrac{a_e}{k}12k\sin(\tfrac{\varphi}{2}-\alpha)\exp(i(\alpha-\varphi))I_1I_2$$

$$+\lambda_e^2\tfrac{a_e}{k}9I_2^2|,$$

$$= 2\lambda_e^2\tfrac{a_e}{k}[I_0^2 + 4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)(\cos\alpha + i\sin\varphi)I_0I_1 + 3I_0I_2(\cos\varphi + i\sin\varphi)$$

$$+4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)(\cos\alpha - i\sin\alpha)I_0I_1 + 16k^2\sin^2(\tfrac{\varphi}{2}-\alpha)I_1^2$$

$$+12k\sin(\tfrac{\varphi}{2}-\alpha)(\cos\alpha - i\sin\alpha + \cos\varphi + i\sin\varphi)I_1I_2 + 3I_0I_2(\cos\varphi - i\sin\varphi)$$

$$+12k\sin(\tfrac{\varphi}{2}-\alpha)(\cos\alpha+i\sin\alpha+\cos\varphi-i\sin\varphi)I_1I_2+9I_2^2],$$

$$=2\lambda_e^2\tfrac{a_e}{k}[I_0^2+4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)\cos\alpha)I_0I_1+4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)$$

$$i\sin\varphi I_0I_1+3I_0I_2\cos\varphi+3I_0I_2 i\sin\varphi+4\bar{k}\sin(\tfrac{\varphi}{2}-\alpha)\cos\alpha I_0I_1-4\bar{k}$$

$$\sin(\tfrac{\varphi}{2}-\alpha)i\sin\alpha I_0I_1+16k^2\sin^2(\tfrac{\varphi}{2}-\alpha)I_1^2+12k\sin(\tfrac{\varphi}{2}-\alpha)$$

$$\cos\alpha I_1I_2-12k\sin(\tfrac{\varphi}{2}-\alpha)i\sin\alpha I_1I_2+12k\sin(\tfrac{\varphi}{2}-\alpha)\cos\varphi I_1I_2+12k\sin(\tfrac{\varphi}{2}-\alpha)i\sin\varphi I_1I_2$$

$$+3I_0I_2\cos\varphi-3I_0I_2 i\sin\varphi+12k\sin(\tfrac{\varphi}{2}-\alpha)\cos\alpha I_1I_2+12k\sin(\tfrac{\varphi}{2}-\alpha)i\sin\alpha I_1I_2$$

$$+12k\sin(\tfrac{\varphi}{2}-\alpha)\cos\varphi I_1I_2-12k\sin(\tfrac{\varphi}{2}-\alpha)i\sin\varphi I_1I_2+9I_2^2],$$

$$=2\lambda_e^2\tfrac{a_e}{k}[I_0^2+8k\sin(\tfrac{\varphi}{2}-\alpha)I_0I_1(\cos\alpha+i\sin\varphi+\cos\alpha-i\sin\varphi)+(3\cos\varphi$$

$$+3i\sin\varphi)I_0I_2+(3\cos\varphi+3i\sin\varphi)I_0I_2+16k^2I_1^2\sin^2(\tfrac{\varphi}{2}-\alpha)+24kI_1I_2(\cos\alpha-$$

$$i\sin\alpha+\cos\varphi+i\sin\varphi+\cos\alpha+i\sin\alpha+\cos\varphi-i\sin\varphi)+9I_2^2],$$

$$\Rightarrow\tfrac{d\sigma(\varphi)}{d\varphi}=2\lambda_e^2\tfrac{a_e}{k}[I_0^2+16k^2I_1^2\sin^2(\tfrac{\varphi}{2}-\alpha)+9I_2^2+8kI_0I_1\sin(\tfrac{\varphi}{2}-\alpha)\cos\alpha$$

$$+6I_0I_2\cos(2\alpha-\varphi)+24kI_1I_2\cos(\varphi-\alpha)\sin(\frac{\varphi}{2}-\alpha)]. \qquad (3.6.5)$$

