ORIGINAL PAPER

THERMAL CONDUCTIVITY OF GRAPHENE FOR COHERENT AND NON-COHERENT HOLE –ELECTRON'S STATES

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Abstract. *In this thesis, we investigate the thermal transport properties of graphene using the Boltzmann approximation. Based on the analytical solution of Boltzmann equation for coherent and non-coherent electron-hole states, the minimum electrical and thermal conductivities are studied. We solve the Boltzmann equation in the chirality basis by considering off-diagonal elements of the distribution function due to the electron-hole coherency effect and calculate the thermal transport properties of graphene. Finally, we obtain the thermal coefficients as functions of temperature. Our results show that the thermal conductivity in non-coherent electron-hole state has a linear behavior at low temperature.*

Keywords: *thermal conductivity-graphene-chirality*

1. INTRODUCTION

Single graphite layers (graphene) have been found in the free state only recently [1], and their transport properties have immediately attracted much attention from both experimental [2 - 4] and theoretical [5 - 16] invest number of very unusual transport properties including (i) the conductivity does not vanish at zero carrier con- centration (minimum conductivity phenomena), (ii) the minimum conductivity does not depend on the temperature. Besides these unconventional transport properties many related phenomena have been studied in graphene such as weak localization [14 - 16], the Klein paradox [17], tunneling conductance of normal metal-insulator- superconductor [18] and n-p [19] junctions, Andreev re- flection [20], Josephson effect [21, 22], photon-assisted electron transport [23], integer [24] and fractional quantum Hall effect [25]. The remarkable transport proper- ties of graphene are usually attributed to the particular spectrum of excitations [26] which consists of two conical bands and is described by a two-dimensional analog of the relativistic Dirac equation. For a review concerning the history, fabrication, fundamental properties, and ing the history, fabrication, fundamental properties, and future applications of graphene we refer to very recent article [26]. To investigate the transport properties (i) and (ii) of graphene several different approaches have been applied including the Kubo formalism [5 - 7, 9 - 11], and direct calculations of the transmission probability (Landauer formula) [8, 11, 12]. In this Letter we start from a direct analytical solution of the Boltzmann equation for Dirac fermions. Though the model is quasi classical, the most remarkable features noted above are reproduced. In what follows we derive analytical expressions for the electrical and thermal conductivity of graphene.

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2. THERMAL CONDUCTIVITY AT NON-COHERENCE HOLE-ELECTRON'S STATES

Dispersing and effective potential of carrier in grapheme with impurities is shown in the following formula:

(1)

1

which in it, q and eZ are in order electrostatic carrier's charge and impure atom charge and R is a camouflage radius or the same Thomas Fermi's radius.

In uniform electrical field, E in Boltzmann's equation is in the following form

$$\left(\frac{\partial f_k}{\partial t}\right)^{coll} = -q\vec{E}v_k\left(-\frac{\partial f^{\circ}(\varepsilon_{k\lambda})}{\partial \varepsilon_{k\lambda}}\right), \kappa = \pm 1 \tag{2}$$

which in it, v_k are speed operator of diagonal elements at chirality basis.

We solve Boltzmann's equation, when an electrical field is zero and there is just temperature gradient.

$$\left(\frac{\partial f}{\partial t}\right)^{\mathrm{coll}} = \frac{\partial f}{\partial t} + \vec{v}.\nabla f + \dot{p}\frac{\partial f}{\partial p} = I[f] \tag{3}$$

After calculation, we can show, density of thermal current in the following form:

$$j_q = -\frac{\nabla T}{e^2 T}\int d\varepsilon\left[\sigma(\varepsilon_{+\lambda})(\varepsilon_{+k}-\mu)^2\left(-\frac{\partial f^{\circ}(\varepsilon_{+k})}{\partial \varepsilon_{+k}}\right) + \sigma(\varepsilon_{-\lambda})(\varepsilon_{-k}-\mu)^2\left(-\frac{\partial f^{\circ}(\varepsilon_{-k})}{\partial \varepsilon_{-k}}\right)\right] \tag{4}$$

This formula in comparison with $J= - K\nabla T$ flow of thermal energy or transmission energy, so we have:

$$K = \frac{1}{e^2 T}\int d\varepsilon\left[\sigma(\varepsilon_{+\lambda})(\varepsilon_{+k}-\mu)^2\left(-\frac{\partial f^{\circ}(\varepsilon_{+k})}{\partial \varepsilon_{+k}}\right) + \sigma(\varepsilon_{-\lambda})(\varepsilon_{-k}-\mu)^2\left(-\frac{\partial f^{\circ}(\varepsilon_{-k})}{\partial \varepsilon_{-k}}\right)\right]$$

