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Dynamical Optical Conductivity of Doped Monolayer Gapped Graphene: Green's Function Approach

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Abstract

We investigated the optical conductivity of monolayer gapped graphene in the presence of electron injection and bias voltage in the context of tight-binding model as a function of frequency. The effect of the dispersion caused by electron injection was also investigated by the use of Green's function approach. The dependence of dynamical optical conductivity on frequency has been investigated in different temperatures and it has been demonstrated that the conversion of temperature doesn't affect this conductance. We have also considered, by applying the bias voltage, the dependence of dynamical optical conductivity on this voltage, in different charge amounts caused by electron injection in constant temperature and frequency. As a result, in the values of $V=t_{||}$ *this conductivity is zero due to the tendency of the system to be insulated. Applying the gap in the system changes the dependence of conductivity on the amount of electron injection merely according to the measure of the gap.*

Keywords: Optical conductivity, Electron injection, Monolayer gapped graphene, Green's function

INTRODUCTION

Graphene as a one-atom-thick layer of graphite, attracts a lot of attention of both theoreticians and experimentalists since it's fabrication [1]. 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 the nearest neighbor hopping tight binding Hamiltonian which at low energy maps on to a Dirac Hamiltonian for massless fermions with Fermi velocity v_F . In electronic industry and semiconductors, remarkable development in nano technology, is attendant with challenges like control of conductivity due to operation of these tools. Combinations of carbon, as monolayer graphene, it can fulfil essential features for industrial applications and since the dynamical optical conductivity of monolayer graphene depends on it's isotopic structure, in this work, we has been investigated the changes of dynamical optical conductivity of the monolayer graphene with electron injection and applying the bias voltage on this material. The optical properties of graphene are of considerable importance for technological applications, all variants of graphene are also of potential interest and should be examined. The dynamical conductivity of graphene has been extensively studied theoretically [2] and experiments have largely verified the expected behavior [3].

THEORETICAL METHOD

Based on the monolayer graphene specific band structure, we can obtain dynamical optical conductivity of it with Green's function approach [4]. According to the honeycomb lattice structure shown in Fig. 1, by using of the tight-binding model, Hamiltonian is given by:

$$H = -t_{\parallel} \sum_{i,l,\delta} (a_{i+\delta}^{\dagger} b_i + h.c.) \tag{1}$$

where $t_{||}$ is the amplitude of in-plane hopping. $a_i^{\dagger}$ (a_i) creates (destroys) one electron in site i and δ is one of the three vectors (a_{01}, a_{02}, a_{03}) shown in Fig. 1. V is the external potential energy difference caused by applying bias voltage and Δ is the gap.

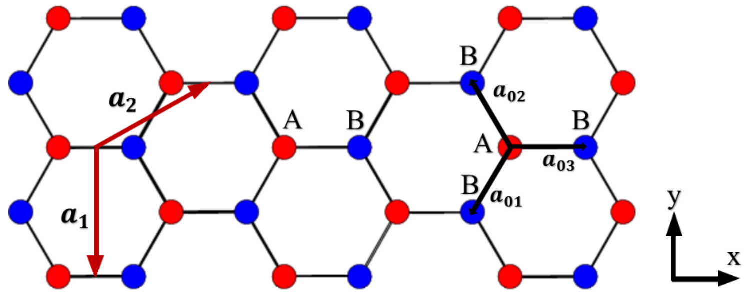

Figure 1: (Color online) Lattice structure of monolayer graphene

With using Fourier conversion and supposing the fermionic creation vector as $\phi^\dagger_k = (a^\dagger_k , b^\dagger_k)$,the matrix shape of Hamiltonian Fourier conversion is as below:

$$H_0(k) = \begin{pmatrix} V-\mu+\Delta & f(\mathbf{k}) \\ f^*(\mathbf{k}) & V-\mu-\Delta \end{pmatrix} \qquad (2)$$

where $f(\mathbf{k}) = -t_{||}\Sigma\exp(i\mathbf{k}.\mathbf{a}_i)$. By using of the Matsubara representation, without impurity injection, Green's function can be obtain as:

$$G_0(k,i\omega_n) = \frac{1}{(i\omega_n+\mu)I - H_0(k)} \qquad (3)$$

where $\omega_n = (2n + 1)\pi/\beta$ is the fermionic Matsubara frequency. By meaning of the simple analysis and regarding $i\omega_n \rightarrow \omega + io+$, the optical conductivity of monolayer graphene in the presence of bias voltage and electron injection in the context of tight-binding model, could be obtained as a function of frequency in different temperatures.