It is seen that Eqs. (3.6.5) give a nonzero backscattering cross section. In particular

$$\langle\frac{d\sigma}{d\varphi}\rangle|_{\varphi=\pi}=\lambda_e^2\frac{a_e}{\bar{k}}[I_0^2+9I_2^2+8k^2I_1^2+4kI_1\sin\frac{\varphi}{2}(I_0-I_2)] \qquad (3.6.6)$$

It is known that from the general theory of scattering [11] that the scattering cross section of fast particles $\bar{k}\gg 1$, is relatively small and nonzero only for small scattering angles $\varphi\ll 1$, when $\bar{q}=2\bar{k}\frac{\varphi}{2}\sim 1$. With the help of power series expansion of the Bessel functions [32]

$$J_n(z)=\sum_{s=0}^{\infty}\frac{(-1)^s}{s!(n+s)!}(\frac{z}{2})^{n+2s} \qquad (3.6.7)$$

keeping the terms up to $\bar{q}^2$ in Eq. (3.6.7), we obtain

$$I_0(\bar{q}) = 1 - \bar{q} + \tfrac{\bar{q}^2}{2^2} + ...,$$

$$I_1(\bar{q}) = 1 - \tfrac{\bar{q}}{2} + ...,$$

$$I_2(\bar{q}) = \frac{\bar{q}}{3} - \frac{\bar{q}^2}{2^3} + ..., \tag{3.6.8}$$

Substituting these expansions in Eq. (3.6.6), we get

$$\langle \tfrac{d\sigma}{d\varphi} \rangle = \lambda_e^2 \tfrac{a_e}{k}[I_0^2 + 9I_2^2 + 8k^2 I_1^2 + 4kI_1 \sin\tfrac{\varphi}{2}(I_0 - I_2)],$$

$$= \lambda_e^2 \tfrac{a_e}{k}[(1 - q + \tfrac{q^2}{4})(1 - q + \tfrac{q^2}{4}) + 9((\tfrac{q}{3} - \tfrac{q^2}{8})$$

$$(\tfrac{q}{3} - \tfrac{q^2}{8})) + 8k^2((1 - \tfrac{q}{2})(1 - \tfrac{q}{2})) + 4k\sin\varphi/2((1 - \tfrac{q}{2}) \times (1 - q + \tfrac{q^2}{4}) - (1 - \tfrac{q}{2}) \times (\tfrac{q}{3} - \tfrac{q^2}{8}))]$$

$$= \lambda_e^2 \tfrac{a_e}{k}[(1 + 8k^2 - 2q + \tfrac{5}{2}q^2 + 2k^2q^2 + \tfrac{5}{4}q^3 + \tfrac{k^2q^2}{3}$$

$$+ \tfrac{37}{192}q^4 - \tfrac{k}{6}q^4 + \tfrac{q^5}{32} - \tfrac{k^2q^5}{120}) + (4k\sin\varphi/2 - \tfrac{22}{3}kq\sin\varphi/2 + \tfrac{25}{6}kq^2\sin\varphi/2 - \tfrac{2}{3}kq^3\sin\varphi/2 - \tfrac{7}{48}kq^4\sin\varphi/2)]$$

$$= \lambda_e^2 \tfrac{a_e}{k}[(1+8k^2-4k\sin\varphi/2+10k^2\sin^2\varphi/2+8k^4\sin^2\varphi/2+10k^3\sin^3\varphi/2+\tfrac{8}{3}k^4\sin^3\varphi/2)$$

$$+(4k\sin\varphi/2 - \tfrac{44}{3}k^2\sin^2\varphi/2 + \tfrac{50}{3}k^3\sin^3\varphi/2 - \tfrac{16}{3}k^4\sin^4\varphi/2$$

$$= \lambda_e^2 \tfrac{a_e}{k}[1 + 8k^2 - \tfrac{14}{3}k^2\sin^2\varphi/2 + \tfrac{80}{3}k^3\sin^3\varphi/2$$

$$+8k^4\sin^2\varphi/2 + \tfrac{8}{3}k^4\sin^3\varphi/2 - \tfrac{16}{3}k^4\sin^4\varphi/2]$$

$$\Rightarrow \langle \frac{d\sigma}{d\varphi} \rangle = \lambda_e^2 \frac{a_e}{k}\{1 + \frac{2}{3}(ka_e)^2[5 + 7\cos^2\frac{\varphi}{2}]\}. \tag{3.6.9}$$

It is seen that the differential cross (3.6.9) for slow electrons $ka_e \ll 1$ is practically isotropic and inversely proportional to the wave vector k of the incident electrons.

