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# Dynamical thermal conductivity of bilayer graphene in the presence of bias voltage

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## HIGHLIGHTS

- Theoretical calculation of dynamical thermal conductivity of biased bilayer graphene.
- The investigation of the effects of chemical potential and temperature on the frequency dependence of thermal conductivity.
- The study of the effect of bias voltage on the thermal conductivity.

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## ABSTRACT

We study dynamical thermal conductivity of doped biased bilayer graphene for both AA and AB-stacking in the context of tight binding model Hamiltonian. The effects of bias voltage and chemical potential on the behavior of dynamical thermal conductivity are discussed for different stacking of bilayer graphene. Green's function approach has been implemented to find the behavior of thermal conductivity of bilayer graphene within linear response theory. We have found that thermal conductivity decreases with chemical potential for different values of temperature and frequency. Also thermal conductivity of AB stacked bilayer graphene versus bias voltage includes a peak for each value of chemical potential. Furthermore we study the frequency dependence of thermal conductivity of AA stacked bilayer graphene for different values of temperature and bias voltage.



## 1. Introduction

Initially studies of graphene were limited to realm of theory where the low energy linear dispersion and chiral nature of the honeycomb carbon lattice were shown to result from a simple nearest neighbor hopping tight binding Hamiltonian which at low energy maps on to a Dirac Hamiltonian for massless fermions with Fermi velocity $v_F$ [1].

Bilayer graphene has attracted experimental and theoretical interest, both for fundamental physics and for possible technological applications [2,3]. This system is composed of two layers, each of which has carbon atoms arranged in a honeycomb lattice with two sublattices.

In contrast to the case of single-layer graphene (SLG) low energy excitations of the bilayer graphene have parabolic spectrum, although, the chiral form of the effective 2-band Hamiltonian persists because the sublattice pseudospin is still a relevant degree of freedom. The pristine or undoped bilayer graphene has attracted a lot of interest since the presence of a single Fermi point and quadratic dispersion can lead to a host of exotic phenomena [4,5]. The low energy properties of the doped bilayer graphene also show interesting feature like enhanced backscattering due to the chirality of the bands present in the system [6].

The low energy approximation in bilayer graphene is valid only for small doping $n < 10^{12}\,\mathrm{cm}^{-2}$, while experimentally doping can obtain 10 times larger densities. For such a large doping, the 4-band model [7] should be used instead of the low energy effective 2-band model. Bilayer is of intense interest as it too shows an unusual quantum Hall effect [7,8] and indeed its low energy tight binding Hamiltonian maps to an equation for chiral fermions with an effective mass based on an interlayer hopping parameter $\gamma$. Electronic gaps in bilayer graphene can be controlled and thus this material is extremely flexible. This can be accomplished in with an electric field applied perpendicular to the plane. It was shown theoretically [7,9] and demonstrated experimentally [10,11] that a graphene bilayer is the only material with semiconducting properties that can be controlled by electric field effect [12]. The size of the gap between conduction and valence bands is

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proportional to the voltage drop between the two graphene planes and can be as large as 0.1–0.3 e, allowing for novel terahertz devices [11] and carbon based quantum dots [13] and transistors [14].

Disorder generates a scattering rate and hence a characteristic energy scale which is the order of fermi energy. Therefore, one expects disorder to have a strong effect in the physical properties of graphene. Indeed, theoretical studies of the effect of disorder in unbiased [15] and biased [16] graphene bilayer show that disorder leads to strong modifications of its transport and spectroscopic properties. Static transport in few-layer graphene has been studied for both without and in the presence of a magnetic field. It is established that charged impurity scattering is primarily responsible for the transport behavior observed in monolayer graphene [17,18]. A comprehensive study of the electronic properties of the graphene in the presence of defects as a function of temperature, external frequency, gate voltage, and magnetic field has been presented by Peres and coworkers [19]. Thermopower of clean and impure biased bilayer graphene has been calculated for Bernal A–B stacking within Born approximation [20]. This work shows band gap through the application of an external electric field leads to greatly enhance the thermopower of bilayer graphene, which is more than four times that of the monolayer graphene and gapless bilayer graphene at room temperature.

