Anderson transition in disordered bilayer graphene

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Abstract
Employing the kernel polynomial method (KPM), we study the electronic properties of the graphene bilayers with Bernal stacking in the presence of diagonal disorder, within the tight-binding approximation and nearest neighbor interactions. The KPM method enables us to calculate local density of states (LDOS) without the need to exactly diagonalize the Hamiltonian. We use the geometrical averaging of the LDOS at different lattice sites as a criterion to distinguish the localized states from extended ones. We find that this model undergoes an Anderson metal–insulator transition at a critical value of disorder strength.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
Graphene (the 2D allotrope of carbon with honeycomb structure) has attracted tremendous interest since its isolation by Novoselov et al [1]. Some of the features that make graphene distinct from previously known materials are properties such as, the possibility to control the charge carrier types from holes to electrons in the same sample by a gate voltage, high mobility of charge carriers (about two orders of magnitude larger than the best silicon-based semiconductors), the anomalous integer quantum Hall effect (IQHE) at room temperature [2, 3]. Among them, the high mobility of carriers which is due to the vanishing of back-scattering, makes graphene favorable in the fabrication of carbon-based electronic devices.

The spectral and transport properties of graphene are well described within the tight-binding approximation. In this model the two upper energy bands, which are due to the π and π* bonds of p z orbitals normal to the honeycomb lattice plane, touch each other with a linear dispersion at the corners of the Brillouin zone (the so called K-points) [4]. In this picture, graphene is a semi-metal whose low energy excitations are massless fermions propagating with a Fermi velocity (vF) of about 1/300 times the speed of light. These excitations are called Dirac fermions, which along with the strong stability of graphene structure (which is related to the in-plane σ bonds), are responsible for the odd properties of graphene [2].

Empowering graphene in electronic devices requires opening a gap in its electronic spectrum. This can be done by confining its geometry either to graphene nano-ribbons or quantum-dots. However, these methods affect the electronic transport because of the formation of rough edges and also enhancement of the Coulomb blockade effects in the small size structures [5]. Moreover, reducing the size tends to decrease the possible conduction channels. Nevertheless, it has been shown that by applying an electric field normal to a graphene bilayer a gap can be opened whose magnitude is proportional to the intensity of the applied electric field [6, 7]. The size of the gap can be as large as 0.1–0.3 eV, thereby making bilayer graphene an attractive candidate in carbon-based transistors [8].

The graphene bilayer consists of two layers of carbon atoms in a honeycomb structure placed on top of each other, making the Bernal stacking [9]. In this stacking the upper layer is rotated 60° relative to the lower one, in such a way that the atoms in one sublattice, i.e. A1 and A2, are on top of each other while the atoms of the B-sublattice in the upper layer are placed on top of the hollow center of hexagons of the lower layer. In the absence of an external perpendicular electric field the band structure of the graphene bilayer consists of four bands, arising from the π-bonding between p z orbitals. Two of these bands touch each other at zero energy with a quadratic dispersion, and so give rise to the massive quasi-particles also called chiral fermions [6]. The other two bands are separated by an energy scale corresponding to the inter-plane hopping energy, t L; one lying below the zero energy and the other above it. The electronic structures of bilayer as
well as multilayer graphene have been extensively investigated recently [6, 8, 10–14].

