A Numerical Study of the Electronic Properties of Graphene Bilayer with Local Disorder

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Abstract. We study the effect of disorder in the normal and superconducting phases of the bilayer graphene. We choose the Bernal stacking configuration to characterize the graphene bilayer, and introduce the kernel polynomial method to provide numerical results for the evolution of optical conductivity with the increase of disorder. The Drude weight is found to decrease very rapidly with the enhancement of disorder and drop to zero at a critical strength $W_c$, suggesting that Anderson metal-insulator transition can take place.

In the superconducting phase, the distribution of the inhomogeneous superconducting gap is obtained by solving self-consistently the Bogoliubov-de Gennes equations under the mean-field description, and the significant suppression of the Drude weight is obtained in the weak disorder region.

1. Introduction

The bilayer graphene (BLG) is an unique semiconductor, the bandgap of which can be gate-controlled [1, 2]. Modifying the electric field applied perpendicularly to the graphene surface, the potential difference between the two A-B Bernal stacking layers is controlled, thereby generating a tunable gap in the band structure. Since the local impurities are very likely to be introduced during the fabrication procedure, it is crucial to study the effect of disorder on the electronic properties of BLG. Very recently the transport properties of BLG affected by the short-range potentials [3], the long-range disorder [4], and the adatom residing at the center of a hexagonal plaquette [5] have been studied theoretically by applying the mean-field descriptions.

The disagreement of whether there exits metal-insulator transition in perfect two-dimensional (2D) graphene compound is still an open question [6, 7]. Although the exact diagonalization method can give precise wave functions of a finite system, the limitation of lattice size still makes it very hard to distinguish the extended states with the localized states providing with very large localization lengths. The kernel polynomial method (KPM) is regarded recently as a distinct method for the disordered systems since it allows for the numerical calculations for dimensions of the order of $D \approx 10^9$ [8].

In this paper, we employ KPM to study the disorder effects on the density of states (DOS) and optical conductivity in the normal and superconducting phases. We find that the Drude weight of optical conductivity decreases very rapidly with the increase of disorder strength, suggesting the existence of Anderson metal-insulator transition (MIT) in BLG. In addition, we check our finding by the lattice size scaling of generalized inverse participation ratio (GIPR) [9], and good agreement has been achieved.

2. The kernel Polynomial method for BLG in the superconducting phase

We study an effective tight-binding model of a double-layer hexagonal lattice with Bernal-staking configuration [1]. Considering the effect of localized disorder in the superconducting phase [10], the
Hamiltonian can be expressed as:

\[ H = -t \sum_{\langle ij \rangle \sigma} c_{i \sigma}^\dagger c_{j \sigma} - t_\perp \sum_{\langle i, i' \rangle \sigma} \{ c_{i \sigma}^\dagger c_{i' \sigma} + c_{i' \sigma}^\dagger c_{i \sigma} \sigma + H.c. \} + \sum_{i s} \epsilon_i c_{i s}^\dagger c_{i s} - \sum_{\langle ij \rangle s} [\Delta_{ij}^{(s)} c_{i s}^\dagger c_{j \sigma} + H.c.], \]

where \( c_{i \sigma} \) (\( c_{i \sigma}^\dagger \)) are the electronic annihilation (creation) operators at sites \( i \) of layer \( s \) (1 or 2) with spin \( \sigma \) (↑ or ↓), \( t \) denote the intralayer hopping integrals between nearest neighbor (NN) sites \( i \) and \( j \) of the same layer, \( t_\perp \) present the perpendicular interorbital hopping parameters between carbon atom \( A_1 \) of layer 1 and \( B_2 \) of layers 2 [1], \( \epsilon_i \) represent the on-site disorder energies, and \( \Delta_{ij}^{(s)} = -V(c_{j \sigma} c_{i \sigma}) \) are the superconducting gap of layer \( s \) under the NN attractive interactions \( V \).

We introduce the kernel polynomial method (KPM) [8] to expend the single particle Green’s function into a series of Chebyshev polynomials of order \( M \), and the NN superconducting gap \( \Delta_{ij}^{(s)} \) can be obtained by [8, 11],

\[ \Delta_{ij}^{(s)} = -V \int_{-E_c}^{E_c} \text{Im} \, G_{ij}^{(s)}(\omega)(1 - 2f(\omega))d\omega, \]

where \( f(\omega) \) represents the Fermi-Dirac distribution function. We obtain the imaginary part of Green’s function as: \( \text{Im} \, G_{ij}^{(s)}(\omega) = -\frac{2}{\pi \omega} \sum_{n=M} \mu_n^{(s)}(i, j)g_n T_n(\bar{\omega}) \), where \( \bar{\omega} \) represent the scaled energies within the interval \([-1, 1]\), \( T_n(\bar{H}) = \cos[n \arccos(\bar{H})] \) denote the Chebyshev polynomials of the first kind, \( \mu_n^{(s)}(i, j) = \langle 0 | c_{i s}^\dagger T_n(\bar{H}) c_{j \sigma}^\dagger | 0 \rangle \) represent the coefficients of the expansion, and \( g_n = \sinh[\lambda(1 - n/M)]/\sinh(\lambda) \) is the Lorentz kernel, which is introduced to overcome the Gibbs oscillation. Then the optical conductivity at finite temperature can be calculated directly by [12],

\[ \sigma(\omega) = \sum_{k q} \frac{|\langle k | J | q \rangle|^2}{2Z_\omega} \frac{[f(E_k) - f(E_q)]}{\delta(\omega - (E_k - E_q))} = \frac{1}{\omega} \int_{-\infty}^{\infty} j(x, x + \omega)[f(x) - f(x + \omega)]dx \]

with \( j(x, y) = \frac{1}{\lambda} \sum_{k q} |\langle k | J | q \rangle|^2 \delta(x - E_k) \delta(y - E_q) \).

