Anderson transition in disordered graphene

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Abstract – We use the regularized kernel polynomial method (RKPM) to numerically study the effect disorder on a single layer of graphene. This accurate numerical method enables us to study very large lattices with millions of sites, and hence is almost free of finite-size errors. Within this approach, both weak- and strong-disorder regimes are handled on the same footing. We study the tight-binding model with on-site disorder, on the honeycomb lattice. We find that in the weak-disorder regime, the Dirac fermions remain extended and their velocities decrease as the disorder strength is increased. However, if the disorder is strong enough, there will be a mobility edge separating localized states around the Fermi point, from the remaining extended states.

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Introduction. – Graphene is the 2D allotrope of carbon in which carbon atoms with \(sp^2\) hybridization are organized in a honeycomb lattice. Recently, the isolation of single graphene sheets has become possible through chemical exfoliation of bulk graphite [1–3], or epitaxial growth, either by chemical vapor deposition of hydrocarbons on metal substrates [4] or by thermal decomposition of SiC [5]. The latter method produces graphene layers with high crystalline quality. Properties such as, tuning the carrier types from hole to electron in the same sample through a gate voltage and remarkably high mobility of charge carriers, even at room temperature, due to the absence of back-scatterings, has made the graphene promising from the technological point of view in building the carbon-based electronic devices [6].

The electronic properties of pure graphene can be modeled with a simple tight-binding picture proposed by Wallace [7] which provides the essential band structure of graphene as a half-filled system with a density of states (DOS) vanishing linearly at the charge neutrality point. In this picture the energy dispersion is linear in momentum near the Fermi points, causing the quasi-particles behave as massless chiral Dirac electrons [8].

In spite of high crystalline quality, disorder cannot be avoided in currently available samples of graphene. Various kinds of intrinsic disorder such as surface ripples and topological defects, as well as extrinsic ones like vacancies, ad-atoms, charge impurities affect the electronic properties of graphene. The presence of a minimal conductivity at zero bias [2] implies the existence of extended states at the charge neutrality points, in contrast to prediction of the scaling theory in 2D [9].

There has been various theoretical and numerical approaches to study the effect of different types of disorder in graphene (as a review, see ref. [6] and references therein). Based on one-parameter scaling theory [10], Ostrovsky and coworkers found a metal-insulator transition in graphene for long-range disorder [11]. The hypothesis of one-parameter scaling was subsequently verified with numerical calculation of Bardarson et al. [12]. They used a transfer operator method to investigate the localization properties of the low-energy effective (Dirac) theory. Similar result for the beta function was obtained independently by Nomura et al. [13] by evaluating the Kubo formula for the conductance. Although these numerical works verify the hypothesis of single-scaling theory, but they predict that Dirac fermions remain delocalized at arbitrary strength of disorder. The effect of roughness on the electronic conductivity was studied in [14], and it was found that all states remain localized in the presence of random effective gauge fields induced by ripples.

Lherbier et al. used a real space and order N Kubo formalism to calculate time-dependent diffusion constant \(D(E,t)\) for the Anderson model on honeycomb lattice [15]. For small values of disorder strength \(W\), they found...
$D(E, t)$ saturates to a constant value in long-time limit, indicating the presence of extended states. At larger values of $W$ they report a decrease in $D(E, t)$ pinpointing the onset of localization.

Most of the analytical methods used in the studies of disorder in graphene, are able to handle restricted regimes of specific types of disorder. Their predictions are valid only on the low-energy scales around the Dirac points, where the inter-valley scatterings from the impurity potential can be ignored. When disorder strength becomes comparable to the band width, it is important to take into account all energy scales simultaneously along with possible interplay between different energy scales. There also remains an important question about whether there is a mobility edge in graphene in the strong-disorder regime or not.

In this paper we use the kernel polynomial method (KPM) [16] based on the expansion of spectral functions in terms of a complete set of polynomials to accurately calculate various spectral properties, including the density of states (DOS). The computation time in KPM method grows linearly with system size. Matrix manipulations can be done on the fly, which reduces the memory usage enormously. Therefore one can study very large lattice sizes in a moderate time. Regularization of KPM method known as RKPM remedies the Gibbs oscillations [17], and therefore is capable to handle any type of disorder with arbitrary strength in essentially the exact way. By this method, one can treat the low-energy and high-energy features of graphene on the same footing, and hence the interplay between the Dirac features and high-energy parts of the spectrum, as well as inter-valley scattering is taken into account. This method enables us to explore new regimes of disorder strength with fascinating properties.