In this paper, we study the effects of electron doping and bias voltage on the frequency behavior of thermal conductivity of both AA and AB stacked graphene bilayer within full band tight binding approximation. Full band calculation beyond Dirac approximation has been implemented to derive in-plane dynamical thermal conductivity spectra. We have exploited Green's function approach to calculate the thermal conductivity, i.e. the time ordered heat current correlation. The effects of electron doping on the dynamical thermal conductivity have been studied via changing the electronic chemical potential. Also we discuss and analyze to show how bias voltage value affects the frequency behavior of the dynamical thermal conductivity. Also we study the behavior of dynamical thermal conductivity of both bernal and simple types of bilayer graphene versus chemical potential and bias voltage for fixed frequency. Finally the comparison between the results of bernal and simple stacking is performed in detail.

## 2. Model and method

To calculate the dynamical thermal conductivity of bilayer graphene we consider bilayer graphene composed of two graphene single layers arranged in both cases of the simple (AA) and Bernal (AB) stacking [14]. In order to derive the dynamical properties of AA-stacked bilayer graphene we must first examine the band structure and provide and expression for the electronic Green's function. We start from a tight binding model incorporating nearest neighboring intralayer and interlayer hopping terms. An on-site potential energy difference between the two layers is included to model the effect of an external voltage. For the case of AA-stacking, an A (B) atom in the upper layer is stacked directly above A(B) atom in the lower layer. Under the nearest neighbor approximation, the single spin tight binding model Hamiltonian for AA-stacked bilayer grapehene ($H_{AA}$) and AB one ($H_{AB}$) is given by

$$\begin{aligned} H_{AA} = & -t_{\parallel}\sum_{i,l,\delta}(b^{\dagger}_{l,i+\delta}a_{l,i}+h.c.)-t_{\perp}\sum_{i}a^{\dagger}_{1,i}a_{2,i}+h.c. \\ & -t_{\perp}\sum_{i}b^{\dagger}_{1,i}b_{2,i}+h.c.+\frac{V}{2}\sum_{i}(a^{\dagger}_{1,i}a_{1,i}+b^{\dagger}_{1,i}b_{1,i}) \\ & -\frac{V}{2}\sum_{i}(a^{\dagger}_{2,i}a_{2,i}+b^{\dagger}_{2,i}b_{2,i}), \\ H_{AB} = & -t_{\parallel}\sum_{i,l,\delta}(b^{\dagger}_{l,i+\delta}a_{l,i}+h.c.)+t_{\perp}\sum_{i}a^{\dagger}_{1,i}b_{2,i}+h.c. \\ & +\frac{V}{2}\sum_{i}(a^{\dagger}_{1,i}a_{1,i}+b^{\dagger}_{1,i}b_{1,i})-\frac{V}{2}\sum_{i}(a^{\dagger}_{2,i}a_{2,i}+b^{\dagger}_{2,i}b_{2,i}). \end{aligned} \tag{1}$$

The first two terms of each above model Hamiltonian are the nearest neighbor intralayer hopping terms for electrons to move within a given plane with a hopping energy $t \approx 3$ eV. The two planes are indexed 1 and 2. According to the crystal structure of the honeycomb lattice, each layer has two inequivalent atoms labelled A and B. This lattice structure has been shown in Fig. 1. The unit cell vectors of bilayer graphene are similar to those of single layer one. Therefore one presents the unit cell vectors of bilayer graphene on the honeycomb lattice structure. According to Fig. 1 the unit cell vectors are given by

$$\mathbf{a}_1 = a\mathbf{i}, \quad \mathbf{a}_2 = \frac{a}{2}\Big(-\mathbf{i}+\sqrt{3}\mathbf{j}\Big), \tag{2}$$