Single and bilayer graphene samples are not free from defects and there are inevitable sources of disorder which may affect the electronic transport in the fabricated samples. Typical forms of disorder include surface ripples, topological defects, vacancies, ad-atoms, charge impurities and the polarization field of the substrate. Scaling theory of localization predicts that all the electronic states are localized in two-dimensional systems once the smallest amount of disorder is introduced [15]. According to this theory, the single and bilayer of graphene are expected to be insulators at zero temperature. However, theoretical as well as experimental studies show that both single and bilayer graphene have a minimum conductivity of the order of the conductance quantum \((e^2/h)\) at the charge neutrality point [16]. It is also shown that the minimum conductivity is at least twice as large in bilayer graphene [14, 17]. The effect of site dilution on the electronic properties of bilayer graphene was extensively studied by Nilsson et al [9], using the coherent potential approximation (CPA). Within this approximation they computed spectral functions, density of states, and self energies as well as the temperature dependence of dc conductivity, and found a minimal dc conductivity \(\frac{e^2}{h}\), independent of impurity concentration. Nevertheless, being a perturbative method, CPA cannot capture the localization properties of electronic states. For bilayer graphene nano-ribbons (BGNs), it has been shown that introducing a small amount of edge disorder by random removal of carbon atoms from the edges, induces an energy gap in the vicinity of the charge neutrality point, hence strongly suppressing the conductivity [18]. The localization properties of electronic states in bilayer graphene has been previously investigated by the transfer matrix method [19]. In this reference it is claimed that all states are localized in the presence of the smallest amount of any kind of disorder (random on-site energy, random intra-layer hopping or random inter-layer hopping). These results are not consistent with the observed minimal conductivity in dc conductivity measurements. This motivates us to investigate the localization properties of disordered bilayer graphene with an alternative method.

In our previous work, we investigated single-layer graphene in the presence of on-site disorder by using the numerically powerful approach of KPM [20]. There, we found that the disordered graphene mono-layer shows an Anderson transition at a critical value of disorder intensity which is of the order of the bandwidth. This metal–insulator transition, driven by short range diagonal disorder due to neutral impurities, was experimentally verified in hydrogen doped graphene by an angular resolved photoemission experiment [21].

In this paper we investigate the localization properties of the electronic states in bilayer graphene in the presence of diagonal disorder. We consider minimal coupling between the two layers of graphene, that is, we take into account only the hopping between \(A_1\) and \(A_2\) sublattices. Here we use the kernel polynomial method (KPM) [22], which consists in the expansion of various spectral functions in terms of a complete set of polynomials. We calculate a different local density of states (LDOS), from which we introduce a quantity for distinguishing the localized states from extended ones. The CPU time in this method grows as the square of the system size, which enables us to study large lattice sizes in a moderate time.

2. Model Hamiltonian

As was mentioned before, we use a minimal tight-binding model for describing the low energy transport properties of the graphene bilayer. In this model we consider only the hopping between the \(p_z\) orbitals residing on the nearest neighbor sites. In this picture the two layers are assumed to be connected only through the hopping among \(A_1\) and \(A_2\) sublattices in the Bernal stacking. The Hamiltonian can be written as:

\[
H = -t \sum_{m=1}^{2} \sum_{(i,j)} a_{m,i}^{\dagger} b_{m,j} + \text{h.c.} - t_{\perp} \sum_{i} a_{1,i}^{\dagger} a_{2,i} + \text{h.c.} + 2 \sum_{m=1}^{2} \sum_{i} \epsilon_{m,i} a_{m,i}^{\dagger} a_{m,i} + \epsilon_{b_{m,i}}^{b^{\dagger}} b_{m,i}^{\dagger} b_{m,i},
\]

in which \(a_{m,i}^{\dagger}\) (\(a_{m,i}\)) creates (annihilates) a \(p_z\)-electron at site \((m, i)\) on the sublattice \(A\), with \(m = 1, 2\), where \(m\) is the index of layers and \(i\) labels the sites on each A sublattice of a given layer. Similarly, \(b_{m,i}^{\dagger}\) and \(b_{m,i}\) are the corresponding creation and annihilation operators in the \(B\) sublattices of the two layers. Here, \(t\) denotes the intra-plane hopping integral between the nearest neighbors and \(t_{\perp}\) is the inter-plane hopping amplitude between two layers. Empirical estimates of the hopping terms are \(t \sim 3.16\) eV, and \(t_{\perp} \sim 0.39\) eV [23, 24]. There are further inter-plane couplings, which for simplicity we ignore in our study. Also, \(\epsilon_{m,i}^{a}\) and \(\epsilon_{m,i}^{b}\) in the last term denote the on-site energies at \(A\) and \(B\) sublattices on each layer, respectively. To introduce disorder in the model, we choose the on-site energies randomly from a uniform distribution in the interval \([-\frac{16}{3}, \frac{16}{3}]\). This is the so called Anderson model with spatially uncorrelated diagonal disorder in which \(W\) is a measure for the intensity of disorder. Hereafter, we assume the unit of energy to be set by \(t\).

