Charge fractionalization and gap states of interacting disordered graphene zigzag nanoribbon

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We investigate the properties of the gap-edge states of half-filled interacting disordered zigzag graphene nanoribbons. We find that the midgap states can display the quantized fractional charge of 1/2. These gap-edge states can be represented by topological kinks with their site probability distribution divided between the opposite zigzag edges with different chiralities. In addition, there are numerous spin-split gap-edge states, similar to those in a Mott-Anderson insulator.

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I. INTRODUCTION

A rectangular graphene nanoribbon (GNR) has two zigzag edges and two armchair edges. When the length of the zigzag edges is longer than the length of the armchair edges, a zigzag graphene nanoribbon (ZGNR) is realized; for the inverse case, an armchair graphene nanoribbon (AGNR) is realized. Electron-electron interactions generate an excitation gap and induce antiferromagnetism between the opposite edges of a ZGNR.

First principles and Hubbard model calculations\textsuperscript{1, 2} and, as well as, the investigation of the topological Zak phase\textsuperscript{3, 4} show that spin-up charges are localized on one zigzag edge and the spin-down charges are localized on the opposite zigzag edge of AGNRs or ZGNRs. The repulsive interaction between electrons is crucial for this effect, as it reduces the double occupancy of spin-up and spin-down electrons. Although numerous one-dimensional insulators, such as polyacetylene, spin chains, Kondo insulators have fractional charges on their boundaries\textsuperscript{5, 10}, no fractional charge was found on the well separated zigzag edges of a GNR\textsuperscript{1, 2, 4, 11}. Antiferromagnetic coupling between well-separated zigzag edges may be responsible for the suppression of the formation of fractional edge charges. This is despite that a local distortion of hopping parameters can lead to formation solitonic states\textsuperscript{12}. One of the key features of a soliton is that, for each of its spin state, half of its spectral weight originates from the conduction band and the other half from the valence band\textsuperscript{7}. In GNRs a soliton connects two neighboring zigzag edges of opposite chirality, which is analogous to a soliton of polyacetylene which connects two different dimerized phases.

An impurity can have a significant effect on redistributing the probability density of an edge state over the opposite zigzag edges\textsuperscript{13}. In the present work we investigate the role of disorder on the zigzag edge properties in the presence of antiferromagnetic coupling. In particular, we investigate whether a fractional zigzag edge charge may appear in the presence of disorder in ZGNRs. However, to investigate the formation of a fractional edge charge of 1/2 one needs to include both electron-electron interactions and disorder in a self-consistent way. In ZGNRs gap states are localized and reside on the zigzag edges and may display charge fractionalization in the presence of disorder (in the following we call these states gap-edge states).

We investigate the effect of the interplay between disorder and electron-electron interactions on the properties of graphene gap-edge states\textsuperscript{14}. In this work we perform such a calculation in a ZGNR, where the number of gap states increases with increasing length of zigzag edges. We find that, among numerous gap states, only midgap states ($E \approx 0$) contribute to the quantized fractional charge 1/2 in the weak disorder regime, where the strength of disorder is smaller than the on-site repulsion. We find that the charge fractionalization of a midgap state is more robust for short-ranged disorder potentials than for long-ranged potentials. The formation of a well-defined fractional charge originates from the left and right edge states that are coupled by a short-ranged disorder potential. Site pseudospin\textsuperscript{15} of midgap states displays a topological kink-like property. In addition, we find that several edge states become spin-split and singly occupied, as in a Mott-Anderson insulator\textsuperscript{16}.

This paper is organized as follows. In Sec. 2 we describe various type of zigzag edge (gap) states; we classify them as type I, II, and III. In Sec. 3 we describe our model and the mean field Hamiltonian. The fractional charge is defined in Sec. 4 using the eigenstates of the Hamiltonian. In Sec. 5 the site probability distribution of type I, II, and III gap states and their number are computed. The distribution of non-integer charge of the gap states is investigated as a function their energy in Sec. 6. In Sec. 7, these results are used to show the quantization of the charge fractionalization of midgap states. We also investigate how the variance of the quantized value of the fractional charge is related to the impurity range. The
summary and discussions are given in Sec. 8.

