YUCOMAT 2013, Herceg Novi, Montenegro

THERMOELECTRIC POWER IN GRAPHENE MONOLAYER

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INTRODUCTION

Thermoelectric power (TP) in graphene monolayer is hereby analyzed in the wide temperature range of 10–300 K, based on semiclassical Boltzmann equation and theory of linear response. The solutions of Boltzmann equation are found in the approximation of relaxation time for different relaxation mechanisms of charge carriers, with temperature dependence of the corresponding relaxation times adopted from the literature. Temperature dependence of graphene thermoelectric power is numerically found and compared with the experimentally observed data. The dependance of graphene thermoelectric power on the concentration of charge carriers is analyzed as well.

THERMOELECTRIC POWER

Thermoelectric power can be determined with Neville Mott formula:

$$Q_x = -\frac{\pi^2}{3}\frac{k_B^2}{e}T\frac{d}{d\mu}\left(\ln\sigma_x(\mu)\right)$$

In the linear response theory within semiclassical approximation TP is determined as:

$$Q_x = -\frac{1}{eT}\frac{\int_0^\infty (\varepsilon-\mu)\tau(\varepsilon)(-\frac{\partial f_0}{\partial\varepsilon})v^2 D(\varepsilon)\,d\varepsilon}{\int_0^\infty \tau(\varepsilon)(-\frac{\partial f_0}{\partial\varepsilon})v^2 D(\varepsilon)\,d\varepsilon}$$

Where $\tau(\varepsilon)$ is relaxation time, $D(\varepsilon)$ is density of states, f_0 is Fermi-Dirac distribution function, and v is charge velocity.

GRAPHENE ELECTRICAL CONDUCTIVITY

Further on, for finding graphene electrical conductivity we shall apply semiclassical Boltcmann transport equation in the approximation of relaxation time

$$\sigma = \frac{e^2}{2}\int_0^\infty \frac{g_s g_v}{2\pi(\hbar v_F)^2}v^2\tau(\varepsilon)(-\frac{\partial f_0}{\partial\varepsilon}) = \frac{e^2}{2}\int_0^\infty D(\varepsilon)v^2\tau(\varepsilon)(-\frac{\partial f_0}{\partial\varepsilon}).$$

To calculate total relaxation time we apply Matthiessen rule, in case of relaxation on charged impurities (long-range Coulomb interaction), and in case of relaxation on neutral impurities (short-range Coulomb interaction), respectively:

$$\frac{1}{\tau_{im}} = \begin{cases} \dfrac{u_0^2}{\hbar\varepsilon_F}; \\ \dfrac{n_d V_0^2}{\hbar}\dfrac{\varepsilon_F}{4(\hbar v_F)^2}. \end{cases}$$

In case of relaxation on phonons, we analyze the temperature ranges $T \geq T_{BG}$ and $T < T_{BG}$ (where T_{BG} is Bloch-Grüneisen temperature), respectively:

$$\frac{1}{\tau_{ph}(\varepsilon)} = \begin{cases} \dfrac{1}{\hbar^3}\dfrac{\varepsilon}{4v_F^2}\dfrac{D^2}{\rho_m v_{ph}^2}k_B T; \\ \dfrac{1}{\pi}\dfrac{1}{\varepsilon_F}\dfrac{1}{k_F}\dfrac{D^2}{2\rho_m v_{ph}}\dfrac{4!\zeta(4)}{(\hbar v_{ph})^4}(k_B T)^4. \end{cases}$$

For numerical calculation of electrical conductivity, we shall adopt the following values of parameters:

$$D = 30{,}4\cdot10^{-19}\,\mathrm{J};\ \rho_m = 7{,}6\cdot10^{-7}\,\frac{\mathrm{kg}}{\mathrm{m}^2};\ v_{ph} = 2\cdot10^4\,\frac{\mathrm{m}}{\mathrm{s}};\ \varepsilon_F = 4{,}168\cdot10^{-19}\,\mathrm{J};$$

$$v_F = 10^6\,\frac{\mathrm{m}}{\mathrm{s}};\quad k_F = 4{,}8\cdot10^8\,\mathrm{m}^{-1};\ n_i^C = 4\cdot10^{15}\,\mathrm{m}^{-2};\ Z = 1;\ \tilde{\varepsilon}_r = 2{,}4;\ \tilde{\gamma} = 4{,}2;$$

$$n_d = 0{,}4\cdot10^{14}\,\mathrm{m}^{-2};\ V_0 = 16\cdot10^{-37}\,\mathrm{Jm}^2;\ T_{BG} = 54\mathrm{K}.$$