3. Kernel polynomial method

Local density of states (LDOS), denoted by \(\rho_i(E)\), is a quantity that measures the contribution of a given lattice site \(i\) in the total density of energy states of the lattice in the interval \([E, E + dE]\), and is defined by the following relation:

\[
\rho_i(E) = \sum_{n=1}^{N} \frac{\langle |i| E_n \rangle^2 \delta(E - E_n)}{\langle |i| E_n \rangle^2}
\]

in which \(\langle |E_n | \rangle\) is the energy eigenvector corresponding to energy eigenvalue \(E_n\). \(\langle |i| E_n \rangle^2\) in equation (2) is the probability of finding an electron with energy \(E_n\) on the site \(i\), which in the absence of disorder is the same for all lattice sites as a result of translational invariance. However for localized states encountered in disordered systems, this probability drastically varies in space. If the Hamiltonian possesses an extended eigenstate with the eigenvalue between
$E$ and $E + dE$, then all sites contribute comparably to this state, while for a localized state only a limited number of sites have appreciable probability of being occupied. Therefore, LDOS would be a suitable quantity to distinguish an extended state from a localized one. This can be accomplished by comparing the geometric and arithmetic averagings of LDOS at different lattice points. The geometric average of LDOS known as typical DOS is defined as

$$
\rho_{typ}(E) = \exp \left[ \frac{1}{K_i K_s} \sum_{K_i} \sum_{K_s} \ln \left( \rho_i^s(E) \right) \right], \quad (3)
$$

where $K_s$ is the number of sites in a given realization that LDOS is calculated and $K_i$ is the number of realizations. On the other hand, the total density of states is obtained by summing up the partial LDOS of all lattice sites, which amounts to the following arithmetic average:

$$
\rho_{av}(E) = \frac{1}{K_i K_s} \sum_{K_i} \sum_{K_s} \rho_i^s(E) = \frac{1}{D} \sum_{n=0}^{D-1} \delta(E - E_n), \quad (4)
$$

where $D$ is the dimension of Hilbert space of the Hamiltonian. For an extended state $\rho_{typ}(E) \approx \rho_{av}(E)$, while in the case of localized states $\rho_{typ}(E) \ll \rho_{av}(E)$. Note that, $\rho_{typ}$ is not necessarily the best quantity to distinguish the onset of localization transition [25]. This criterion is known to slightly overestimate the critical value $W_c$ of the Anderson transition. For example, for a 3D cubic lattice this criterion gives $W_c/t \sim 17.5$, which is slightly larger than the known value of 16.5 [22].

LDOS is a site dependent quantity which we employ the KPM [22] to compute. The basic idea of KPM is to expand the spectral functions, such as $\rho_i(E)$, in terms of orthogonal polynomials. In principle, one can use any kind of orthogonal polynomials. In this paper, we use Chebyshev polynomials. Therefore, we expand LDOS as

$$
\rho_i(E) = \frac{1}{\pi \sqrt{1 - E^2}} \left[ \mu_0 + 2 \sum_{n=1}^{N} \mu_n T_n(E) \right], \quad (5)
$$

where the coefficient $\mu_n$ is given by [22]

$$
\mu_n = \int_{-1}^{1} \rho_i(E) T_n(E) \, dE = \frac{1}{D} \langle i | T_n(\hat{H}) | i \rangle. \quad (6)
$$

