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Anisotropic resistivity of the monolayer graphene in the trigonal warping and connected Fermi curve regimes

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ABSTRACT

In the present study, the anisotropic resistivity of the monolayer graphene has been obtained in semi-classical regime beyond the Dirac point approximation. In particular, detailed investigations were made on the dependence of conductivity on the Fermi energy. At low energies, in the vicinity of the Dirac points, band energy of the monolayer graphene is isotropic at the Fermi level. Meanwhile, at the intermediate Fermi energies anisotropic effects such as trigonal warping is expected to be the origin of the anisotropic resistivity. However, besides the band anisotropy there also exists an other source of anisotropic resistivity which was introduced by scattering matrix. At high energies it was shown that the band anisotropy is less effective than the anisotropy generated by the scattering matrix. It was also shown that there exist two distinct regimes of anisotropic resistivity corresponding the trigonal warping and connected Fermi curve at intermediate and high energies respectively.

1. Introduction

Two-dimensional crystals of carbon atoms (a single sheet of graphite) [1] were first fabricated in 2004 by Novoselov et al. [2]. Discovery and fabrication of graphene provided a matchless opportunity for novel experimental observation of electronic transport properties which has also provided a rich field of theoretical studies over the last 10 years. The experimental realization of a graphene has prompted much excitement and emotion in both the experimental and theoretical physics. From a fundamental point of view, discovery of graphene was important not only in providing the first realization of Dirac Hamiltonian and relativistic massless particles [3–7] but also in providing a way for designing graphene-based electronic devices. The discovery of these extraordinary properties in graphene-based systems in recent years opens unprecedented expectancy for the investigation of low dimensional systems.

The energy bands of graphene touch together in the edge of the hexagonal Brillouin zone known as Dirac points. The energy spectrum of carriers is linear at the Dirac points. This fact has many significant consequences especially on the electric transport in graphene. Therefore the electrical transport in graphene becomes a very active research field in recent years because of its potential application in nano-material and instrumentation of nano-scale materials. It should be noted that it was shown that the graphene based nano-structures such as nano-ribbons could have finite energy gap at the Dirac points [8–21].

As mentioned before in the pure graphene the energy band in the edge of the hexagonal Brillouin zone meets each other. This fact provides a theoretical perception to realize unusual transport properties in this material. Graphene is a gapless semiconductor with a minimal conductivity which can be considered as the nearly universal value of the order of $4e^2/h$ [22–27]. Meanwhile this conductivity depends on externally imposed conditions such as the temperature and doping. The band structure of the graphene has been obtained in the 1947 by Wallace [28] however, the universal value of the minimal conductivity in the pure graphene is not completely understood until the recent years.

In the present work it was shown that the Fermi energy, ϵ_F, determines different transport regimes. Unlike the linear energy dispersion at low energies (typically when $0 < \epsilon_F \leq 1\,\mathrm{eV}$) in the vicinity of the Dirac points, small corrections, such as second order of Dirac equation, [29] would lead to revision in effective Hamiltonian of graphene at higher energies. These corrections which appear in the energy dispersion by introducing an additional quadratic term result in deformation of the Fermi line. The deformation of the Fermi circle around a K-point in which the circular Fermi curve at the Dirac points changes to a trigonal is known as trigonal warping. In fact breaking the symmetry of the effective Hamiltonian at the Dirac points results in trigonal warping [29–32]. This effect has been reported in graphene-related structures such as bilayer and multi-layer graphene and even in carbon nano-tubes [33–35]. It was also shown that, by increasing the Fermi energy beyond the hopping energy, t, another

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regime will appear in which the shape of the Fermi curves and the behavior of the anisotropic resistivity (AR) are changed simultaneously.

