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Role of acoustic phonons in frequency dependent electronic thermal conductivity of graphene

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ABSTRACT

We study the effect of the electron–phonon interaction on the finite frequency dependent electronic thermal conductivity of two dimensional graphene. We calculate it for various acoustic phonons present in graphene and characterized by different dispersion relations using the memory function approach. It is found that the electronic thermal conductivity $\kappa_e(T)$ in the zero frequency limit follows different power law for the longitudinal/transverse and the flexural acoustic phonons. For the longitudinal/transverse phonons, $\kappa_e(T) \sim T^{-1}$ at the low temperature and saturates at the high temperature. These signatures qualitatively agree with the results calculated by solving the Boltzmann equation analytically and numerically. Similarly, for the flexural phonons, we find that $\kappa_e(T)$ shows $T^{1/2}$ law at the low temperature and then saturates at the high temperature. In the finite frequency regime, we observe that the real part of the electronic thermal conductivity, $\mathrm{Re}[\kappa_e(\omega, T)]$ follows ω^{-2} behavior at the low frequency and becomes frequency independent at the high frequency.

In recent times, Graphene [1–3] has attracted a lot of attention both in the fundamental and applied research due to its unique electronic and optical properties. These properties include anomalous high electrical conductivity, high thermal conductivity, quantum Hall effect, effect of impurities on the electric properties, etc. [4–17] which make the use of this material quite promising for the fabrication or design of the electronic devices. Among these properties, electrical conductivity, Hall effect have been discussed several times in literature, while there is lack of discussions in the electronic contribution to the thermal conductivity. Thus, in the present work, we focus on the electronic thermal conductivity of graphene.

In the literature, it is argued that the unusual high thermal conductivity of graphene [18,19] is mainly contributed by the phonons and the electronic contribution is small, hence neglected. However, in real systems, the total thermal conductivity is expressed as the sum of the electronic and the phononic thermal conductivity. In different temperature limits, these thermal conductivities show different temperature behavior. In the high temperature limit, due to larger number of phonons the electronic thermal conductivity shows temperature independent behavior [20–22] due to the scattering by electron–phonon interactions. On the other hand, the phononic thermal conductivity shows T^{-1} behavior due to the dominating scattering mechanism by phonon–phonon interactions. In the opposite limit i.e. the low temperature limit, the electronic and the phononic thermal conductivities are due to the interactions of electrons and phonons with impurities, boundaries, defects. These different scenarios of the electronic thermal conductivity in both low and high temperature limits make this study important.

In case of metals, it has been depicted that at the low temperature i.e. $T \ll \Theta_D$, Θ_D being the Debye temperature, only the acoustic phonons within the phonon sphere of radius k_{ph} with $k_{\mathrm{ph}} \ll k_D$, where k_D is the radius of Debye sphere, play a role in the electronic thermal conductivity [20–22]. In these three dimensional systems, it leads to T^{-2} behavior of the electronic thermal conductivity. In such systems, the radius of the Fermi sphere is larger than the radius of the Debye sphere i.e. $2k_F \gg k_D$. Thus all phonons can scatter off the electrons. But in the systems where $k_F \ll k_D$, only small number of phonons can scatter off the electrons. These phonons are restricted within the energy range $v_s k_{\mathrm{ph}} \leq 2v_s k_F$. This can be explained by introducing the new temperature scale known as Bloch Grüneisen (BG) temperature which is smaller than the Debye temperature [23]. This scale defines two regimes i.e. low temperature ($T \ll \Theta_{\mathrm{BG}}$) and high temperature ($T \gg \Theta_{\mathrm{BG}}$) regimes for the electron–phonon interaction in graphene. In the low temperature regime ($T \ll \Theta_{\mathrm{BG}}$), the acoustic phonons with linear dispersion relation yield inverse temperature behavior to the electronic thermal conductivity (i.e.

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$\kappa_e \sim T^{-1}$) and then change to the temperature independent behavior in the high temperature regime ($T \gg \Theta_{BG}$) [24,25]. However, because of the two dimensional nature of the graphene, there are also other acoustic phonons known as flexural phonons or out of plane phonons which obey quadratic dispersion relation and hence give different power law behavior to the electronic thermal conductivity. Thus the role of the different acoustic phonons is very important to understand the transport or the electronic thermal conductivity of graphene. However most of the studies have considered only the zero frequency limit. But for the generation of the integrated circuits, high frequency communication devices, the study of the electronic thermal conductivity in the dynamical regime is important as it may degrade the issue of the heat dissipation within the systems [26–29].

With this motivation, we have examined the electronic thermal conductivity both in the zero frequency and the finite frequency regime using the memory function approach [30–34]. The advantage of using memory function approach is that it directly deals with the dynamics of the transport [35]. Here we discuss the dynamical behavior of the electronic thermal conductivity due to the interactions of electrons with different acoustic phonons and also its difference with the behavior in normal metals. In the zero frequency limit, our findings for the electronic thermal conductivity of graphene agrees qualitatively with the results calculated by solving the Boltzmann equation analytically and numerically [40,24,25]. In the finite frequency regime, our findings may be important from both the fundamental and the application points of view and may inspire important experimental studies in future.

