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Critical wavefunctions in disordered graphene

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Abstract
In order to elucidate the presence of non-localized states in doped graphene, a scaling analysis of the wavefunction moments, known as inverse participation ratios, is performed. The model used is a tight-binding Hamiltonian considering nearest and next-nearest neighbors with random substitutional impurities. Our findings indicate the presence of non-normalizable wavefunctions that follow a critical (power-law) decay, which show a behavior intermediate between those of metals and insulators. The power-law exponent distribution is robust against the inclusion of next-nearest neighbors and growing the system size.

(Some figures may appear in colour only in the online journal)

Graphene is a two-dimensional atomic crystal [1] with the highest known charge carrier mobility [2] and thermal conductivity [3] at room temperature. Both properties indicate graphene as a raw material for transistor use; however, the 'graphenium inside' era is quite far off [4]. Keeping in mind the design of transistors, the problem turns out to be how to alchemize it into a semiconductor [5–7]. One alternative is to dope graphene. This leads immediately to the question of quantum percolation in two dimensions, which has been the subject of debate for many years [8, 9]. In the literature, usually it is found that 'there is no true metallic behavior in two dimensions' as a consequence of the fact that all eigenstates are localized even when the disorder is weak [10]. For graphene, there has been a debate about this point [11–13]. Recently, disordered graphene has been classified using arguments of symmetry around the Dirac point [14]; this classification allows a minimal conductivity behavior. Experimentally, the minimal conductivity was measured for graphene doped with potassium [15, 16]. Furthermore, it has been found that a metal transition can be observed when graphene is doped with H [17]. Also, using a non-interacting electron model enriched with first-principles calculation, a metal–insulator transition has been found [18–20]. In this paper, we present numerical evidence that shows a very interesting scenario. We have characterized the probability distribution of the moments associated with the wavefunction using the inverse participation ratios. The scaling of this quantity is frequently used to discriminate between an eigenstate being extended or localized. We found states in doped graphene which do not follow the usual exponential localization; instead, these are critical, i.e., the wavefunction decays spatially as a non-normalizable power law. This behavior evidenced the multifractality of the wavefunction [21, 22]. Notice that in the original development of the scaling theory, critical states were not considered [10].

As a model we use the tight-binding Hamiltonian,

$$\mathcal{H} = -t\sum_{\langle i,j\rangle} c_i^\dagger c_j - t'\sum_{\langle\langle i,j\rangle\rangle} c_i^\dagger c_j + \varepsilon\sum_{\ell} c_\ell^\dagger c_\ell, \qquad (1)$$

where the nearest neighbor, $t = 2.79$ eV, and next-nearest neighbor (NNN), $t' = 0.68$ eV, hopping parameters are included; these values have been taken from [23]. The impurity sites, ℓ, have been distributed randomly in the lattice with a concentration C, and ε is the impurity self-energy.

In order to investigate localization, we introduce the inverse p-participation ratios (IPRs),

$$\|\Psi_{\mathbf{k}}\|_{2p} = \sum_{i}^{N} |\Psi_{\mathbf{k}}(\mathbf{r}_i)|^{2p}, \qquad (2)$$

where $\Psi_{\mathbf{k}}$ is the wavefunction associated with the eigenstate $\mathbf{k}$ with energy $E_{\mathbf{k}}$, which solves the Schrödinger equation