**Model and method.** – From the single-particle point of view, disorder can affect the non-interacting electrons in graphene, mainly through spatial variations of on-site energy (diagonal disorder) or changes in the hopping integrals due to the variations in the distances or angles of the $p_z$ orbitals (off-diagonal disorder). In what follows we study the graphene with on-site uncorrelated disorder. We consider non-interacting electrons moving on a honeycomb lattice in the presence of local diagonal disorder. The basic model to describe this kind of problem is the Anderson model:

$$H = -t \sum \langle cj|c_j + \text{H.c.}] + \sum_j e_j c_j^\dagger c_j. \quad (1)$$

The first term describes hopping between nearest-neighbor sites and $e_j$‘s in the second term are the random on-site potential uniformly distributed in the interval $[-W/2, W/2]$. In eq. (1), the energy $t$ is associated with nearest neighbor hopping integral, which is about $2.7 \text{eV}$ in graphene. This model has recently been studied by transfer-matrix method in ref. [18], where it was found that all states are localized, in agreement with scaling theory of localization in 2D. However, our results are in contradiction with this finding.

In our work, to investigate the localization properties, we employ the so-called typical DOS as a quantity which determines whether a given state with energy $E$ is extended or localized [16]. The return probability for an extended state at a given energy $E$ is zero [19]. Therefore the self-energy of an extended state acquires an imaginary part to account for the decay of return probability, while the self-energy for localized states remains purely real. This reflects itself in the local density of states (LDOS):

$$\rho_s(E) = \sum_k |\langle s|E_k\rangle|^2 \delta(E - E_k), \quad (2)$$

where $|s\rangle$ denotes a localized basis state at site $s$, while $|E_k\rangle$ is an energy eigen-vector corresponding to energy $E_k$. Examining LDOS at $K_s$ sites provides a measure to distinguish localized states from extended ones. To do so, one defines the typical DOS which is a geometrical average of LDOS’s:

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

where $K_s$ is the number of realizations used in numerical calculations. We also need the total spectral weight which can be obtained from the following arithmetic averaging:

$$\rho(E) = \frac{1}{K_s} \sum_{s} \sum_{r} \rho_s^r(E) = \frac{1}{D} \sum_{k=0}^{D-1} \delta(E - E_k), \quad (4)$$

where $D$ is the dimension of the Hilbert space on which the Hamiltonian $\hat{H}$ is acting.

The core quantity in both eqs. (3) and (4) is the LDOS. In order to calculate quantities of this sort, the KPM method [16] employs a complete basis set.

The basic idea behind the KPM is to expand the spectral function, say, $\rho_s(E)$, in terms of orthogonal polynomials, $\phi_m(E)$. In general, all types of orthogonal polynomials can be used. In the case of, e.g., Chebyshev polynomials one has

$$\rho_s(E) = \frac{1}{\pi \sqrt{1 - E^2}} \left[ \mu_0 + 2 \sum_{m=1}^{M} \mu_m T_m(E) \right], \quad (5)$$

where

$$\mu_m = \int_{-1}^{1} \rho_s(E) T_m(E) dE = \frac{1}{D} \langle s|T_m(\hat{H})|s\rangle. \quad (6)$$

Here, $\hat{H}$ is obtained from $H$ by a simple linear transformation to ensure that the eigenvalues of $\hat{H}$ are in $[-1, 1]$. The same procedure when applied to eq. (4) gives

$$\mu_m = \int_{-1}^{1} \rho(E) T_m(E) dE = \frac{1}{D} \text{Tr} [T_m(\hat{H})]. \quad (7)$$

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Fig. 1: (Color online) $\rho$ (solid line) and $\rho_{\text{typ}}$ (dotted line) for different values of disorder strength $W$ in the weak-disorder regime ($W \lesssim t$). In this regime the disorder only renormalizes the Fermi velocity of Dirac quasi-particles. Our results are stable with respect to change in both lattice size, as well as $M$.

Equations (7) and (6) can be evaluated with a recursive relation first discussed by Wang [20]. The Tr in eq. (7) can be most conveniently evaluated with a simple stochastic summation employing the recursion relation among Chebyshev polynomials [16]. However, since $M$ in eq. (5) is finite in computer implementations, one faces the classic problem of Gibbs oscillations. There are standard attenuation factors suggested in the literature which minimize such unwanted oscillations [16,20]. Due to peculiar Dirac dispersion in graphene, none of the so-called $g$-factors worked. The solution around this problem is to use regulated (Gaussian broadened) polynomials to calculate the moments [17]:

$$\langle \phi_m(x) \rangle_\sigma \equiv \frac{1}{2\pi\sigma^2} \int dx' e^{-(x'-x)^2/2\sigma^2} \phi_m(x').$$

Our present calculation is based on using Legendre polynomials in (8) with $\sigma$ equal to $4/M$.

Results and discussions. – To investigate the Anderson transition in graphene, we use eq. (1) with different values of $W$ and then calculate the LDOS via the RKPM method with $M$ equal to 5000–12000 on a lattice with $10^6$ sites. The result for different values of $W$ is shown in fig. 1. As can be seen in fig. 1 the average DOS for various values of $W \lesssim t$ resembles that of perfect graphene. The typical DOS, $\rho_{\text{typ}}$, is non-zero everywhere, indicating that none of the states are localized in this regime. The role of disorder at weakly disordered regime is to slow down the Dirac quasi-particles, with their Dirac nature preserved. This result is in agreement with other works [21,22]. Figure 2 shows the renormalization of the Dirac fermion’s velocity. By increasing the disorder strength, the slope of $\rho$ decreases. Therefore, according to $\rho(\omega) \propto |\omega|/v_F^2$, the velocity of quasi-particles decreases when $W$ increases [15,21].