where $\mathbf{i}$ and $\mathbf{j}$ are unit vectors along $x$ and $y$ directions, respectively. In Eq. (1), $a_{l,i}$ denotes the annihilates operator for an electron which is on an A-atom site with site label $i$ in the graphene layer indexed by $l$. Also $b^{\dagger}_{l,i+\delta}$ creates an electron in sheet $i$ on the neighboring site at the position $i+\delta$, where $\delta$ is one of the three possible nearest-neighbor vectors given by $\mathbf{a}_{01}$, $\mathbf{a}_{02}$ and $\mathbf{a}_{03}$ which are presented in Fig. 1. Furthermore the primitive vectors of the triangular sublattice have property $|\mathbf{a}_1| = |\mathbf{a}_2| = \sqrt{3}a_{cc}$ with $a_{cc}$ being the nearest carbon–carbon distance. The third term in Eq. (1) corresponds to the interlayer hopping between graphene sheets. The hopping parameter between an A (B) site in one layer and the nearest A(B) site in the other layer is given by $t_{\perp}$. In the simple AA stacked type, we have $t_{\perp} \approx 0.2$ eV [21,22]. $V$ is the potential energy difference between the first and second layers induced by a bias voltage. Since for every attainable carrier density, it is possible to find a bias voltage to make the potential difference between the two layers as $V$. In terms of Fourier transformation of operators, one can rewrite the clean tight binding part of the Hamiltonian in Eq. (1) as

$$H_{AA(AB)} = \sum_{\mathbf{k}}\phi^{\dagger}_{\mathbf{k}}H_{0AA(0AB)}(\mathbf{k})\phi_{\mathbf{k}}, \tag{3}$$

in which the vector of fermion creation operators is defined as $\phi^{\dagger}_{\mathbf{k}} = (a^{\dagger}_{1,\mathbf{k}}, b^{\dagger}_{2,\mathbf{k}}, a^{\dagger}_{2,\mathbf{k}}, b^{\dagger}_{1,\mathbf{k}})$. $a^{\dagger}_{l,\mathbf{k}}$ and $b^{\dagger}_{l,\mathbf{k}}$ are the Fourier transformation of $a^{\dagger}_{l,i}$ and $b^{\dagger}_{l,i}$, respectively, that are expressed as

$$\begin{aligned} a^{\dagger}_{l,\mathbf{k}} &= \frac{1}{\sqrt{N}}\sum_{i}e^{-i\mathbf{k}\cdot\mathbf{R}_i}a^{\dagger}_{l,i}, \\ b^{\dagger}_{l,\mathbf{k}} &= \frac{1}{\sqrt{N}}\sum_{i}e^{-i\mathbf{k}\cdot\mathbf{R}_i}b^{\dagger}_{l,i}, \end{aligned} \tag{4}$$

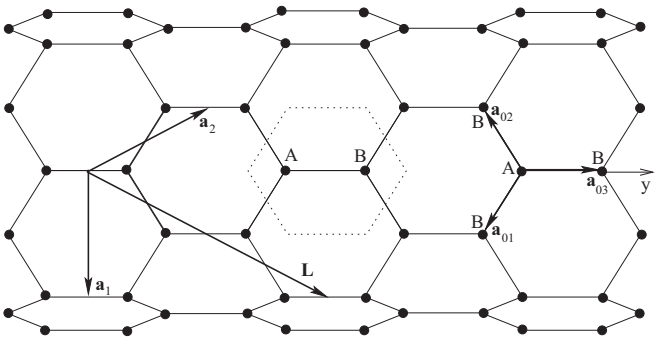


**Fig. 1.** The structure of honeycomb structure is shown. The light dashed lines denote the Bravais lattice unit cell. Each cell includes two nonequivalent sites, which are indicated by A and B. $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive vectors of unit cell. $\mathbf{a}_{01}$, $\mathbf{a}_{02}$ and $\mathbf{a}_{03}$ are three vectors that connect nearest neighbor sites.