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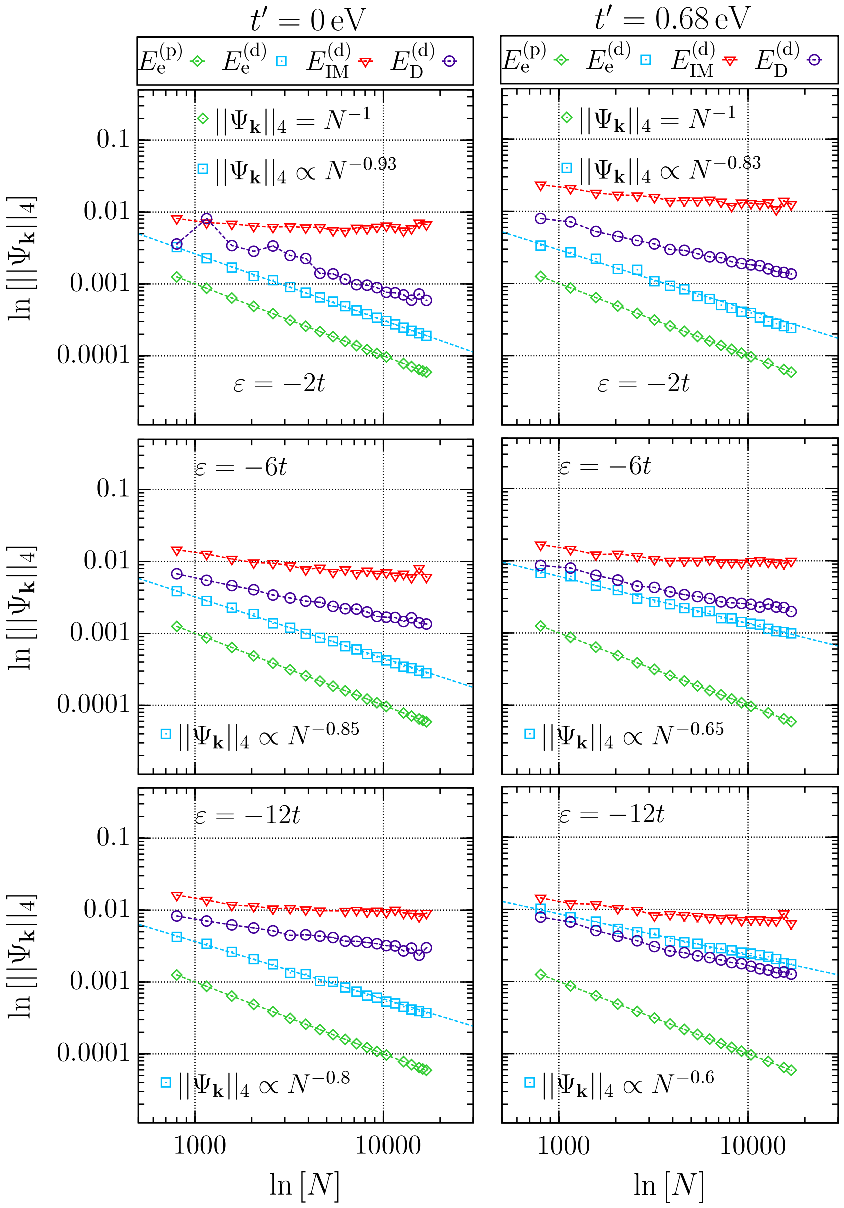

Figure 1. The $p = 2$ IPR behavior as a function of N for several selected energies, using different impurity self-energies (from top to bottom) and without and with NNN interaction (left and right columns, respectively). The selected energies are the Dirac point energy (E_D, (dark blue online) circles), the maximal localized state (E_IM, (red online) triangles) and $E_\mathrm{e} = E_\mathrm{D} - 0.4t$ ((blue online) squares) for doped graphene$^{(\mathrm{d})}$. In all cases, doped graphene has a 5% impurity concentration. For the state with energy E_e, we present in all cases the scaling exponent that results from the fitting, shown in the figures with (blue online) lines. For comparison proposes, we include the case of pure graphene for the energy $E_\mathrm{e}^{(\mathrm{p})}$ ((green online) diamonds). Each data point is obtained from an average over 95 disordered configurations.

$\mathcal{H}\Psi_\mathbf{k} = E_\mathbf{k}\Psi_\mathbf{k}$. The index i belongs to the sum over sites, N is the total number of sites and p is an integer. When $p = 1$, $\|\Psi_\mathbf{k}\|_2 = 1$ because of the normalization condition. If the wavefunction of the eigenstate follows the power law, $\Psi(\mathbf{r})_\mathbf{k} \sim |\mathbf{r}|^{-\alpha}$, the p-IPRs are scaled as [24],

$$\|\Psi_\mathbf{k}\|_{2p} \simeq \begin{cases} N^{-(p-1)} & \left(0 \le \alpha < \dfrac{1}{p}\right) \\ N^{-p(1-\alpha)} & \left(\dfrac{1}{p} \le \alpha < 1\right), \\ N^{0} & (1 \le \alpha) \end{cases} \qquad (3)$$

when $p > 1$. The N^{-1} behavior corresponds to a metal, while N^0 corresponds to an insulator. Notice that here $N \propto L^2$, where L it is the length of the sample.

To evaluate equation (2), we calculated all the eigenvalues and eigenvectors of $\mathcal{H}$ by numerical diagonalization. In order to take the disorder into account in a proper way, for each combination of self-energy, concentration, and sample size without and with NNN interaction, we performed averages over 95 disordered realizations. Since for any given disordered realization and for a finite-size lattice, the spectrum is discrete, the energy eigenvalues are never equal to the chosen value of the energy (more precisely, the probability of coincidence is