Dynamical optical conductivity is obtained as the response of electrical current to different frequencies. Using the low of conservation of charge, we have the relation of electrical current density as below:

$$J_e = \frac{dP}{dt} = i[H,P] \quad (4)$$

where P is the polarization operator. Transport matrix coefficients are as below:

$$L_{ab}(\omega) = \frac{1}{\beta\omega} \lim_{i\omega_n \to \to \omega + io^+} \int_0^\infty d\tau e^{i\omega_n \tau} \langle T_\tau (J_x^a(\tau) J_x^b(0)) \rangle \quad (5)$$

where $(a, b) = (1, 2)$, $\beta = 1/k_B T$ and the bosonic Matsubara frequency is $\omega_n = 2n\pi/\beta$. By the use of Lehmann theorem and summation of Matsubara frequencies, we can calculate the transport matrix coefficients and obtain the dynamical optical conductivity from the relation below [5]:

$$\sigma = k_B \beta \sigma_0 L_{11} \quad (6)$$

RESULTS AND CONCLUSIONS

Here we present results for the longitudinal conductivity which is evaluating Eq. (6) numerically. Also the calculation is performed within full Brillouin zone beyond Dirac cone approximation. We have obtained the electronic spectrum of the disordered tight binding model by means of Green's function approach which gives the optical conductivity by calculating the energy current correlation function. In the obtaining the following numerical results, the intralayer nearest neighbor hopping parameter ($t_{||}$) is set to 1. As it's shown in Fig. 2, the results obtained for the dynamical optical conductivity in terms of the frequency are the same in all temperatures. As a result of increase in electron injection, from the amount of $\mu > 0.8\, t_{||}$, the conductivity is reduced and that is becouse of the increase in despersion caused by electron injection.

It's seen in Fig. 3 that the dynamical optical conductivity of this system is zero for different amounts of bias voltage in constant frequency and temperature for $V > t_{||}$ and $\mu > 1.2\, t_{||}$ that the dispersion caused by electron injection and the system's tendency to be insulated are the reasons respectively.

The effect of electron injection on the dynamical optical conductivity in different frequencies and in the consant bias voltage and temperature is shown in Fig. 4 and as it's seen, for $\mu \gg t_{||}$, similar to Fig. 3, the conductivity tends to a constant amount and in $\mu = t_{||}$ reaches its maximum value.

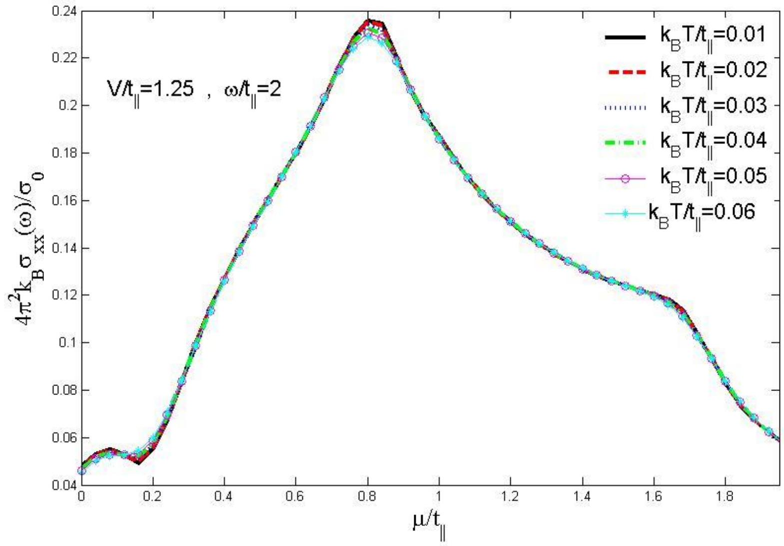

Figure 2: (Color online) The dependence of dynamical optical conductivity of doped monolayer gapped graphene in V/t|| = 1.25 and ω/t|| = 2 for different temperatures.