3.7 The electron scattering by magnetic impurities

In a planar loop of current, the magnetic dipole moment vector $\vec{\mu}$ is defined in terms of the current I_L , the area $\mathbf{A}$ of the loop, and the unit vector $\vec{n}$ perpendicular to the plane of the loop. To find $f_{1,2}(\varphi)$ that control the scattering cross section, it is necessary to specify the operator Eq. (3.4.3). With account of Eqs. (3.3.1) and (3.3.2) after ignoring small terms proportional to A^2 and U, we get

$$\hat{V}_{1,2}(\vec{r}) = -\frac{\lambda_1}{r^3}[2\hat{L}_z \pm 1], \tag{3.7.1}$$

where $\lambda_1 = \frac{ed_m}{(a_m c\hbar)}$ is the dimensionless coupling parameter and $\hat{L}_z = i(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y})$ is z projection of the dimensionless angular momentum operator. Eq. (3.5.4) contains $V_{1,2}$ that is obtained by acting on the wave functions (3.4.2). The result reads

$$V_{1,2}(\vec{r}) = \frac{\lambda_1}{r^3\sqrt{2}}[2y\bar{k} \mp 1] \tag{3.7.2}$$

The integrals (3.5.4) in this case take the form

$$\begin{aligned} f_{1,2}(\varphi) &= -\tfrac{1}{4\sqrt{\pi k}} \textstyle\int \exp(-i\bar{\mathbf{q}}.\mathbf{r}')\hat{V}_{1,2}(r')d^2r', \\ &= -\tfrac{1}{4\sqrt{\pi k}} \textstyle\int \exp(-i\bar{\mathbf{q}}.\mathbf{r}')\tfrac{\lambda_1}{r^3\sqrt{2}}[2y\bar{k} \mp 1]d^2r', \\ &= -\tfrac{\lambda_1}{4\sqrt{\pi k}} \textstyle\int \exp(-i\bar{\mathbf{q}}.\mathbf{r}') \times [2y\bar{k} \mp 1]\tfrac{d^2r'}{r^3\sqrt{2}}, \\ &= -\frac{\lambda_1\sqrt{a_m}}{4\sqrt{\pi k}} \int \exp(-i\bar{\mathbf{q}}.\mathbf{r}') \times [2\bar{k}y' \mp 1]\frac{d^2r'}{r'^3}. \end{aligned} \tag{3.7.3}$$

where, a_m is radius of magnetic dipole here, $\bar{q} = qa_m$ is the dimensionless transferred momentum. The integration in Eq. (3.7.3) is performed in the same coordinate system coordinate system as in the previous section with the y'-axis along the vector $\mathbf{q}$ (see Fig 3.1). Changing to the cylindrical coordinates r', ϕ', with $y' = r'\cos(\phi' - \frac{\varphi}{2})$= $r'\cos\phi'\cos\frac{\varphi}{2} + r\sin\phi'\sin\frac{\varphi}{2}, ...$

We can rewrite Eq. (3.7.3) as follows:

$$f_{1,2}(\varphi) = -\tfrac{\lambda_1\sqrt{a_m}}{4\sqrt{\pi k}} \int \exp(-i\bar{\mathbf{q}}.\mathbf{r}') \times [2\bar{k}(r'\cos\phi'\cos\tfrac{\varphi}{2} + r\sin\phi'\sin\tfrac{\varphi}{2}) \mp 1]\tfrac{d^2r'}{r'^3},$$

$$= -\frac{\lambda_1\sqrt{a_m}}{4\sqrt{\pi k}} \int_1^\infty \frac{dr'}{r'^2}\int_0^{2\pi} \exp(-i\bar{q}r'\cos\phi') \times [2\bar{k}r'\cos\phi'\cos\frac{\varphi}{2} \mp 1]\frac{d^2r'}{r'^3}. \quad (3.7.4)$$