We have following figure for the non-coherence electron – hole in the low temperatures say that $\frac{T}{T_f} \ll 1$. According to this figure we conclude that in the low temperatures, conductivity change with temperature as linear.

$$\kappa = \frac{\pi^2 k_\beta^2 \sqrt{\alpha}}{3h} T$$

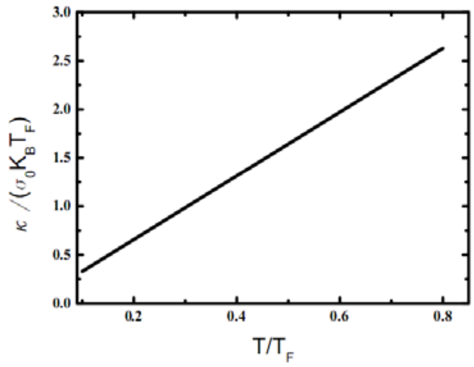

Fig. 1. Thermal conductivity in low temperature for non-coherent electron-hole states.

And we introduce non-coherence hole-electron's parameter in the following form:

$$\alpha = 4\varepsilon_{k+}^2 \tau^2(k)/\hbar^2$$

By usage of first-grade's relaxation time approximation,

$$\tau \approx \frac{1}{k}\frac{\hbar^2 v_\circ}{4R^2 V_\circ^2} \quad Rk \ll 1$$

is independent of K and is in the following form

$$\alpha = \hbar^4 v_\circ^4 / 4R^4 V_\circ^4 \tag{5}$$

3. THERMAL CONDUCTIVITY AT COHERENT HOLE-ELECTRON'S POSITION

In non-coherence hole-electron's position, we can relinquish from off-diagonal elements of distribution function. But, totally, we describe the particle by Dirac Hamiltonian, it means:

$$H = -i v_f \sigma.\nabla = \hbar v_F(\sigma_x k_x + \sigma_y k_y), \vec{k} = -i\nabla = (k_x, k_y) \tag{6}$$

That $v_F \approx 10^6 ms^{-1}$ is Fermi's speed (speed of graphene's carriers) and σ_x and σ_y are Paoli spinors. Necessarily, it is not only at ψ_{k+} or ψ_{k-} states, but also, in the superposition of these states and in this case, coherent hole-electron's states occurs. In this state, distribution function of non-coherence hole-electron's parameter is very little, it means $\hat{f}(k)$ is little, and is, as a matrix 2×2 with off-diagonal and off-zero elements. With temperature gradient, the answer results from (3) formula and pay attention to off-diagonal elements, time evolution of distribution function results from (7) formula.

$$I[f] = \frac{i}{\hbar}[H_\circ, \rho] + \vec{v}.\nabla f = \frac{-i}{\hbar}[U, \rho]$$

$$I(f) = \left(\frac{df}{dt}\right)^{coll} = \frac{i}{\hbar}[H_0, \rho] + \left(-\vec{v}_k.\frac{\nabla T}{T}(\varepsilon - \mu)\left(-\frac{df_0}{d\varepsilon}\right)\right) \tag{7}$$

With pay attention to timeevolutionof matrix of density after every scatteringis in the following form:

$$\hat{\rho} \to \hat{\rho}(t=0) + \frac{i}{\hbar}\int_0^\infty dt e^{-\frac{i}{\hbar}\hat{H}_\circ t}\left[\hat{\rho}(t=0), U\right] e^{-\frac{i}{\hbar}\hat{H}_\circ t} \tag{8}$$

and from $\sigma = \sigma_0 + nq^2 \frac{\hbar \omega_F}{2 u_0^2}$ formula, results (9) formula.