$\hat{H}$ in the above equation is the rescaled Hamiltonian, which can be obtained by a simple shift and scaling transformation of the original Hamiltonian to ensure that eigenvalues of $\hat{H}$ lie in the interval $[-1, 1]$. A similar procedure for the expansion of the total DOS gives the following moments:

$$
\mu'_n = \int_{-1}^{1} \rho_{av}(E) T_n(E) \, dE = \frac{1}{D} \text{Tr}[T_n(\hat{H})]. \quad (7)
$$

The moments given in equations (6) and (7), which were first discussed by Wang [26], can be evaluated by using the recursion relation between Chebyshev polynomials. The matrix elements are computed on the fly, without saving any matrix, which is a key aspect of KPM. The summation over the diagonal matrix elements required in the trace in equation (7) can be performed stochastically, which dramatically reduces the computer time. These considerations make it possible to study reasonably large systems, even on a desktop computer [22].

When the series expansion of equation (5) is used in numerical calculations, it has to be truncated at a finite order $N$. This truncation leads to the infamous Gibbs oscillations in the LDOS. To relieve this effect, some standard damping factors [27] (called $g$-factors) have been suggested [22, 26], by using equation (5) which can be re-written as follows:

$$
\rho_i(E) = \frac{1}{\pi \sqrt{1 - E^2}} \left[ \mu_0 g_0 + 2 \sum_{n=1}^{N} \mu_n g_n T_n(E) \right]. \quad (8)
$$

In our work, we found that the following (Jackson’s) positive $g$-factor

$$
g_n = \left( N - n + 1 \right) \cos(\frac{\pi n}{N+1}) + \sin(\frac{\pi n}{N+1}) \cot(\frac{\pi}{N+1}) \frac{N+1}{N+1}, \quad (9)
$$

is suitable to damp the oscillations arising in the calculation of LDOS [22].

4. Results and discussions

We operate with the Hamiltonian given in equation (1) with different strengths of disorder ($W$) to investigate the Anderson
transition on bilayer graphene and then calculate LDOS by means of KPM. We carried out the calculations for the lattices consisting of $L = 20 \times 10^3 - 80 \times 10^3$ sites. In order to obtain reliable results, the order of expansion, $N$, has to be reapportioned, depending on the system size, as $N \sim L^2$. The number of random lattice sites used in averaging the LDOS is $K_s = 15$ for each of the $K_r = 15$ different realizations. In figure 1(a) we compare the total and typical DOS corresponding to $L = 80 \times 10^3$ sites and $N = 4000$ moments for $W/t = 0.5$ and $1.0$. As can be seen in this figure, $\rho_{typ}$ is nonzero and almost equal to $\rho_{av}$ for the entire energy bandwidth, indicating that none of the states are localized for these strengths of disorder. The four sharp peaks located near $E/t \approx \pm 1.0$ in the $W/t = 0.5$ plot are the Van-Hove singularities due to the four saddle points in the band structure of the clean bilayer graphene. Therefore, this disorder strength does not appreciably alter the overall spectral features of the clean bilayer graphene. There are also four jumps near $E/t = \pm 3$, corresponding to the four extrema in the energy surfaces. As can be seen in figure 1(b), for $W/t > 1.0$, these singularities tend to smear out. One has to note that the total bandwidth of clean bilayer graphene is very close to the value $3t$ of a mono-layer sample, due to the dominant in-plane energy scale, $t$. However, as we will see shortly, when the disorder is introduced, the presence of the second layer causes the states in bilayer graphene to resist more against Anderson localization than the mono-layer.

The results for the larger values of the disorder strength are displayed in figure 2. As can be seen in this figure, the average density of states still resembles that of the clean graphene bilayer up to $W/t = 2$. Beyond $W/t \sim 2$, the spectral properties start to significantly deviate from the clean bilayer. The typical DOS starts to vanish at two bounds of the energy spectrum. This behavior is quite similar to the localization behavior of 3D bands, where a mobility edge sets in, rendering the states at the tails localized. A further increase in the disorder strength eventually localizes the entire spectrum beyond $W/t \sim 8$.