This paper is organized as follows. In Sec. 1, first we discuss the basic idea of the thermal conductivity and its relation with the memory function. Then the model Hamiltonian considering only the electron–phonon interactions in graphene is discussed. Later, we discuss the phonon dispersion relation of different acoustic phonons. With these descriptions, we calculate the finite frequency and temperature dependent electronic thermal conductivity for different acoustic phonons. In Sec. 2, the results are presented in the two subsections. In one subsection, we discuss the electronic thermal conductivity in the zero frequency limit. In other subsection, the results for the finite frequency in different BG regimes has been discussed. Finally, in Sec. 3, we conclude.

1. Theoretical framework

1.1. Thermal conductivity

The thermal conductivity is defined as the rate of flow of heat across a unit area of cross section in a unit temperature gradient [36]. Mathematically, this can be depicted from the following expression

$$J_Q = -\kappa \nabla T. \tag{1}$$

Here J_Q is the thermal current density and is defined as,

$$J_Q = \frac{1}{m}\sum_{\mathbf{k}} \mathbf{k}.\hat{n}(\epsilon_{\mathbf{k}} - \mu) c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}}, \tag{2}$$

where $c_{\mathbf{k}}$ ($c^{\dagger}_{\mathbf{k}}$) is the annihilation (creation) operator having momentum $\mathbf{k}$, $\epsilon_{\mathbf{k}}$ is the electron energy dispersion of graphene, μ is the chemical potential, m is the electron mass and $\hat{n}$ is the unit vector parallel to the direction of heat current. And in Eq. (1) ∇T is the temperature gradient and κ is the thermal conductivity. The latter is known as response due to the change in the temperature gradient and is generally analyzed by various approaches [20,21] where the gradient of the temperature is considered as static. But in the present work, we assume that ∇T is not static, while it oscillates with the external driving frequency ω. This oscillation leads to the dynamical variation of the thermal conductivity. Here we set $\hbar = 1$ and $k_B = 1$ in our calculations.

To compute it, we employ the memory function approach. Following the latter approach, the dynamical thermal conductivity at complex frequency z and temperature T is defined as [22]

$$\kappa(z,T) = \frac{i}{T}\frac{\chi^0_{Q\,Q}(T)}{z + M_{Q\,Q}(z,T)}, \tag{3}$$

where $\chi^0_{Q\,Q}(T)$ is the static thermal current–thermal current correlation function i.e. $\chi^0_{Q\,Q}(T) = \frac{\pi}{24}\frac{k_F^3}{m^2 v_F}T^2$, where k_F is the Fermi wave vector and v_F is the Fermi velocity, $M_{Q\,Q}(z,T)$ is the thermal memory function.

It is known that within the perturbation theory, the thermal memory function can be expressed to the leading order in the electron–phonon coupling, as [37,35,22]

$$M_{Q\,Q}(z,T) = \frac{\langle\langle [J_Q, H]; [J_Q, H]\rangle\rangle_{z=0} - \langle\langle [J_Q, H]; [J_Q, H]\rangle\rangle_z}{z\chi^0_{Q\,Q}(T)}. \tag{4}$$

This is the complex memory function in which the imaginary part of the memory function describes the thermal scattering rate and the real part describes the mass enhancement factor. In the present work, we focus on the thermal scattering rate which leads to the real part of the thermal conductivity. Here for simplicity, we have ignored the mass enhancement contribution to the thermal conductivity. To calculate it, we require the total Hamiltonian that is discussed in the next subsection.

1.2. Model Hamiltonian

We consider a two dimensional graphene with only electron–phonon interactions. The Hamiltonian of such a system is described as

$$H = H_0 + H_{ep} + H_{ph}, \tag{5}$$

where $H_0 = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$ and $H_{ph} = \sum_q \omega_q \left(b^{\dagger}_q b_q + \frac{1}{2}\right)$ corresponds to the Hamiltonians of the free electrons and phonons respectively. Here ω_q is the phonon energy dispersion, b_q ($b^{\dagger}_q$) is the phonon annihilation (creation) operator having phonon wave vector $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ and σ is the electron spin. H_{ep} describes the electron–phonon interactions and is given as $H_{ep} = \sum_{\mathbf{k}\mathbf{k}'\sigma}\left[D(\mathbf{k}-\mathbf{k}')c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma} b_{\mathbf{k}-\mathbf{k}'} + H.c.\right]$, where $D(q)$ is the electron–phonon matrix element. The latter is usually written in the following form [38,39]

$$D(\mathbf{q}) = \frac{D_0 q}{\sqrt{2\rho_m \omega_q}}\left(1 - \left(\frac{q}{2k_F}\right)^2\right)^{1/2}. \tag{6}$$

Here D_0 is the deformation potential coupling constant, ρ_m is the graphene mass density and ω_q is the phonon energy dispersion.

1.3. Phonon dispersions

Before proceeding to compute the thermal scattering rate and the corresponding electronic thermal conductivity for the sake of completeness, we will first discuss the phonon dispersion relations in this subsection.

The thermal transport due to the electron–phonon interactions significantly depends on the characteristics of the phonon which are further determined by the two dimensional structure of the graphene. In graphene, there are two carbon atoms per hexagonal

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