The effects of edges on the electronic localization properties of graphene

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Abstract. In this numerically work, we study the effects of edges on the electronic properties of graphene lattices in the quantum Hall regime using a proposed quantity called participation ratio, that is employed to analyze the localization properties of edge states. We use the tight-binding model to include the effects of the magnetic field and disorder. The effect of the edges on the energy levels of the system is studied through Hofstadter’s butterfly-like spectrum. Using the participation ratio and analyzing the contributions of the armchair and zigzag edges separately, we find that there are energy regions where the wave functions are clearly more localized in a specific edge type. The zigzag preferential localization is a reminiscence of the case without magnetic field and the armchair localization which is dependent on the disorder and the strength of the magnetic field, comes from the presence of magnetic field in the system. The results obtained contribute to the understanding of the localization properties of graphene lattices with edges.

1. Introduction

Graphene is a two-dimensional (2D) material formed by six carbon atoms in a honeycomb lattice with two hexagonal sublattices [1, 2]. Its valence and conduction bands are degenerate at the six corners of the Brillouin zone. The energy value where the bands are degenerate is known as Dirac point. From the perspective of its electronic properties, graphene is a gap-less semiconductor, and its charge carriers, for low energies and close to the Dirac point, present a linear scattering, and act as massless Dirac fermions [1, 3–5]. Due to this fascinating feature, graphene has attracted a lot of attention and efforts to develop devices in fields such as electronics, spintronics and quantum computing [6, 7].

The observation of the quantum Hall effect for graphene in 2005 represented an important landmark, proved the genuine two-dimensional behavior of the charge carriers [3]. Edge states are known to play an important role in the quantum Hall regime [8–12]. For graphene, in particular, it was recently shown through scanning tunneling microscopy and spectroscopy that the quantum Hall edge states display the characteristics of confinement by an atomic edge, without edge-state reconstruction [13]. Due to its electronic properties, graphene shows unconventional electronic transport and disorder effects. Kleftogiannis [14] done a study on the localization properties of wave functions in graphene flakes varying the disorder, obtaining an abnormal behavior for graphene flakes with zigzag edge termination where the wave function got less localized as the disorder was increased due to the interplay between the destructive and diffusive interference mechanism.
The edge states in the quantum Hall regime are manifested in the presence of states among the Landau levels (LL’s) [15–17]. Depending on their proximity with the Landau levels, as we will show later, these states can localize exclusively in only a determined edge type. Shed light on the localization properties and nature of these states is the purpose of this paper. This work is organized as follows. In section 2, we describe the tight binding Hamiltonian employed and we introduce the participation ratio quantity, and give details on the considerations taken to define the edge regions. In section 3.1, we focus on the case of graphene sheet without a magnetic field to unveil the nature and localization particularities of the edge states. In Section 3.2, we study the localization properties of graphene in the presence of a perpendicular magnetic field. Also, we analyze the energy spectra as a function of the magnetic flux in search of signatures and to establish the role of disorder in the localization properties. Finally, in section 4, we draw our conclusions.

2. Numerical model
We consider graphene’s tight-binding Hamiltonian up to first neighbours (see Equation (1)) [18].

$$H = \sum_i \epsilon_i c_i^\dagger c_i - \sum_{<ij>} t(e^{i\phi_{ij}} c_i^\dagger c_j + H.c.),$$