Increasing $W$ to the strong-disorder regime, $W \gtrsim t$, we observe a mobility edge in graphene in fig. 3. The mobility edge starts at the Fermi energy and keeps moving to both the left and right side separating localized states around the Fermi point of graphene. We find that in the intermediate disorder regime ($W \sim t$) states at the

Fig. 2: (Color online) Average DOS as a function of energy. By increasing $W$ in weakly disordered region, the velocity of Dirac fermions decreases.

Fig. 3: (Color online) For $W > t$ a mobility edge starts to appear. $\rho_{\text{typ}}$ is zero around the Fermi energy. Therefore localized states fall into a “gap” separating extended states of the valence and conduction bands.

The idea of band gap opening in graphene has already been proposed by several groups. Pereira et al. [23] by selectively producing vacant sites in only one sub-lattice, found the appearance of a clean gap without any states in it. Substrate-induced band gap, which is accompanied by breaking the particle-hole symmetry is another possible scenario [24].

However, our result suggest the possibility of disorder-induced gap in graphene. This gap is defined as the distance between the upper and lower mobility edges around the Fermi point of graphene. We find that in

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Fermi point start to localize, thereby opening a small gap around it (fig. 3). The states inside the gap are localized and cannot contribute in transport phenomena. Upon increasing disorder strength, this gap rises slowly up to $W \sim 2t$, above which its growth speeds up with a high slope (fig. 4). This behavior can be assigned to cross-over from weak to strong localization regimes. Naumis also obtains such disorder-induced gap, using a real space renormalization group scheme [25] for vacancy-doped graphene. Nevertheless this gap continuously grows from zero as a function of doping ratio.

Finally with increasing $W$ beyond $W_c/t = 2.5 \pm 0.5$, all states in the band become localized. The “error” $\pm 0.5$ here needs clarification: One might argue that the typical DOS is not the best quantity to distinguish localized states from extended ones. Our benchmark runs for the known results of the critical $W$ for the 3D cubic systems gives $W^{3D}_c/t = 16.0 \pm 0.5$. Therefore the possible intrinsic error in finding $W_c$ in this method is less than 0.5.

**Conclusion.** For the Anderson model, in weak-disorder regime, we observe that the Dirac fermions remain delocalized up to $W^* \approx t$. In this regime, the effect of disorder is to decrease the velocity of Dirac fermions, hence resulting in a renormalized Dirac cone. However, upon increasing the disorder strength beyond $W^*$ in this model, we observe a mobility edge, in agreement with ref. [25]. Our results support the idea proposed by Suzuura and Ando [26] which explains the suppression of weak localization in graphene. According to their argument, the change in relative weights of the two components of chiral electrons wave functions induces a new Berry phase, when these electrons move along a closed path. If the inter-valley scatterings are negligible, this new phase changes the sign of the wave function in a given path with respect to its time-reversed counterpart, leading to a destructive interference of the two paths, hence leaving the low-energy states extended. A similar result has also been obtained in recent theoretical work on chemiabsorbed adatoms attached to the carbon atoms in graphene [27]. Another single-impurity study using the scattering formulation indicates the possibility of localization due to bound-state formation for strong enough scattering strength [28]. Although our method is not able to estimate the contributions of inter-valley and intra-valley scatterings separately, we speculate that the relative intensity of inter-valley scattering might be small. We think the localization of all the electronic states, obtained by transfer matrix method [18], might be due to size limitations, which makes their method inconclusive in the weak-disorder limit ($W/t < 1$). We have performed a careful finite-size scaling specially in the weak-disorder regime.

Figure 5 shows the finite-size analysis at $W/t = 0.3$ for the lattice sizes $N = 4 \times 10^4$, $16 \times 10^4$, $36 \times 10^4$ near the Dirac point. As can be seen in the figure, the typical DOS remains non-zero as one increases the lattice size. This clearly means that states near the Dirac point remain extended in the weak-disorder regime. It should be noted that the number of moments, $M$ used in the polynomial expansion must be large enough ($M \propto N^4$). Upon increasing the disorder strength, when it becomes comparable with the hopping energy ($W \sim t$), the inter-valley scatterings get significant and the weak localization will be eventually recovered around the Fermi points [29–32]. In the very strong-disorder regime ($W > 2t$), localization quickly spreads over all the energy spectrum. In this case the system is no longer homogeneous in the sense that it divides into regions with different chemical potential and transport is described in terms of percolation in the real space [33,34]. A recent study employing the same method as ours on graphene nano-ribbons agrees with our results [35].

Some aspects of our predictions are qualitatively verified in the recent ARPES measurements of graphene samples dosed with atomic hydrogen [36]: i) The very observation of metal-insulator transition at finite amount of short-range disorder due to adsorbed hydrogen atoms. ii) The observed gap is due to the emergence of a mobility edge around the charge neutrality point in agreement with our work and ref. [25].
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