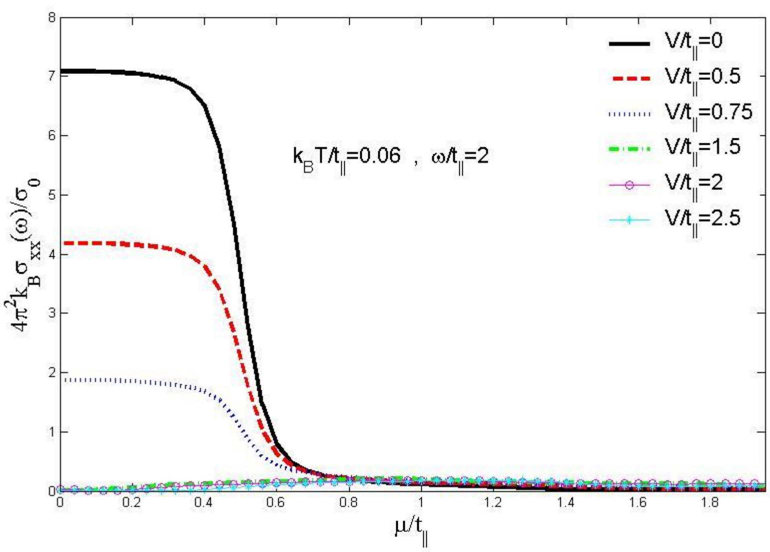

Figure 3: (Color online) The dependence of dynamical optical conductivity of doped monolayer gapped graphene in *kBT/t*|| = 0.06 and *ω/t*|| = 2 for different bias potentials.

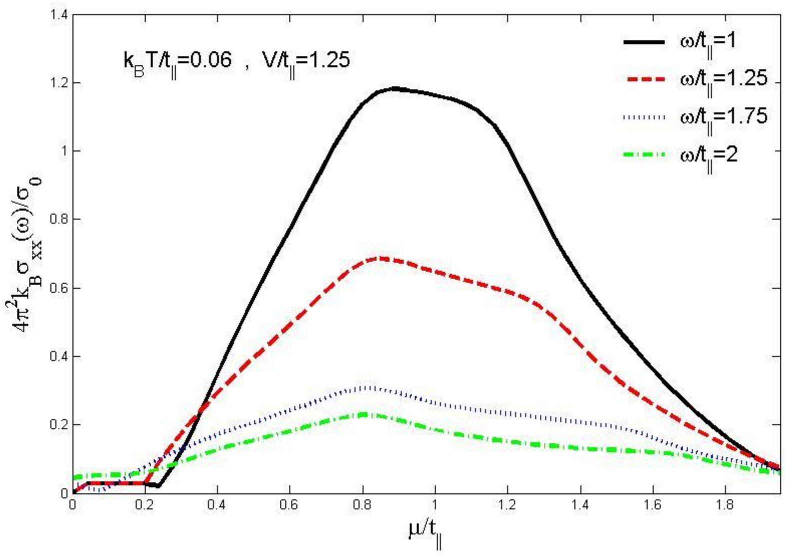

Figure 4: (Color online) The dependence of dynamical optical conductivity of doped monolayer gapped graphene in $k_BT/t_{||} = 0.06$ and $V/t_{||} = 1.25$ for different frequencies.

REFERENCES

[1] K. S. Novoselov, A. K. Geim, S. V. Morosov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva and A. A. Firsov, Science 306, 666 (2004).

[2] T. Ando, Y. Zhang, and H. Suzuura, J. Phys. Soc. Jpn 71, 1318 (2002).

[3] R. R. Nair, B. Blake, A. N. Grigeronke, K. S. Novoselov, T. J. Booth, T. Stauber, N. M. R. Peres, and A. K. Geim Science 320, 1308 (2008).

[4] J. Nilsson, A. H. Castro Neto, F. Guinea, and N. M. R. Peres, Phys. Rev. B, 76, 165416 (2007).

[5] G. D. Mahan, many Particle Physics, Plenumn Press, New York, 1993.