3. Results
We define the on-site disorder energies \( \epsilon_i \) as random variables distributed uniformly between \(-W/2\) and \( W/2\), and set \( t = 1.0 \) and \( t_\perp/t = 0.15 \). Since the intraorbital hoppings \( t \) of graphene have been found experimentally as 3.1eV, the interorbital hoppings are approximated as \( t_\perp \approx 0.47\text{eV} \) in our study. We
findings in figure 1. In the normal state, the effects of disorder on DOS in the normal and superconducting phases, and show our compare firstly the effects of disorder on DOS in the normal and superconducting phases, and compare the results to scale the GIPR [9], graphene. To measure the Anderson localization of electronic states in BLG, we introduce a polynomial series [6]. For the BLG, the localization effect of disorder is assumed to be weaker than that in the single layer graphene, where the DOS close to the Dirac points is enhanced significantly by disorder. While, the superconducting phase can introduce an energy gap in DOS around the Dirac energy region, which can survive the relatively weak disorder as shown in figure 1(c).

The existence of extended states in single layer graphene has been predicted by the numerical study [6]. For the BLG, the localization effect of disorder is assumed to be weaker than that in the single layer graphene. To measure the Anderson localization of electronic states in BLG, we introduce a polynomial series [6] to scale the GIPR [9], $G_2(\omega) = \frac{\sum_i \rho(r_i, \omega)^2}{(\sum_i \rho(r_i, \omega))^2}$, where the local DOS ($\rho(r_i, \omega)$) can be obtained directly in KPM. Considering the hopping integrals between the two layers, there appears a transition from a weakly localized state to a delocalized state as shown in figure 2(a).

Figure 2 presents the evolution of the matrix element density $j(x, y)$ of BLG with the enhancement of the disorder strength $W$ in the normal phase. It is obvious to find from equation (3) that the main contribution to the low-energy optical conductivity comes from the density of $j(x, y)$ concentrated near the straight line $x = y$. Different from the single layer graphene, two pairs of neighboring two peaks with central symmetry are found inside the straight line $x = -y$ as shown in figure 3(a). With the increase of $W$, we find that the density of $j(x, y)$ spreads in the entire energy plane, but the density around line $x = y$ reduces gradually, suggesting the appearance of the Anderson localization.

![Figure 2](image2.png)

**Figure 2.** The lattice size scaling of the generalized inverse participation ratio for an electronic state with energy $\omega = 1.0$ for single layer and double layer graphene. The disorder strength are set as: (a) $W = 2.0$ and (b) $W = 8.0$.

compare firstly the effects of disorder on DOS in the normal and superconducting phases, and show our findings in figure 1. In the normal state, the effect of disorder on DOS of BLG is quite similar to that in the single layer graphene, where the DOS close to the Dirac points is enhanced significantly by disorder. While, the superconducting phase can introduce an energy gap in DOS around the Dirac energy region, which can survive the relatively weak disorder as shown in figure 1(c).

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Figure 3 presents the evolution of the matrix element density $j(x, y)$ of BLG with the enhancement of the disorder strength $W$ in the normal phase. It is obvious to find from equation (3) that the main contribution to the low-energy optical conductivity comes from the density of $j(x, y)$ concentrated near the straight line $x = y$. Different from the single layer graphene, two pairs of neighboring two peaks with central symmetry are found inside the straight line $x = -y$ as shown in figure 3(a). With the increase of $W$, we find that the density of $j(x, y)$ spreads in the entire energy plane, but the density around line $x = y$ reduces gradually, suggesting the appearance of the Anderson localization.

![Figure 3](image3.png)

**Figure 3.** The matrix element density $j(x, y)$ for the bilayer graphene in the normal phase with disorder strength: (a) $W=0$, (b) $W=2.0$, and (c) $W=8.0$. The other parameters are $M = 2000$, $\lambda = 5.0$, $N = 200 \times 200$, and $R = 200$. 

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As shown in figure 4(a), the two peaks in the optical conductivity of perfect BLG (solid line) near energy $\omega = 2.0$ correspond to the appearance of the two pairs of neighboring two peaks in $j(x, y)$ along the line $x = -y$ shown in figure 3(a). The Drude weight decreases rapidly with the increase of disorder in the normal phase, suggesting that there exists the Anderson MIT in disordered BLG. In figure 4(b), we present the disorder effect on the optical conductivity in superconducting phase. In the weak disorder case, the Drude weight is found to be zero since the superconduction gap survive disorder. On the other hand, strong disorder can suppress the superconducting gap and make the electronic states to be localized, as a result the Drude weight maintains its zero value in the strong disorder region.

In summary, we use the kernel polynomial method to study numerically the effect of disorder in bilayer graphene, and the existence of Anderson metal-insulator transition is predicted by examining the evolution of optical conductivity with the increase of disorder. The scaling of the generalized inverse participation ratio also provides evidence for the electron delocalization in bilayer graphene. Comparing with the single layer graphene, delocalized electronic states are more likely to be found in bilayer graphene with interlayer coherence.

Acknowledgments

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