The term with $\sim \sin\phi'\sin\frac{\varphi}{2}$ gives no contribution to integral (3.7.4). The integration over r' is taken from 1 (in the dimension coordinates it corresponds to integration from a radius a of the nanomagnet). Acting in the same manner as in the previous section, we obtain

$$f_{1,2}(\varphi) = \frac{\lambda_1}{2}\sqrt{\frac{a_m\pi}{\bar{k}}}[2i\bar{k}\cos\frac{\varphi}{2}I_1(\bar{q}) \pm I_0(\bar{q})], \quad (3.7.5)$$

where $I_0(\bar{q})$ and $I_1(\bar{q})$ are given by the first two expansions of (3.6.8). With the help of Eqs. (3.4.10) and (3.7.5), we obtain the differential cross-section of electron scattering by magnetic impurity

$$\tfrac{d\sigma(\varphi)}{d\varphi} = 2|f_1^*(\varphi)f_2(\varphi)|$$

$$= ((2\tfrac{\lambda_1}{2}\sqrt{\tfrac{a_m\pi}{\bar{k}}}2i\bar{k}\cos\tfrac{\varphi}{2}I_1(\bar{q}) + I_0(\bar{q}))((2\tfrac{\lambda_1}{2}\sqrt{\tfrac{a_m\pi}{\bar{k}}}2i\bar{k}\cos\tfrac{\varphi}{2}I_1(\bar{q}) - I_0(\bar{q}))$$

$$= \tfrac{\lambda_m^2 a_m}{\bar{k}}[4i^2\bar{k}^2\cos^2\tfrac{\varphi}{2}I_1^2(\bar{q}) - 2i\bar{k}\cos\tfrac{\varphi}{2}I_1(\bar{q})I_0(\bar{q}) + 2i\bar{k}\cos\tfrac{\varphi}{2}I_1(\bar{q})I_0(\bar{q}) - I_0^2(\bar{q})]$$

$$= \tfrac{\lambda_m^2 a_m}{\bar{k}}[-4I_1^2(\bar{q})\bar{k}^2\cos^2\tfrac{\varphi}{2} - I_0^2(\bar{q})]$$

$$= \lambda_m^2\frac{a_m\pi}{\bar{k}}[4I_1^2(\bar{q})\bar{k}^2\cos^2\frac{\varphi}{2} + I_0^2(\bar{q})]. \quad (3.7.6)$$

Here we introduced $\lambda_m = \frac{ed_m\sqrt{\pi}}{2a_mc\hbar}$ to be consistent with the previous section. From Eq. (3.7.6) one can see that the backscattering cross section

$$\frac{d\sigma(\varphi)}{d\varphi}|_{\varphi=\pi} = \lambda_m^2\frac{a_m\pi}{\bar{k}}I_0^2(\bar{q}), \quad (3.7.7)$$

is not equal to zero. The electron scattering by magnetic impurities may be important for slow electrons $\bar{k} = ka_m \ll 1$. For the fast electrons $\bar{k} \gg 1$ this type of scattering gives negligible contribution. To see the dependence of cross-section (3.7.6) on φ in the limit $\bar{k} \ll 1$, we use the first two relations of Eq. (3.6.8). The result reads

$$\tfrac{d\sigma(\varphi)}{d\varphi} = \lambda_m^2 \tfrac{a_m \pi}{\bar{k}} [4(1 - 2\bar{k}\sin\tfrac{\varphi}{2} + \bar{k}^2 \sin^2\tfrac{\varphi}{2})\bar{k}^2\cos^2\tfrac{\varphi}{2}$$