where $c_i$ ($c_i^\dagger$) annihilates (creates) an electron at site $i$ and the sum runs over nearest-neighbor sites. The external magnetic field $B$, perpendicular to the graphene sheet, is included by means of a Peierls’ substitution [19] $\phi_{ij} = 2\pi \frac{e}{h} \int_i^j A \cdot dl$ in hopping parameter ($t=2.7$ eV for graphene). Considering the Landau gauge, $\phi_{ij} = 0$ along the x-direction and $\phi_{ij} = \pm \pi(x/a)\phi/\phi_0$ along the ±y-direction, with $\phi/\phi_0 = B a^2 \sqrt{3} e/2 h$ ($a=2.46$ Å, is the lattice constant for graphene) per unit cell. We consider disorder through on-site white-noise fluctuations [20], by sorting uncorrelated orbital energies within $\epsilon_i \leq |W/2|$. We focus the analysis on the lowest Landau levels for small magnetic flux $\phi/\phi_0 = 0.025$, a value where the lattice effects on the electronic spectra (Landau levels) are negligible. For these calculations, we have considered a graphene square lattice with $M \times N$ corresponding to M atoms in the armchair direction times N atoms in the zigzag direction. In this way, the dimensions of the lattices that are periodically repeated are given by $L_x = (N - 1)a/2$ and $L_y = (M - 1)a\sqrt{3}/2$.

Figure 1. Schematic representation of the graphene lattice, where the shaded area corresponds to the edge area $\Omega$ used in the calculation of the participation ratio. In the presence of a magnetic field, the width of the edge area $\Omega$ is defined as twice the magnetic length $\ell_B$. 
To accomplish our purpose of identifying and analyzing edges states, we define here a quantity named participation ratio \( (PR) \) [21], see Equation (2), that corresponds to the sum of the probability amplitudes \( |a_i|^2 \) of the wave function only over atomic sites \( i \) contained in a specific area \( \Omega \) close to the edge (see Figure 1):

\[
PR = \frac{1}{\Omega} \sum_{i \in \Omega} \frac{1}{|a_i|^4}.
\]  

(2)

When the system is under a perpendicular magnetic field \( B \), the width of the edge area \( \Omega \) is defined as two times the magnetic length \( \ell_B \) from the edge, as shown in Figure 1. This definition follows a semi-classical picture, in which charged carriers in the presence of \( B \) complete a cyclotron orbit when in the bulk region, but are reflected when close to the edges, describing skipping orbits whose maximum distance from the edge (seen as a hard wall) is \( 2\ell_B \) [22–24].

For finite graphene lattices we can, in principle, consider magnetic fields as low as we desire in this model (differently from the case where periodical boundary conditions are applied, when the magnetic field phase should be commensurable to at least one of the dimensions of the system). However, note that for the defined participation ratio to be able to differentiate edge from bulk states, we are restricted to cases where both lattice dimensions, \( L_x \) and \( L_y \), are greater than \( 4\ell_B \). The results we show here are for lattice dimensions of about 30 times \( \ell_B \).

When the magnetic field is zero, it is necessary to redefine the width of the \( \Omega \) region, due to the fact that in the case of \( B \neq 0 \), the edge region defined relying on the magnetic length, but without magnetic field, there is not such a quantity. Therefore, we considered the edge region as the line of atoms of atoms at each edge, as shown in Figure 1 and as it is going to be seen in section 3.1, the major contribution of the probability amplitude of the localized states is mainly here (sharply localized states). Observe that this line of atoms includes both sublattices, both for the zigzag and for the armchair edges.

For normalized wave-functions, the participation ratio values will vary from zero to one. Zero value of participation ratio corresponds to the case of a wave-function that has no amplitudes over the defined edge region \( \Omega \). On the other hand, an participation ratio with maximum value (one) means that the wave function has amplitudes only within the \( \Omega \) region. Intermediate values of participation ratio will allow one to appreciate the fraction of the wave function amplitudes contained within the edge area.

3. Discussion

3.1. Participation ratio for systems without magnetic field

In this section we focus on understanding the origin of the particular edge localization found in the quantum Hall regime, and with this aim we studied the same graphene systems but without magnetic field. Figure 2(a) shows the comparison between the partial participation ratio for a system without magnetic field, considering widths in the edge region of atoms. Here is possible to see that the main contributions occur at the very first line and because of this, there is not need to consider inner lines of atoms. Also, it is important to point out that the existence of preferential localization in the zigzag edge around the energy \( E/t = 0 \), implies that the preferential localization over the zigzag edges in the quantum hall regime near \( n = 0 \) is a reminiscence of the case without magnetic field. The nature of these states explains furthermore its robustness with respect to magnetic flux and disorder.