$$\left(\frac{df}{dt}\right)^{coll} = \frac{i}{\hbar}\begin{pmatrix} 0 & f_{21}(\varepsilon_{k+} - \varepsilon_{k-}) \\ f_{12}(\varepsilon_{k-} - \varepsilon_{k+}) & 0 \end{pmatrix} + \frac{\nabla T}{T}\begin{pmatrix} -v_{11}(\varepsilon_+ - \mu)\left[-\frac{\partial f^\circ(\varepsilon_{k+})}{\partial E_{k+}}\right] & \frac{v_{12}}{2E_{k+}}\left[(\varepsilon_- - \mu) f^\circ_{E_{k-}} - (\varepsilon_+ - \mu) f^\circ_{E_{k+}}\right] \\ \frac{v_{21}}{2\varepsilon_{k-}}\left[(\varepsilon_+ - \mu) f^\circ_{E_+} - (\varepsilon_- - \mu) f^\circ_{E_{k-}}\right] & -v_{22}(\varepsilon_- - \mu)\left[-\frac{\partial f^\circ(\varepsilon_{k-})}{\partial \varepsilon_{k-}}\right] \end{pmatrix} \tag{9}$$

With analytical solving of above equation, off-diagonal elements of distribution function results from following form:

$$f_{11}^1 = qEv_{11}\tau(k)\left\{\left(1+\frac{1}{2\alpha}\right)\left[-(\varepsilon_+ - \mu)\frac{\partial f^\circ(\varepsilon_{k+})}{\partial \varepsilon_{k+}}\right] + \frac{1}{2\alpha}\left[-(\varepsilon_- - \mu)\frac{\partial f^\circ(\varepsilon_{k-})}{\partial \varepsilon_{k-}}\right] + \frac{1}{2\alpha E_{k+}}\left((\varepsilon_+ - \mu) f^\circ_{\varepsilon+} - (\varepsilon_- - \mu) f^\circ_{\varepsilon_{k-}}\right)\right\} \tag{10}$$

$$f_{22}^1 = qEv_{22}\tau(k)\left\{\left(1+\frac{1}{2\alpha}\right)\left[-(\varepsilon_- - \mu)\frac{\partial f^\circ(\varepsilon_{k-})}{\partial \varepsilon_{k-}}\right] + \frac{1}{2\alpha}\left[-(\varepsilon_+ - \mu)\frac{\partial f^\circ(\varepsilon_{k+})}{\partial \varepsilon_{k+}}\right] + \frac{1}{2\alpha E_{k-}}\left((\varepsilon_- - \mu) f^\circ_{\varepsilon-} - (\varepsilon_+ - \mu) f^\circ_{\varepsilon_{k+}}\right)\right\} \tag{11}$$

$$f_{12}^1 = \frac{qEv_{12}\tau(k)\left(\frac{1}{2}+\frac{1}{2\alpha}\right)}{1+2i\varepsilon_{k+}\tau(k)/\hbar}\left\{\frac{1}{\varepsilon_{k+}}\left((\varepsilon_+ - \mu) f^\circ_{\varepsilon_{k+}} - (\varepsilon_- - \mu) f^\circ_{\varepsilon_{k-}}\right) + \left[-(\varepsilon_+ - \mu)\frac{\partial f^\circ(\varepsilon_{k+})}{\partial \varepsilon_{k+}} - (\varepsilon_- - \mu)\frac{\partial f^\circ(\varepsilon_{k-})}{\partial \varepsilon_{k-}}\right]\right\} \tag{12}$$

$$f_{21}^1 = \frac{qEv_{21}\tau(k)\left(\frac{1}{2}+\frac{1}{2\alpha}\right)}{1+2i\varepsilon_{k-}\tau(k)/\hbar}\left\{\frac{1}{\varepsilon_{k+}}\left((\varepsilon_- - \mu) f^\circ_{\varepsilon_{k-}} - (\varepsilon_+ - \mu) f^\circ_{\varepsilon_{k+}}\right) + \left[-(\varepsilon_- - \mu)\frac{\partial f^\circ(\varepsilon_{k-})}{\partial \varepsilon_{k-}} - (\varepsilon_+ - \mu)\frac{\partial f^\circ(\varepsilon_{k+})}{\partial \varepsilon_{k+}}\right]\right\} \tag{13}$$