$$+(1 - 4\bar{k}\sin\tfrac{\varphi}{2} + 6\bar{k}^2\sin^2\tfrac{\varphi}{2} - 4\bar{k}^3\sin^3\tfrac{\varphi}{2} + \bar{k}^4\sin^4\tfrac{\varphi}{2})],$$

$$= \lambda_m^2 \tfrac{a_m \pi}{\bar{k}} [4\bar{k}^2\cos^2\tfrac{\varphi}{2} - 8\bar{k}^3\sin\tfrac{\varphi}{2}\cos^2\tfrac{\varphi}{2} + 4\bar{k}^4\sin^2\tfrac{\varphi}{2}\cos^2\tfrac{\varphi}{2}$$

$$+(1 - 4\bar{k}\sin\tfrac{\varphi}{2} + 6\bar{k}^2\sin^2\tfrac{\varphi}{2} - 4\bar{k}^3\sin^3\tfrac{\varphi}{2} + \bar{k}^4\sin^4\tfrac{\varphi}{2})],$$

$$\Rightarrow \frac{d\sigma(\varphi)}{d\varphi} = \lambda_m^2 \frac{a_m \pi}{\bar{k}} \{1 - 4\bar{k}\sin\frac{\varphi}{2} + 2\bar{k}^2[2 + \sin^2\frac{\varphi}{2}]\}. \tag{3.7.8}$$

The cross section (3.7.8) comparing with cross section (3.6.9) contains linear term $\sim \bar{k} = ka_m$. For very slow electrons $ka_m \ll 1$, it is practically isotropic as Eq. (3.6.9)

Chapter 4

Transport Cross-Section

In this Chapter, we discuss the transport scattering length in 2D and transport cross-section by electric and magnetic dipole.

4.1 Transport scattering length in 2D

Electronic transport in graphene towards high mobility is that, strong carrier scattering perturbs the intrisic response of Dirac fermions in graphene and limits potential applications of graphene based on devices. Multiple scattering mechanisms including Coulomb scattering, lattice disorder scattering and electron phonon scattering play roles in realistic graphene devices. Moroever, different types and preparations of graphene are characterized by different dominant scattering mechanisms.The scattering strength is usually quantified by mobility, the ratio of Carrier drift velocity to an applied electric field. Carrier mobility is typically defined as [33]

$$\begin{aligned} \vec{\mu} &= \tfrac{\vec{v}}{\vec{E}}, \\ &= \frac{\vec{\sigma}}{en}, \end{aligned} \tag{4.1.1}$$

where $\vec{v}$ is the Drude carrier drift velocity, $\vec{E}$ is applied electric field, assuming to be small, $\vec{\sigma}$ is conductivity,n is carrier density. Total cross-section scattering classified as elastic and inelastic. For intermediate and heavy elements, the elastic cross-section is constant at low energy and exhibit some variation at higher energy. We are usually more interested in light elements as far as elastic scattering is concerned, for all elements of interest. In case of inelastic scattering, cross-section is relatively small for light nuclei. Heavy nuclei can not serve as good moderators in thermal reactors. The scattering length in quantum mechanics, describes low-energy scattering. It is defined as the following low-energy limit

$$\lim_{k\to 0} k \cot \delta(k) = -\frac{1}{a}, \tag{4.1.2}$$

where a is the scattering length, k is the wave number , δk is the s-wave phase shift. The elastic cross section, σ_e, at low energies is determined solely by the scattering length [34]

$$\lim_{k\to 0} \sigma_e = 4\pi a^2 \tag{4.1.3}$$

When a slow particle scatters off a short ranged scattered (e.g, an impurity in a solid or a heavy particle) it cannot resolve the structure of the object since its de Broglie wave length is very long. The idea is that it should not be important what precise potential $V(r)$ one scatters off, but only how the potential looks at long length scales. In quantum physics, the scattering amplitude is the amplitude of the out going spherically wave relative to the incoming plane wave in a stationary-state scattering process. The latter is described by the wave function,

$$\psi(r) = e^{ikz} + f(\theta)\frac{e^{ikr}}{r}, \tag{4.1.4}$$

where e^{ikz} is the incoming plane wave with the wave number, $\frac{e^{ikr}}{r}$ is the outgoing spherical wave, θ is the scattering angle and $f(\theta)$ is the scattering amplitude. The transport cross section or transport scattering length in 2D problems is the quantity which controls the collision time that enters in all kinetic coefficients. It is given by the relation:

$$\sigma_{tr} = \int_0^{2\pi} (1 - \cos\varphi)\frac{d\sigma}{d\varphi} d\varphi \tag{4.1.5}$$