2. Model

Anisotropic transport generally has been discussed in terms of the asymmetry of the scattering between two states on the Fermi surface. In the present work we have employed an analytical approach which was introduced by Výborný et al. in [36]. They have described an analytical approach in which the anisotropic transport can be obtained within the semiclassical Boltzmann method [36]. We consider the Boltzmann equation for non-equilibrium distribution function, $f_\lambda(\vec{k}, \varepsilon)$, as

$$-e\vec{\varepsilon}.\vec{v}_\lambda(\vec{k})(-\partial_\varepsilon f_0) = \sum_{\lambda'}\int \frac{d^2k'}{(2\pi)^2}\omega_{\lambda\lambda'}(\vec{k},\vec{k}')[f_\lambda(\vec{k},\varepsilon) - f_{\lambda'}(\vec{k}',\varepsilon)], \tag{1}$$

where $\omega_{\lambda\lambda'}(\vec{k},\vec{k}')$ denotes the scattering rate between the following states: $|\vec{k}\lambda\rangle$ and $|\vec{k}'\lambda'\rangle$. In this approach the following solution has been proposed for non-equilibrium distribution function:

$$f_\lambda(\phi,\theta) - f_0 = -e\varepsilon v_\lambda(-\partial_\varepsilon f_{0\lambda})(a_\lambda(\phi)\cos(\theta) + b_\lambda(\phi)\sin(\theta)) \tag{2}$$

where ϕ and θ are angles along the $\vec{k}$ (wave vector) and $\vec{\varepsilon}$ (electrical field) respectively. λ and λ' are the band indices, f_0 is the equilibrium distribution function and the velocity, $\vec{v}_\lambda$, $(\vec{v}_\lambda = (1/\hbar)\nabla_k\epsilon_{\vec{k}})$ is given by the band dispersion energy. The electric field and the wave vector have been denoted by $\vec{\varepsilon} = \varepsilon(\cos\theta, \sin\theta)$ and $\vec{k} = k(\cos\phi, \sin\phi)$ respectively.

The Taylor series of the distribution function is given as

$$f(\vec{k},\vec{\varepsilon}) = f_0 + \varepsilon_x\partial_{\varepsilon_x}f + \varepsilon_y\partial_{\varepsilon_y}f + \sum \varepsilon_i\varepsilon_j\partial_{\varepsilon_i}\partial_{\varepsilon_j}f + \cdots \tag{3}$$

For a two band system ($\lambda = \pm$) by using the above equations it can be shown that in order to have the non-equilibrium distribution function following relations have to be satisfied [36]:

$$\cos(\phi) = \varpi_\pm(\phi)a_\pm(\phi) - \int d\phi'[\omega_{\pm\pm}(\phi,\phi')a_\pm(\phi') + \omega_{\pm\mp}(\phi,\phi')a_\mp(\phi)] \tag{4}$$

$$\sin(\phi) = \varpi_\pm(\phi)b_\pm(\phi) - \int d\phi'[\omega_{\pm\pm}(\phi,\phi')b_\pm(\phi') + \omega_{\pm\mp}(\phi,\phi')b_\mp(\phi)] \tag{5}$$

in which we have assumed

$$\varpi_\lambda(\phi) = \sum_{\lambda'}\int d\phi'\,\omega_{\lambda\lambda'}(\phi,\phi') \tag{6}$$

$$\omega_{\lambda\lambda'}(\phi,\phi') = (2\pi)^{-2}\int k'\,dk'\omega_{\lambda\lambda'}(k,k') \tag{7}$$

where $a_\pm(\phi)$ and $b_\pm(\phi)$ take the form of the Fourier series that can be described by

$$a_\pm(\phi) = a_0 + a_{c1}^\pm\cos\phi + a_{c2}^\pm\cos2\phi + \cdots + a_{s1}^\pm\sin\phi + a_{s2}^\pm\sin2\phi + \cdots \tag{8}$$

$$b_\pm(\phi) = b_0 + b_{c1}^\pm\cos\phi + b_{c2}^\pm\cos2\phi + \cdots + b_{s1}^\pm\sin\phi + b_{s2}^\pm\sin2\phi + \cdots \tag{9}$$