For lower and for higher temperatures, expression for electrical conductivity is transformed, respectively:

$$\sigma = \frac{4\pi e^2}{h^2}\int_0^\infty dx\{k_B T\,x + \varepsilon_F[1 - \frac{\pi^2}{6}(\frac{k_B T}{\varepsilon_F})^2]\}\tau(x)\frac{e^x}{(e^x+1)^2};\quad x = \frac{\varepsilon-\mu}{k_B T};\quad \mu = \varepsilon_F - \frac{\pi^2}{6}\frac{(k_B T)^2}{\varepsilon_F};$$

$$\sigma = \frac{4\pi e^2}{h^2}\int_0^\infty dx\{k_B T\,x + \frac{1}{4\ln 2}\frac{\varepsilon_F^2}{k_B T}]\}\tau(x)\frac{e^x}{(e^x+1)^2};\quad x = \frac{\varepsilon-\mu}{k_B T};\quad \mu = \frac{1}{4\ln 2}\frac{\varepsilon_F^2}{k_B T}.$$

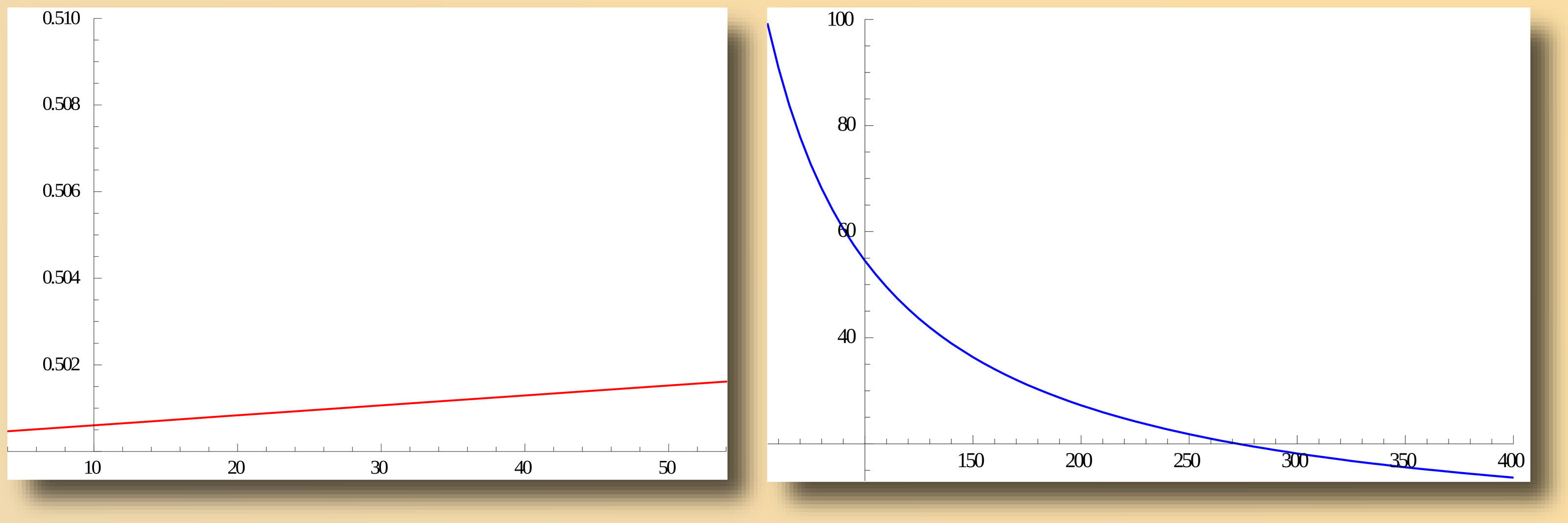

Figure 1. Temperature dependance of graphene electrical conductivity in case of relaxation on charged impurities, for temperature ranges $T<<T_{BG}$ (left) and $T>T_{BG}$ (right)