4.2 Transport crosssection by electric and magnetic dipoles

From Eqn. (3.6.9), the differential cross section by the electric dipoles are given by

$$\langle\tfrac{d\sigma}{d\varphi}\rangle = \lambda_e^2\tfrac{a_e}{\bar{K}}\{1+\tfrac{2}{3}(Ka_e)^2[5+7cos^2\varphi/2]\} = \lambda_e^2\tfrac{a_e}{\bar{K}}\{1+\tfrac{2}{3}k^2a_e^2[5+7\cos^2\varphi/2]\},$$

$$= \lambda_e^2\frac{a_e}{\bar{K}}\{1+\frac{10}{3}k^2a_e^2+\frac{14}{3}k^2a_e^2\cos^2\varphi/2\}. \quad (4.2.1)$$

From Eqn. (4.1.5)

$\sigma_{tr} = \int_0^{2\pi}(1-cos\varphi)\frac{d\sigma}{d\varphi}d\varphi = \int_0^{2\pi}\frac{d\sigma}{d\varphi}d\varphi - \int_0^{2\pi}\cos\varphi\frac{d\sigma}{d\varphi},$

$= \lambda_e^2\frac{a_e}{\bar{K}}\{1+\frac{10}{3}k^2a_e^2+\frac{14}{3}k^2a_e^2\cos^2\varphi/2\}d\varphi - \int_0^{2\pi}\cos\varphi\lambda_e^2\frac{\alpha_e}{\bar{k}}\frac{d\sigma}{d\varphi}d\varphi$

. Therefore, from this equation:

$$\sigma_{tr}^e = \lambda_e^2\frac{a_e}{\bar{k}}\{1+\frac{9}{2}\bar{k^2}\}. \quad (4.2.2)$$

From Eqn. (3.7.8),the differential cross section by the magnetic dipoles are given by

$$\frac{d\sigma(\varphi)}{d\varphi} = \lambda_m^2\frac{a_m}{\bar{k}}\{1-4\bar{k}\sin\varphi/2+2\bar{k^2}[2+\sin^2\varphi/2]\} \quad (4.2.3)$$

By substitution of Eqn. (4.2.3) into Eqn. (4.1.5), we obtain:

$$\sigma_m^{tr} = \int_0^{2\pi}(1-\cos\varphi)\tfrac{d\sigma}{d\varphi}d\varphi$$

$$= \int_0^{2\pi}(1-\cos\varphi)\lambda_m^2\tfrac{a_m}{\bar{k}}\{1-4\bar{k}\sin\varphi/2+2\bar{k^2}[2+\sin^2\varphi/2]\}d\varphi,$$

$$= \lambda_m^2\frac{\pi a_m}{\bar{k}}\{1-4\bar{k}\sin\varphi/2+2\bar{k^2}[2+\sin^2\varphi/2]\}. \quad (4.2.4)$$

The ratio of these quantities in the limit $\bar{k} = ka_{e,m} \ll 1$ is equal to

$$\tfrac{\sigma_{tr}^e}{\sigma^m} = \frac{\lambda_e^2\frac{a_e}{\bar{k}}\{1+\frac{9}{2}\bar{k^2}\}}{\lambda_m^2\frac{\pi a_m}{\bar{k}}\{1-4\bar{k}\sin\varphi/2+2\bar{k^2}[2+\sin^2\varphi/2]\}},$$

$$= \frac{1}{2}\{\frac{c}{v_F}\frac{d_e}{d_m}\frac{a_m}{a_e}\}^2. \quad (4.2.5)$$