II. TYPES OF ZIGZAG EDGE STATES

In the following we classify possible zigzag edge states. In the absence of electron-electron interactions and disorder, zigzag edge states near the center of the band are degenerate [12, 13, 17, 18]. For a given degenerate pair there is some ambiguity in choosing single electron wave functions: suppose $\phi_L$ and $\phi_R$ are two such degenerate states and that $\phi_L$ and $\phi_R$ are located on the left and right edges, respectively, see Figs. 1(a) and (b) (We will classify these $\phi_L$ and $\phi_R$ as type I states). If these states are chiral, then one has A-carbon chirality and the other B-carbon chirality. However, the bonding edge state $\frac{1}{\sqrt{2}}(\phi_L + \phi_R)$ and antibonding edge state $\frac{1}{\sqrt{2}}(\phi_L - \phi_R)$ are also degenerate with the same energy, see Fig. 1(c). The probability density of these edge states is fractionalized equally between the left and right zigzag edges [12]. It is similar to fractionalization occurring at the end points of a long insulating one-dimensional wire [5, 6].

Consider now the other case where electrons move in a disorder potential in the absence electron-electron interactions. Impurities may also couple the edge states $\phi_L$ and $\phi_R$ and break the degeneracy between them. The resulting edge states are approximately bonding and anti-bonding states [13] (however, they are more localized along the GNR direction due to disorder). Such a state has opposite chiralities on the opposite zigzag edges and has approximately a half-integer edge charge. This state will be classified as a type II state. Under certain conditions it may exhibit charge fractionalization of $1/2[12]$ (a fractional charge is defined precisely in Sec. 4). Disorder can also generate a third type of edge state whose site probability distribution is divided unevenly between two zigzag edges (a type III state). For type II and III states the variation of the site pseudospin [15] of each sublattice basis represents a topological kink [19] (the opposite zigzag edges consist of atoms from opposite sublattices). As the coordinate position varies from one edge to the opposite edge the chirality of the wave function changes from A- to B-carbon sites, i.e., the pseudospin rotates by $\pi$, as shown schematically in Fig. 3.

In the presence of electron-electron interactions, but without disorder, an excitation gap $\Delta$ separates the conduction and valence bands [11]. In this case there are no states inside the gap, but chiral zigzag edge states are present near the gap edges. For the occupied states near $E \approx -\Delta/2$ one of the chiral edge states of $\phi_L$ and $\phi_R$ is occupied by a spin-up electron while the other state is occupied by a spin-down electron, see Fig. 2 (for the unoccupied states near $E \approx \Delta/2$ it is the opposite). As $\phi_L$ and $\phi_R$ are spatially separated there is no repulsive energy, and these states have thus degenerate energy. This is the physical origin of edge antiferromagnetism [11, 2].

To investigate the formation of a gap-edge state with a fractional edge charge of $1/2$ one needs to include...
both electron-electron interactions and disorder in a self-consistent way. Such a model is described in the next section.

III. MODEL

We consider a periodic ZGNR with $N$ carbon atoms, length $L$ and width $w$. Electron-electron interactions play an important role in ZGNRs as it induces an energy gap $\Delta [1,11]$. The system becomes an insulator in the half-filled case. Electron-electron interactions are modeled through on-site repulsion $U$, whose value depends on the type of substrate on which the GNR is formed (a substrate can provide screening of electron-electron interactions). The zigzag edge magnetism is larger for stronger values $U$.