With pay attention to, share's unbalance sentences of distribution function at density of thermal current and putting elements of distribution function at an unbalance state, we have

$$J_q = \frac{\hbar^2 v_0{}^2}{2\pi R^2 v_0{}^2}\frac{-\nabla T}{T}\left[\int \left((\varepsilon_+ - \mu)^2\left(\frac{-\partial f(\varepsilon_{k+})^0}{\partial \varepsilon_{k+}}\right) + (\varepsilon_- - \mu)^2\left(\frac{-\partial f(\varepsilon_{k-})^0}{\partial \varepsilon_{k-}}\right)\right)d\varepsilon \right.$$
$$+ \frac{2}{\alpha}\left[\int \int \left((\varepsilon_+ - \mu)^2\left(\frac{-\partial f(\epsilon_{k+})^0}{\partial \varepsilon_{k+}}\right) + (\varepsilon_- - \mu)^2\left(\frac{-\partial f(\epsilon_{k-})^0}{\partial \varepsilon_{k-}}\right)\right)d\varepsilon\right]$$
$$\left. + \frac{2}{\alpha}\left[\int (\varepsilon_+ - \mu)^2 f(\varepsilon_{k+})^0 - (\varepsilon_- - \mu)^2 f(\varepsilon_{k+})^0 \frac{d\varepsilon}{\varepsilon_+}\right]\right] \qquad (14)$$

Because of the sentences accordance to $\left((\varepsilon_- - \mu)f^{\circ}_{\varepsilon_{k-}} - (\varepsilon_+ - \mu)f^{\circ}_{\varepsilon_{k+}}\right)$ in the non-balancing distribution function, integral is diverge. So we introduce energy of ε_c. If we consider relaxation time as τ then energy time uncertainty will be $\Delta E\tau \sim \hbar$. In fact ε_c is uncertainty of energy that occur between two sequences scattering events by time difference $\tau(k_F)$ than to each other. So we have

$$\varepsilon_C \sim \tau^{-1}(k_F)\hbar$$

$$\varepsilon_C \sim \frac{4R^2 V_0{}^2 k_F}{\hbar v}$$

In coherence electron – hole state $\alpha \ll 1$ and in the low temperatures thermal conductivity as following

$$\kappa = \kappa_{\circ}\left\{1 + \frac{2}{\alpha}\left(1 - \frac{1}{2}\ln\frac{\alpha}{4}\right)\right\}$$

Similarly, we can with the presence of an electrical field,investigate electrical conductivity at coherent hole-electron's state.

4. CALCULATION OF THERMAL CONDUCTIVITY BY USE OF TRANSPORT COEFFICIENTS

For calculation of thermal conductivity's equation,thermal conductivity should relate thermal current to temperature gradient,if there is no electrical current,so we have

$$J_q = \frac{L_{21}}{L_{11}} J_Z + \left(L_{22} - \frac{L_{12}L_{21}}{L_{11}}\right)\left(-\frac{dT}{dZ}\right) = \Pi J_Z + k_e\left(-\frac{dT}{dZ}\right) \qquad (15)$$

In non-current and non-zero temperature gradient at Z axis, we can write

$$J_q = \left(L_{22} - \frac{L_{12}L_{21}}{L_{11}}\right)\left(-\frac{dT}{dZ}\right) \qquad (16)$$

Thus, thermal conductivity of electrons is in the following form

$$k_e = -\frac{J_q}{dT/dZ} = \left(L_{22} - \frac{L_{12}L_{21}}{L_{11}}\right) = \left(L_{22} - L_{21}S\right) \tag{17}$$

After calculations, we have thermal conductivity's formula

$$\begin{aligned} k_e &= \frac{\pi^2}{3}\frac{k_B{}^2 T\sigma_0}{e^2} - \sigma_0\left(1+e^{-\beta\mu}\right)\left(\left[k_B T\ln\left[1+e^{-\beta\mu}\right] + \frac{\mu}{1+e^{\beta\mu}}\right]\right)^2 \\ &= \frac{\sigma_\circ k_B^2 T_F}{e^2\overline{T}}\left[\frac{\pi^2\overline{T}^2}{3} - \left(\overline{T}\right)\ln(1+e^{-\frac{\overline{\mu}}{\overline{T}}}) + \frac{\overline{\mu}}{1+e^{\frac{\overline{\mu}}{\overline{T}}}}\right] \end{aligned} \tag{18}$$

By usage of Mott's famous formula, we have

$$\kappa_e = \frac{\sqrt{\alpha}}{h}\frac{T_F k_B^2}{\overline{T}}\left[\frac{\pi^2\overline{T}^2}{3} - \left(\overline{T}\right)\ln(1+e^{-\frac{\overline{\mu}}{\overline{T}}}) + \frac{\overline{\mu}}{1+e^{\frac{\overline{\mu}}{\overline{T}}}}\right] \tag{19}$$

In this formula, α is non-coherence hole-electron's parameter.