The large ratio $\frac{c}{v_F} \approx 300$ results in that the transport cross section of electric dipoles always dominates over the transport cross section of magnetic dipoles. Even the nonmagnetic impurities with the gigantic magnetic dipole moments cannot change the sign of inequality.

$$\frac{\sigma^e_{tr}}{\sigma^m_{tr}} \gg 1. \tag{4.2.6}$$

We can estimate the magnetic moment of these nanoinclusions as

$$d_m = \frac{Nn\mu_B 4\pi a_m^3}{3}, \tag{4.2.7}$$

where N is the number of Bohr magnetons μ_B per atom, $n = 10^{22}cm^{-3}$ is the density number of atoms on nanomagnet. Taking where a number $N = 10[35]$ and $a_m = k10^{-7}cm$, (k is the radius of nanomagnet in nm) and $\mu_B = 10^{-20}$, we get $d_m \approx k^3 10^{-18}$ The typical value of the electric dipole moment is $d_e = 10^{-18}$ and we set $a_e = 10^{-18}cm$. with these parameters, we get

$$\begin{aligned} \frac{\sigma^e_{tr}}{\sigma^m_{tr}} &= \frac{1}{2}\left\{\frac{c}{v_F}\frac{d_e}{d_m}\frac{a_m}{a_e}\right\}^2 \\ &= 50[c(v_F k^2)] \gg 1. \end{aligned} \tag{4.2.8}$$

Even for the large nanomagnets of the order of $10nm$. It would be interesting to compare the transport cross sections of electric dipoles and charged impurities. The latter is formed by the Coulomb scattering potential $U(r) = \frac{-Ze^2}{r}$. For evaluation we neglect the screening effects. The Fourier component of $U(r)$ in $2D$ case is

$$U(\mathbf{q}) = \frac{-\pi Z e^2}{k \sin\frac{\varphi}{2}} \tag{4.2.9}$$

According to equations (3.5.9) and (4.2.9), the electron differential cross section is $\frac{d\sigma(\varphi)}{d\varphi} = \frac{k|U(q)^2|}{2\pi\hbar^2 v_F^2}(\cos^2\varphi/2)$,

Therefore,

$$\frac{d^c_\varphi}{d\varphi} = \frac{k|U(q)^2|}{2\pi\hbar^2 v_F^2}(\cos^2\varphi/2),$$

$$= \frac{k\pi^2 Z^2 e^4}{k^2\sin^2\varphi/2}\cos^2\frac{\varphi}{2}\cdot\frac{1}{2\pi\hbar^2 v_F^2},$$

$$= \frac{\pi Z^2 e^4}{2\hbar^2 v_F^2 k}\cot^2\varphi/2,$$

$$\text{since } \frac{\cos^2\frac{\varphi}{2}}{\sin^2\varphi/2} = \cot^2\varphi/2$$

$$= \frac{\pi Z^2 e^4}{2\hbar^2 v_F^2 k} \cot^2 \varphi/2. \qquad (4.2.10)$$

The corresponding transport cross-section is obtained by substitution of Eq. (4.2.10) into Eq. (4.1.5). After integration over $d\varphi$, we get

$$\sigma_{tr}^c = \int_0^{2\pi} (1 - \cos\varphi) \frac{d\sigma}{d\varphi} d\varphi$$

$$= \int_0^{2\pi} (1 - \cos\varphi) \frac{\pi Z^2 e^4}{2\pi\hbar^2 v_F^2} \cot^2 \varphi/2 d\varphi,$$

$$= \frac{\pi Z^2 e^4}{2\hbar^2 v_F^2} \int_0^{2\pi} (1 - \cos\varphi) \cot^2 \varphi/2 d\varphi,$$

$$= \frac{\pi Z^2 e^4}{2\hbar^2 v_F^2 k} [\int_0^{2\pi} \cot^2 \varphi/2 d\varphi - \int_0^{2\pi} \cos\varphi \cot^2 \varphi/2 d\varphi],$$