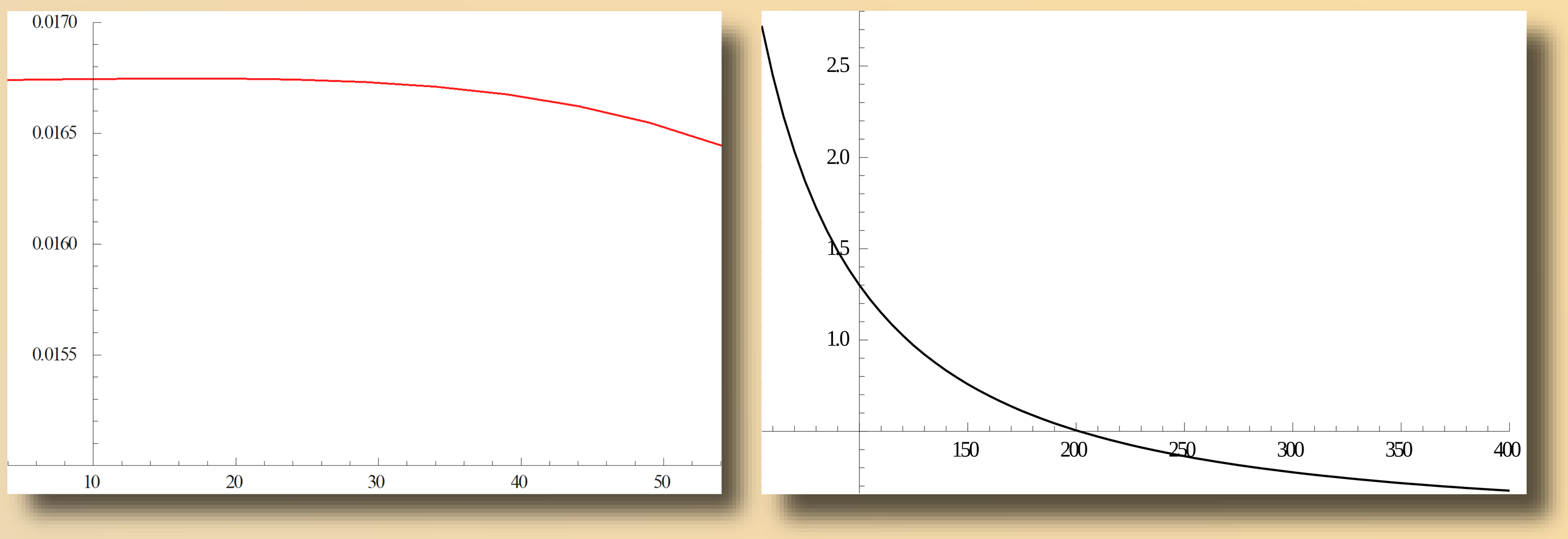

Figure 2. Temperature dependance of graphene electrical conductivity in case of relaxation on neutral impurities, for temperature ranges $T << T_{BG}$ (left) and $T > T_{BG}$ (right)