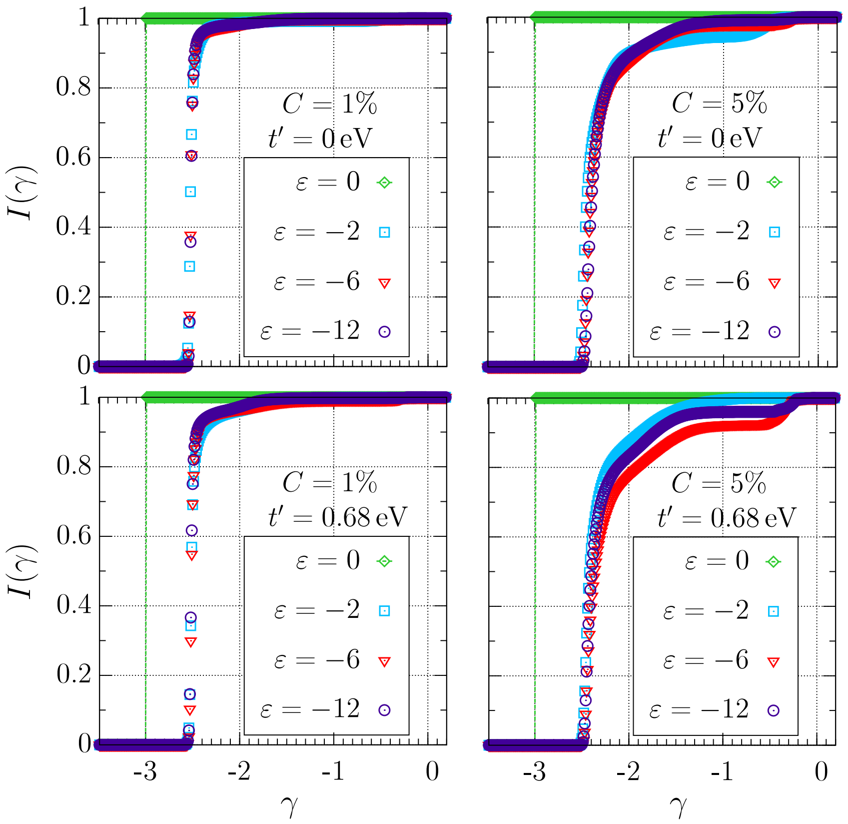

Figure 2. Integrated distribution of exponents for different impurity configurations using lattices with $N = 16\,928$ sites. Extended states are at $\gamma = -3$ and localized ones at $\gamma = 0$. We observe that for pure graphene ((green online) diamonds), the distribution is a step function at $\gamma = -3$; meanwhile for doped graphene the distribution is shifted and it is no longer a step function. Each data point is obtained from an average over 35 disordered realizations.

almost zero). Thus, we compute $\|\Psi_{\mathbf{k}}\|_{2p}$ by averaging over an energy window around the chosen energy, by counting the number of states which fall into the window [21, 25]. We verified that the final results do not change much with the width of the window. In this work, we used an energy window of $0.02t$. To test the convergence of the data, we performed arithmetic and geometric averages. The two approaches gave us similar results, but here we only present the arithmetic averages. Thus, the number of samples used can be considered as reasonably reliable. The $p = 2$ IPR behavior is shown in figure 1 as a function of N for several selected energies, using different impurity self-energies without and with NNN interaction. For the energy $E_e = E_D - 0.4t$, far from the Dirac energy, we compare the behavior for pure graphene ((green online) diamonds) with doped graphene ((blue online) squares). For pure graphene, the state is extended since the $p = 2$ IPR goes like N^{-1}, as shown in figure 1. For doped graphene, is clear that the $p = 2$ IPR can be fitted with a line, which suggests a non-localized, power-law behavior, which is the main result of this work. Near the Dirac energy, it is known that resonant states can appear at an energy E_r obtained by solving the corresponding Lifshitz equation, using the pure graphene Green's function [26, 27]. These resonant states are well characterized when ε is bigger than the bandwidth, and leads to a tendency for increased localization at the band center due to frustration effects [28]. To test this point, in this work we took an energy window around E_r. Then we selected the energy value E_{IM} for which $p = 2$ IPR is at the maximum in the window, and we performed an averaging over disordered realizations. This allows following the most localized state. For these states, E_{IM}, shown in figure 1 as (red online) triangles, the $p = 2$ IPR scales as $\propto N^0$, suggesting localized states (notice that for $\varepsilon = -2t$, the solution of the Lifshitz equation is not necessarily a resonant state; however, here we treat this case like the others). From this scaling analysis is clear that doped graphene, even in the absence of NNN interaction, presents a rich localization behavior, as has been suggested in [29], due to frustration effects [28], as well as in experiments [17].