In following diagram, thermal conductivity is indicating with calculating above sentences of (19) formula.

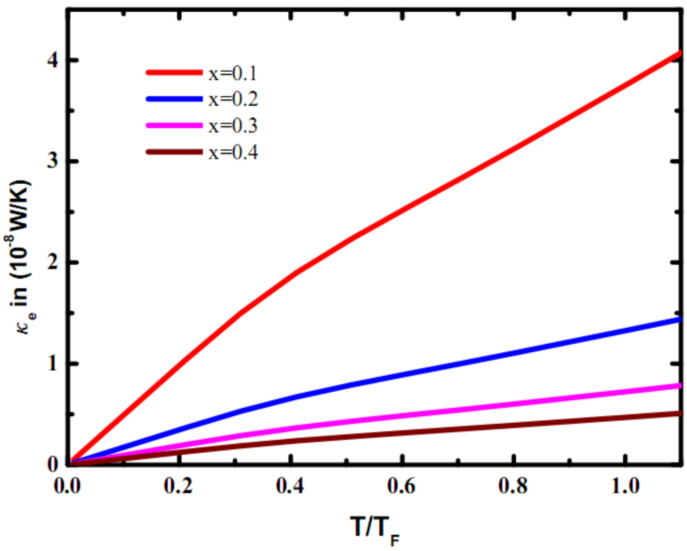

Fig. 2. Thermal conductivity than the temperature for the different scattering values α. In here $x = \left(1/\sqrt{\alpha}\right)$.

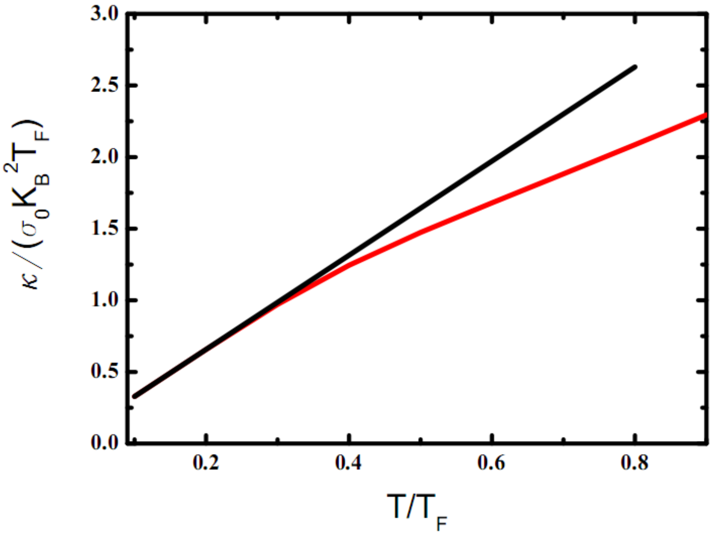

Fig. 3. Thermal conductivity than the temperature with considering higher order of relation (19), (red diagram). Linear behavior thermal conductivity in terms of temperature in low temperatures (dark diagram).

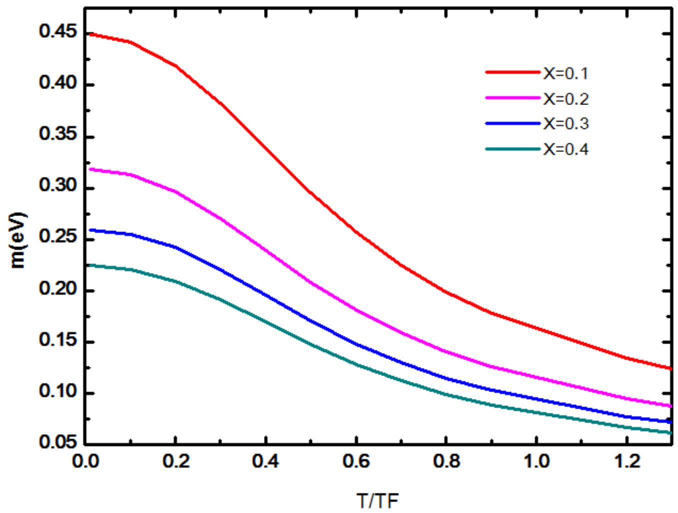

Fig. 4. Thermal conductivity in terms of the temperature.

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