$$= \frac{\lambda_c^2}{k}. \qquad (4.2.11)$$

where $\lambda_c = \frac{\pi Z e^2}{\hbar_{v_F}}$

Comparing Eq.(4.2.11) and Eq.(4.2.2),we get

$$\frac{\sigma_{tr}^c}{\sigma_{tr}^e} = \frac{\frac{\lambda_c^2}{k}}{\lambda_e^2 \frac{a_e}{k} \{1 + \frac{9}{2} \bar{k}^2\}},$$

$$= 4\pi Z^2 \frac{e a_e}{d_e}. \qquad (4.2.12)$$

If $Z = 1$ and $ea_e = d_e$ then, the ratio of the transport cross-sections of charged and polar impurities for slow electrons is 4π.

In Fig 4.1, we present the normalized transport cross sections $\sigma_{tr}^{c,e,m}$ divided by $\lambda_c^2 a_e$, $\lambda_e^2 2\pi a_e$,$\lambda_m^2 \pi a_m$, respectively, versus $\bar{k}$. These curves are denoted by letters c, ed, md. It is seen that σ_{tr}^c and σ_{tr}^e are comparable for $0.25 < \bar{k} < 1$. This allows us to claim that the electron scattering by impurities with electric dipoles must be taken into account while analyzing the electron mobility in graphene.

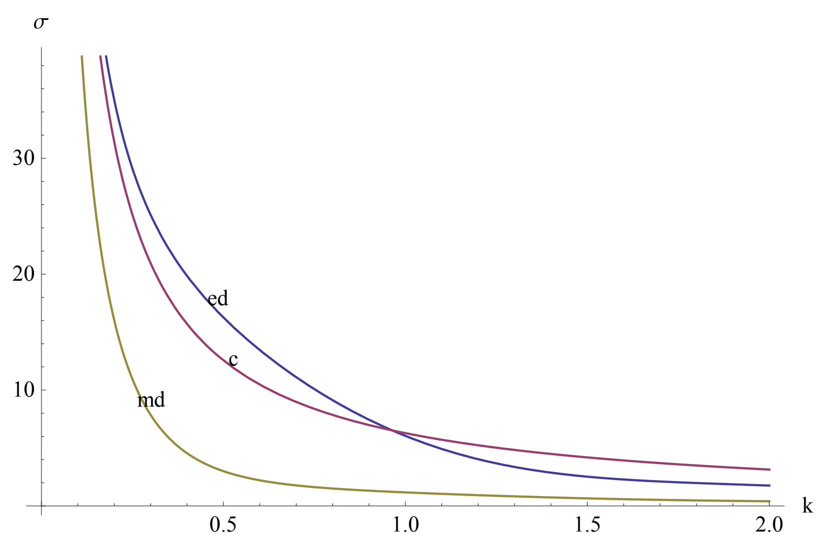

Figure 4.1: The electron transport, cross section by electric dipole (curve, ed), electric charge (coulomb) (curve, c), and magnetic dipole (curve, md) versus dimensionless wave vector k

Chapter 5

Conclusion

5.1 Conclusion

We studied the scattering processes by magnetic impurities with magnetic moment transversal and parallel to the graphene. The interaction of an electron with the magnetic field of the dipole is described by the vector potential $\vec{A}$ is spin independent. However, the electron - magnetic dipole interaction U is spin dependent. The spin dependence leads the wave equations from two component to four component and makes the problem of scattering more complicated. The spin dependent electron scattering in 2DEG has been studied by different researchers and our calculations of the scattering cross section by the nanomagnets located over the graphene plane shows its anisotropy with respect to the spin direction. The analysis of the electron scattering by impurities with electric and magnetic dipole moments in graphene has shown that the electric dipoles are dominant scatterers even compared with nanomagnetic impurities with gigantic magnetic moments.
Moreover, with the help of specially developed Born approximation the derived differential cross-section and the transport cross-section proved that scattering cross-section and the transport cross-section are dominant when the magnetic dipole of the remote nanomagnet is transverse to the electron beam in the graphene plane.

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