It is well-known that the range of an impurity potential is important in determining properties of the Dirac electrons in ZGNRs[20–22]. We model disorder by placing randomly $N_{\text{imp}}$ defects or impurities at carbon sites $\vec{R}_j$. We take the following simple discrete model for the disorder potential at lattice site $\vec{r}_i$

$$V_i = \sum_{j}^{N_{\text{imp}}} \epsilon_j e^{-|\vec{r}_i - \vec{R}_j|^2/d^2},$$  

where $d$ is the range of the potential. Note that when $d = 0$ the disorder potential is defined such that it is finite only for $\vec{r}_i = \vec{R}_j$ (in a continuous model this implies that the effective range is equal to the size of a carbon atom $\sim a_0$). When $d \sim a_0(d \gg a_0)$ the potential is short (long)-ranged (here $a_0 = 1.73a$ is the unit cell length of the ZGNR and $a = 1.42\text{Å}$ is the C-C distance). The strength of the potential $\epsilon_j$ is chosen randomly from the energy interval $[-\Gamma, \Gamma]$. The values of $\epsilon_j$ and $d$ depend on the type of charged impurities in the substrate and defects in graphene. Defects have $d \sim a_0$ while impurities have $d \gg a_0$. In the self-consistent Born approximation disorder strength is characterized by the parameter $\Gamma \sqrt{n_{\text{imp}}}$[23], where $n_{\text{imp}} = N_{\text{imp}}/N$ is the ratio between the numbers of impurities and total carbon atoms. The number of impurities or defects is also relevant in determining the strength of the disorder potential. Defects with a short-ranged potential are more relevant to the quantization of a fractional charge, as we will see below.

We include both electron-electron interactions and disorder in a tight-binding model at half-filling. The interplay between on-site repulsion $U$ and disorder can be treated using the self-consistent Hartree-Fock approximation (HFA). When $U = 0$ disorder can be treated exactly in this method while in the other limit, where disorder is absent, interaction effects can be represented well by the HFA, which widely used in graphene related systems[14][24][26]. Its results are consistent with those of density functional theory[1][11]. When both disorder and interactions are present the self-consistency provides an excellent approximation[27]. The total Hamiltonian in the HFA is

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} V_i c_{i\sigma}^\dagger c_{i\sigma}$$

$$+ U \sum_{i\sigma} (n_{i\uparrow} \langle n_{i\downarrow} \rangle + \langle n_{i\uparrow} \rangle n_{i\downarrow} - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle)$$

$$- \frac{U}{2} \sum_i (n_{i\uparrow} + n_{i\downarrow}),$$

where $c_{i\sigma}^\dagger$ and $n_{i\sigma}$ are the electron creation and occupation operators at site $i$ with spin $\sigma$. Since the translational symmetry is broken, the Hamiltonian is written in the site representation. In the hopping term the summation is over the nearest neighbor sites (the hopping parameter is $t \sim 3eV$). The eigenstates and eigenenergies are computed numerically by solving the tight-binding Hamiltonian matrix self-consistently. The self-consistent occupation numbers $\langle n_{i\sigma} \rangle$ in the Hamiltonian are the sum of the probabilities to find electrons of spin $\sigma$ at site $i$

$$\langle n_{i\sigma} \rangle = \sum_{E_{c} \leq E_{F}} |C_{i}(E_{\sigma})|^2.$$

The sum is over the occupied eigenstates energy $E_{\sigma}$ below the Fermi energy $E_F$. Note that $\{C_{i}(E_{\sigma})\}$ represents an eigenvector of the tight-binding Hamiltonian matrix with energy $E_{\sigma}$. For notational simplicity, we suppress its dependence on $E_{\sigma}$ from now on. We will define the weak disorder regime as the regime where the ratio between disorder strength and interaction strength is $\kappa \equiv \Gamma \sqrt{n_{\text{imp}}}/U \ll 1$. In this work the band is half-filled: the filling factor is $f = N_{c}/2N = 1/2$ ($N_{c}$ is the number of electrons). Below we use $U/t = 1$ unless stated otherwise.