In order to obtain the exponent distribution of the power-law behavior, we introduce the integrated distribution of exponents [24],

$$I(\gamma) = \frac{1}{N}\sum_{\mathbf{k}} \Theta(\gamma - \log_N[\|\Psi_{\mathbf{k}}\|_8]), \tag{4}$$

where Θ is the step function. It is worth mentioning that one can also define $I(\gamma)$ using any p value. However, it is better to use a high p to obtain a better approximation for α in equation (3). In this work, we use $p = 4$ since it narrows the interval for the possible values of α, and at the same time, it is numerically more stable than higher values. Since we are dealing with disorder, to compute $I(\gamma)$ we used two methods which give very similar results: first $\|\Psi_{\mathbf{k}}\|_8$ was obtained after

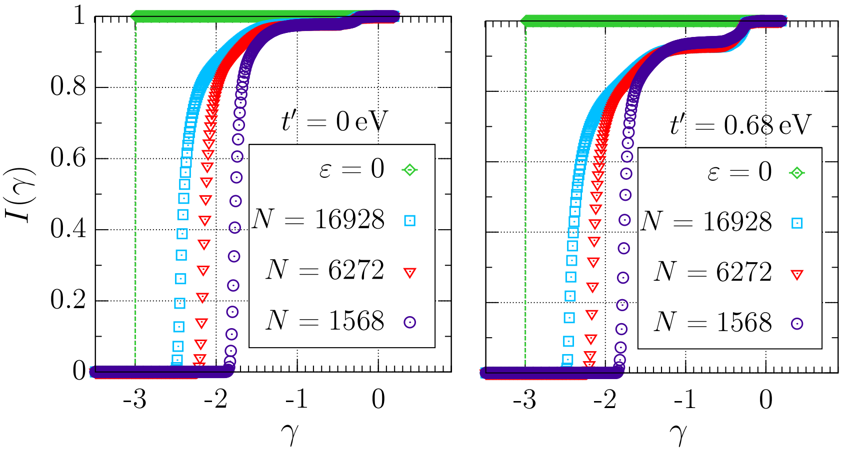

Figure 3. Example of the integrated distribution of exponents for different sample sizes using a fixed concentration of impurities (5%) with self-energy $\varepsilon = -6t$. The left panel corresponds to the model without NNN interaction, and the right panel, that with NNN. Pure graphene is also shown, corresponding to the jump at $\gamma = -3$.

averaging over disordered realizations, and then $I(\gamma)$ was computed; in the second method, $I(\gamma)$ was computed by using all the $\|\Psi_{\mathbf{k}}\|_8$ resulting from the realizations. The exponent distribution is plotted in figure 2, averaging over 35 disordered configurations for several impurity types and two different concentrations, 1% and 5%. For pure graphene, all the states have the same scaling behavior, and a step is observed at $\gamma = -3$. This means that all states have the same scaling, and thus all are extended, as expected from Bloch's theorem. However, for doped graphene, we observe two main effects. First there is a shift to higher values of γ and, second, the jump is no longer a discontinuity. Instead, we observe states that have a distribution of γ values. In all cases, we observed that the minimal value of γ is approximately $-5/2$, which means that the most extended states follow a power law that goes as $r^{-3/8}$. States with $\gamma \approx 0$ are exponentially localized. Since no clear jump is observed in the values of γ, it seems that there is a range of values for the exponents of the critical wavefunctions. Also, it is worth mentioning that the presence of the NNN interaction preserves this behavior, which allows its experimental verification since the NNN is always present.

To verify that such behavior is preserved as the system grows, in figure 3 we present the distribution $I(\gamma)$ for different sample sizes. We can observe that the behaviors are similar at all sizes, although $I(\gamma)$ moves slightly to the left as N grows, i.e., towards low values of gamma instead of to higher values as a function of the lattice sizes, indicating that we are moving away from having localized states, in clear contrast to what we expect for a generic disordered 2D electron gas. From this analysis, we can conclude that there are many non-exponentially localized states, and that the power-law behavior is not a finite-size lattice effect. From the values of γ, we see that these states are critical and non-normalizable. Finally, a careful check of such states reveals that localized states are near the Dirac point and at the band edges, while the power-law non-normalizable states are near the middle part of the valence and conduction bands, in agreement with previous theoretical arguments [28, 29].

In conclusion, using a scaling analysis of the participation ratio, we have shown that the presence of disorder in graphene does not exponentially localize all states; instead, some states are critical with a distribution of exponents. This result is robust against the inclusion of NNN interactions, in which the chirality is not preserved. Although it is quite surprising that the localization behavior presented is qualitatively different from the usual 2D case, that is exponential localization in contrast to the power law found, the honeycomb lattice has some specific symmetries which makes the problem essentially different from that of a generic disordered 2D electron gas [22, 28]. This result is not only important for graphene, but also leads to a revival of an old discussion concerning the possibility of having anomalous quantum percolation in two-dimensional systems [8, 9].

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