Provided that the coefficients $a_\pm$ and $b_\pm$ are known by solving Eqs. (4) and (5) the non-equilibrium distribution functions are given for each band as follows:

$$f_+(\phi,\theta) - f_{0+} = -e\varepsilon v_+(-\partial_\varepsilon f_{0+})\left[a_+\cos\theta + b_+(\phi)\sin\theta\right]$$
$$f_-(\phi,\theta) - f_{0-} = -e\varepsilon v_-(-\partial_\varepsilon f_{0-})\left[a_-(\phi)\cos\theta + b_-(\phi)\sin\theta\right]$$

3. Anisotropic conductivity beyond the Dirac point

Tight binding Hamiltonian of pure graphene in the nearest neighbor approximation is given by

$$H_0 = -t\sum_{\langle i,j\rangle}(a_i^\dagger b_j + h.c) \tag{10}$$

in which the operators $a_i^\dagger$ and b_j refer to the creation and annihilation of an electron in sublattices A and B respectively and $t=2.7$ eV denotes the hopping parameter.

The matrix representation of the Hamiltonian in the bases $\psi = (\psi_A, \psi_B)$ is as follows:

$$H_0 = \begin{pmatrix} 0 & H_{AB}(\mathbf{k}) \\ H_{AB}^*(\mathbf{k}) & 0 \end{pmatrix}, \tag{11}$$

where $H_{AB}(\mathbf{k}) = t(e^{-i\mathbf{k}.\vec{\delta}_1} + e^{-i\mathbf{k}.\vec{\delta}_2} + e^{-i\mathbf{k}.\vec{\delta}_3})$ and we have defined nearest neighbors position vectors by $\vec{\delta}_1 = (a/2)(1, \sqrt{3})$, $\vec{\delta}_2 = (a/2)(-1, \sqrt{3})$, $\vec{\delta}_3 = a(-1, 0)$ in which the carbon–carbon distance is denoted by $a=1.42$ Å.

The eigen-states may then be written as

$$\psi_k = \frac{1}{\sqrt{2}}\begin{pmatrix} \lambda e^{i\bar{\varphi}_k} \\ 1 \end{pmatrix}, \tag{12}$$

in which

$$\bar{\varphi}_k(\phi) = \tan^{-1}\left(\frac{\mathrm{Im}\,H_{AB}(\vec{k})}{\mathrm{Re}\,H_{AB}(\vec{k})}\right), \tag{13}$$

and

$$\phi = \tan^{-1}\left(\frac{k_y}{k_x}\right), \tag{14}$$

Then the band energies are given by

$$\epsilon_{k\lambda} = \lambda t(1 + 4\cos(3a/2k_x)\cos(\sqrt{3}a/2k_y) + 4\cos^2(\sqrt{3}a/2)k_y)^{1/2} \tag{15}$$

where $\lambda = \pm 1$ is the band index. Unlike the Dirac point Hamiltonian here the energy spectrum is anisotropic in k-space.

In the presence of the impurities the Hamiltonian of the system reads

$$H = H_0 + V_{im} \tag{16}$$

in which $V_{im}(\vec{r}) = v\sum_j\delta(\vec{r} - \vec{r}_j)$ stands for short range impurity potential in which summation is over the position of the impurities and v is the strength of the impurity potential. The scattering rates are defined through the relations:

$$\omega_{++}(\phi,\phi') = \frac{\pi}{\hbar}n_i(v^2 + v^2\cos(\bar{\varphi}_k - \bar{\varphi}_{k'}))$$
$$\omega_{--}(\phi,\phi') = \frac{\pi}{\hbar}n_i(v^2 + v^2\cos(\bar{\varphi}_k - \bar{\varphi}_{k'})) \tag{17}$$

$$\omega_{+-}(\phi,\phi') = \frac{\pi}{\hbar}n_i(v^2 - v^2\cos(\bar{\varphi}_k - \bar{\varphi}_{k'}))$$
$$\omega_{-+}(\phi,\phi') = \frac{\pi}{\hbar}n_i(v^2 - v^2\cos(\bar{\varphi}_k - \bar{\varphi}_{k'})) \tag{18}$$

where n_i is the density of the impurities. Scattering rates can be