These edge states are not quantum Hall states and therefore, they can not travel along the edges. Figure 2(b) also confirms that in the case of \( B \neq 0 \), there are edge states near all the Landau levels with exception of \( n=0 \), which are quantum Hall edge states and localize only along the armchair edge as we claimed in the previous section.
3.2. Participation ratio computed separately for zigzag and armchair edges

We now go one step further and propose here the use of the participation ratio not only to compute the fraction of the wave function amplitudes over the entire edge area, but only over each type of edge: zigzag or armchair. These quantities are now addressed as zigzag participation ratio or armchair Edge Fraction. As depicted in Figure 2(a) and Figure 2(b), the Ω region (from Equation 2) will now correspond to only one edge type. The width of the edge region is kept $2\ell_B$, as previous definition. Observe that in the corners, which are highlighted in these figures, there is a superposition of zigzag and armchair edge areas considered in this way (a small superposition if the lattice dimensions are much bigger than the magnetic length). Therefore, to avoid that the sum of the zigzag and armchair participation ratios is higher than the total participation ratio previously computed, the contribution of the corners to the zigzag or armchair participation ratio is divided by two.

Figure 2(b) show the zigzag and the armchair participation ratios, for a graphene lattice of $17\times17\text{nm}$ ($80\times140$ atoms) and magnetic flux $\phi/\phi_0 = 0.025$, considering disorder amplitude of $W/t=0.4$. These plots provide interesting new observations about the nature of the edge states, specially for those between the $n=0$ and $n=1$ Landau levels. Although most of the states are not equally distributed between the two edge types, there are clearly edge states that concentrate predominantly in the zigzag edges, for energies close to the $n=0$ Landau level, or in the armchair edges, for a thinner energy range close to the $n=1$ Landau level. That happens for all the disorder intensities investigated. To the best of our knowledge, this behaviour was not addressed in previous works. And it can have impact on the understanding and design of magneto transport experiments in graphene. These states in only one edge type are edge states in the sense that their wave functions are localized on the edges, however they are clearly not circulating quantum Hall edge states.

4. Conclusions

In this paper we investigated edge states of pristine graphene with edges in the presence of a perpendicular magnetic field through a new quantity named participation ratio. We identified edge states that are localized preferentially along either the armchair or zigzag edge depending on its nature. By means of energy spectra we determined the role of disorder in the system,
founding that the edge states localized in the zigzag edges are robust to disorder, differently to the armchair edge case, where the edge states are highly dependent on disorder. We also unveiled the nature of the zigzag preferential localization near Landau level \( n=0 \), founding that it is the reminiscence of the case without magnetic field, and that the edge states which are preferentially localized in the armchair edge in the energy regions near all the Landau levels (except \( n=0 \)) are quantum Hall edge states. We expect the participation ratio to be an useful tool for future works dealing with systems in the quantum Hall regime.

By means of energy spectra figures we identified the energy regions where preferential localization occurred and related anti-crossings to this behaviour. Also we determined the role of disorder in the system, founding that the edge states localized in the zigzag edges are robust to disorder, differently to the armchair edge case where the edge states are highly dependant on disorder due to the broadening of the Landau levels and their proximity. Also we established the role of disorder near the Landau levels and the effect on the preferential localization.

Also was possible to identify concentrations of the wave function in a specific edge type, when were considered separately the armchair and zigzag contribution. The localization particularities were unveiled applying this quantity to the case of \( B = 0 \), where we established that the zigzag preferential localization near Landau level \( n=0 \), is a reminiscence of the case without magnetic, besides that the edge states localized in the armchair edge in the regions near the Landau levels (except \( n=0 \)) are quantum Hall edge states that circulate all over the edges.

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