IV. QUANTIZED FRACTIONAL CHARGE

Using the eigenvectors $\{C_{i}\}$ we define the fractional charge. If an electron is added into or removed from a gap state it can become fractionalized into charges located on the opposite zigzag edges. Suppose $\langle n_{i\sigma}^0 \rangle$ is the ground state site occupation number after an electron with spin $\sigma$ and energy $E$ is removed from a gap state represented by an eigenvector $\{C_{i}\}$. It can be written as

$$\langle n_{i\sigma}^0 \rangle = \langle n_{i\sigma} \rangle - |C_{i}|^2,$$

where $\langle n_{i\sigma} \rangle = \sum_{E_{c} \leq E_{F}} \langle n_{i\sigma} \rangle$ is the ground state site occupation number before the removal. The fractional boundary charge is defined using this $\langle n_{i\sigma}^0 \rangle$[28]:

$$q = \sum_{i} f_{i}(1 - \langle n_{i\sigma}^0 \rangle).$$

Here the average site occupation is set to $1$. For the fractional charge located on the left edge the sampling
function \( f_i \) is centered around the fractional charge. The fractional charge located on the right edge is similarly defined. The left and right fractional charges decay exponentially, and their overlap is negligible for a large width, \( w \). We can rewrite \( q \) as

\[
q = \sum_i f_i (1 - \langle n_i \rangle) + \sum_i f_i |C_i|^2 = \sum_i f_i |C_i|^2.
\]

(6)

Here, due to the random potential, the sum \( \sum_i f_i (1 - \langle n_i \rangle) \) vanishes since the site occupation number fluctuates around the mean value: \( \langle n_i \rangle = (n_{\text{imp}}) = 1 \pm \delta_i \), where \( \delta_i \) is a random number. The resulting fractional charge is equal to the total probability on the A- or B-carbon sites

\[
q_A = \sum_{i \in A} |C_i|^2, \quad q_B = \sum_{i \in B} |C_i|^2.
\]

(7)

Note that \( q_{A,B} \) depend on energy \( E_\sigma \). For type I either \( q_A \approx 1 \) or \( q_B \approx 1 \), and for type II \( q_A \approx 1/2 \) and \( q_B \approx 1/2 \). For a type III state \( q_A \) can deviate significantly from 1/2 and 1. For any type of gap state \( q_A + q_B = 1 \), which follows from the normalizations of the wave functions. In the following we will denote disorder-averaged values as \( \overline{q}_A \) and \( \overline{q}_B \).

It is important that the fractional charge is quantized to a high precision[28]. Several conditions must be met; 1) fractional charges must not overlap, 2) the fractional charge profile decays fast, and 3) the charge fluctuation must be small. Note that, the wider the ZGNR, the better the fractional quantization as the overlap between fractional charges on the left and right zigzag edges decreases. Also the edge wave functions decay exponentially[15], as their site probability distributions show, see below. The charge fluctuations will be estimated in Sec. 6.

V. SITE PROBABILITY DISTRIBUTION OF GAP-EDGE STATES

To study the shape of fractional charges of gap-edge states we need to investigate the properties of the site probabilities of their eigenvectors \( \{C_i\} \). We now investigate the site probability distribution of \( |C_i|^2 \) for various gap states. Its shape displays the amount of charge fractions located on the zigzag edges. For this purpose we need to analyze the site probabilities of gap-edge states of a single disorder realization (their energy spectrum is given in Fig. 4). The site probability distribution of two states near gap energy \( |E| \approx \Delta/2 \) are plotted in Fig. 5. One of these, shown in Fig. 5(a), is for \( n_{\text{imp}} = 0.01 \) and \( \Gamma = 0.5t \). The site probability decays along the perpendicular direction to the left of the zigzag edge. This state is chiral with significant probability only on A-carbon sites (type I). Another edge state is shown in Fig. 5(b). It is in the intermediate disorder regime with an impurity concentration \( n_{\text{imp}} = 0.1 \) and \( \Gamma = 0.5t \). Its site probability is significant on both the left and right zigzag edges.

However, their overlap is not negligible. Note that the chirality is opposite on the left and right zigzag edges.

There are also edge states in the gap, i.e., with energy \( |E| < \Delta/2 \). The site probability distribution of two gap-edge states in the intermediate disorder regime with \( n_{\text{imp}} = 0.01 \) and \( \Gamma = 2t \) are plotted in Fig. 6; these are both localized. The state shown in Fig. 6(a) is localized without fractionalization (type I). The site probability distribution of the other state shown in Fig. 6(b) is approximately fractionalized into two parts; each with an approximate value of 1/2 near the left and right zigzag edges (type II). Note also that their overlap is negligible (the overlap between fractional charges on the left and right zigzag edges decreases even further when the width of the ZGNRs is larger) A charge fractionalization of 1/2 is thus expected for this midgap state[5] (type II).