Figure 3 shows the intensity plot of LDOS in the $xy$-plane of the lattice for different values of disorder near the charge neutrality point, $E = 0$. As can be seen, by increasing the disorder strength, spatial distribution of the DOS tends to clump into clusters. This means that the wavefunctions corresponding to $E = 0$ are spatially localized mainly on the atoms which have appreciable LDOS. This provides the possibility of real space visualization of the localization transition by means of scanning tunneling spectroscopy [28]. At the disorder strength $W/t = 8.0$, these clusters of nonzero LDOS become entirely disconnected in such a way that the energy states around $E = 0$ would no longer contribute to the electric conduction.

To rule out the possibility of finite size artifacts, we perform a finite size scaling analysis. Let us define $R(E)$ as the ratio of the typical to average DOS for a given electronic mode at energy $E$ [29]:

$$R(E) = \frac{\rho_{typ}(E)}{\rho_{av}(E)}.$$  \hspace{1cm} (10)

Since the arithmetic averages of positive numbers are always greater than the geometric average, one always has,

$$R(E) \leq 1, \quad \forall E.$$  \hspace{1cm} (11)

In the absence of disorder the equality is realized, while turning the disorder on, reduces $R(E)$ from 1. We computed this quantity for different values of disorder strength and different lattice sizes. The results for two energies $E = 0$ and $E = 0.2$ are depicted in figures 4 and 5, respectively. The lattice sizes are $L = 2 \times 10^3, 4 \times 10^4, 6 \times 10^4$ and $8 \times 10^4$. As can be seen in a wide range of disorder strengths, this ratio tends to converge almost to the same curve with increasing $L$, which indicates the validity of our results on the infinite lattice size. We have checked that increasing the order of expansion from $N = 4000$ to 12 000, does not appreciably change our results.
Figure 3. LDOS map for various disorder intensities for $E \in [0.0, 0.01]$. In the weak disorder regime, the electron density is almost uniformly distributed over the entire lattice. By increasing $W/t$ to 8, the electron density becomes confined in disconnected regions of lattice.

Figure 4. The ratio of typical to average DOS ($R(E)$), computed at the band center ($E = 0$), versus the strength of disorder for different lattice sizes $L = 2 \times 10^4, 4 \times 10^4, 6 \times 10^4, 8 \times 10^4$.

Figure 5. The ratio of typical to average DOS ($R(E)$), computed at $E = 0.2$, versus the strength of disorder for different lattice sizes $L = 2 \times 10^4, 4 \times 10^4, 6 \times 10^4, 8 \times 10^4$.

5. Conclusion

In summary, using the KPM method to find the local density of states, and studying their geometrical averages, we investigated the effect of uncorrelated disorder on the electronic states of the graphene bilayer. The localization behavior of bilayer graphene is reminiscent of 3D bands, i.e. the localization starts from the states at the edges of the energy spectrum. The states near the charge neutrality point $E = 0$ remain extended up to a very large value of disorder strength $W/t \sim 8$. Therefore, our finding shows that bilayer graphene remains metal in the presence of on-site disorder up to a critical value of disorder at which it undergoes the Anderson metal–insulator transition. This critical value is about three times larger than the critical value that we obtained for the Anderson transition in single-layer graphene [20]. The inter-layer hopping seems to be responsible for such a drastic difference between the localization properties of mono-layer and bilayer graphene. Roughly speaking, when an electron faces a large energy barrier in one layer it can keep on propagating by hopping to the other layer, while this help from inter-layer hopping does not exist for graphene mono-layers. This difference manifests itself in more than twice as large a minimal conductivity of bilayer graphene compared to mono-layer samples. Similar enhancement has been reported comparing graphene and bilayer graphene nano-ribbons with edge disorder, where it has been shown that in the regime that the Fermi energy lies in the energy gap the localization length in BGN is about twice as large as GNRs [18]. The precise understanding of how the (small) inter-layer hopping can lead to such a remarkable difference in the localization properties remains an open question which requires further investigation.

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