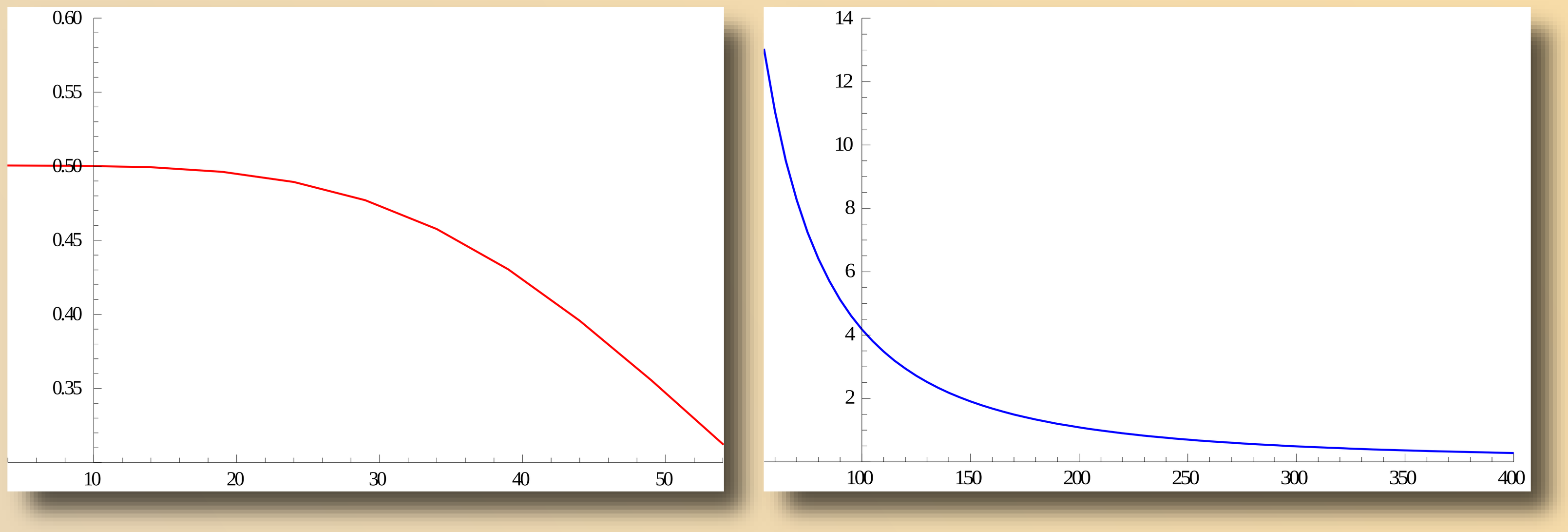

Figure 3. Temperature dependance of graphene electrical conductivity in case of relaxation on both charged impurities and phonons, for temperature ranges $T << T_{BG}$ (left) and $T > T_{BG}$ (right)

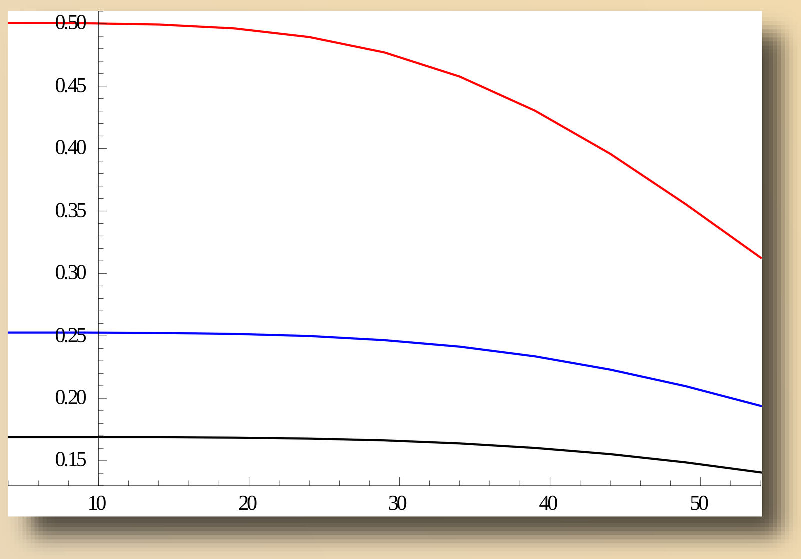

Figure 4. Low-temperature dependance of graphene electrical conductivity (for $T << T_{BG}$) in case of relaxation on both charged impurities and phonons, for several concentrations of impurities as parameters

CONCLUSION

It is obtained that graphene electrical conductivity decreases with temperature for all relaxation mechanisms. Numerical calculations and graphs are presented separately in low-temperature and high-temperature regions, due to different temperature dependences of chemical potentials and relaxation times in these regiouns.

For relaxation on neutral impurities, graphene electrical conductivity is almost temperature independent till 300 K (cf. Fig. 2), which is in excellent agreement with experimental data.

For relaxation on phonons, electrical conductivity is analyzed until T_{BG} temperature with degenerate phonons, and above T_{BG} temperature with non-degenerate phonons. It is found that low-temperature electrical conductivity is lower than the high-temperature one.

It is also obtained that graphene electrical conductivity decreases with increase of impurity concentration.