Another edge state (type III) is displayed in Fig. 7. Its site probability is distributed unevenly between the left and right zigzag edges. When a disorder potential breaks the inversion symmetry, the analysis of the Zak phase suggests that the boundary charge may deviate from integer and half-integer values[8, 11, 29]. Type II and III gap-edge states represent a topological kink. The site pseudospin value[15] rotates by approximately \( \pi \) as the coordinate position varies from one edge to the opposite edge[12]; therefore, the chirality of the wave function changes from the A- to B-carbon sites. An example is shown in Fig. 8. In interacting disordered ZGNRs, type II and III kinks coexist. A kink is rather similar to a
FIG. 5: (a) Site probability distribution of a type I edge state near the gap edge with energy $E/t = -0.107$ for $\Gamma/t = 0.5$, $d = 0$, and $n_{imp} = 0.01$. The green (blue) color represents the probability on A(B)-carbon sites. (b) The site probability distribution of a type II edge state outside the gap for $\Gamma/t = 0.5$, $d = 0$, and $n_{imp} = 0.1$. The energy is $E/t = -0.154$. In both figures $L = 125.4\,\text{Å}$, and $w = 7.1\,\text{Å}$.

FIG. 6: Site probability distribution of localized type I (a) and II (b) gap-edge states with energies $E/t = -0.071$ and $-0.024$, respectively. The parameters are $d = 0$, $n_{imp} = 0.01$, $\Gamma/t = 2.0$, $L = 125.4\,\text{Å}$, and $w = 7.1\,\text{Å}$.

soliton, which represents a domain wall connecting two different dimerized phases of a polyacetylene$^7$.

A short-ranged disorder potential affects the localization properties and changes the site probability distribution along the ribbon direction$^{21}$. The localization properties can be studied by computing the disorder-averaged value of the typical DOS (TDOS)$^{30}$. A finite TDOS in the limit $L \to \infty$ is an indication of delocalized states. The TDOS is shown in Fig. 9 as a function of energy, $E$, for $L = 307.4\,\text{Å}$. The TDOS is nearly zero in the interval $|E| \lesssim \Delta/2$ and displays little finite-size dependence on $L$, which suggests that the corresponding states are localized. The TDOS changes rapidly near the energy $E \approx \pm\Delta/2$, suggesting that the critical energy of the localization/delocalization transition is $E_c \approx \Delta/2$ (in the absence of disorder the states with energy $|E| > \Delta/2$ are delocalized). The ordinary one-dimensional localization theory$^{31}$ does not apply here$^{32}$.

It is interesting to note that most of the gap states are spin-split, i.e., singly occupied, see Fig.4 (a Mott-Anderson insulator has also singly occupied states$^{16}$). Some states are nearly spin degenerate, but their wave functions are different. In GNRs it appears that the gap states are spin-split when both zigzag edges and an external potential are present$^{4, 25}$. Conversely, the states far away from the gap (non-edge states) are nearly spin degenerate. Spin splitting may affect edge antiferromag-
FIG. 7: Site probability distribution of a localized type III gap-edge state with energy $E/t = 0.11$. The parameters are $d = 0, n_{imp} = 0.1, \Gamma / t = 0.5, L = 125.4\AA$, and $w = 7.1\AA$.

netism. Magnetic properties of the gap states will be given in Appendix.

VI. DISTRIBUTION OF NON-INTEGER EDGE CHARGES

The degree of type I, II, and III gap-edge states can be quantified by $q_A$ or $q_B$, defined in Eq. (7). The gap-edge states that are localized on the left zigzag edge have $1/2 < q_A < 1$ and $0 < q_B < 1/2$. (Conversely, the edge states localized on the right edge have $0 < q_A < 1/2$ and $1/2 < q_B < 1$). We perform disorder averaging over numerous disorder realizations to obtain the distribution of type I, II, and III states as a function of energy. These results may show at what energy the quantization of fractional charge may appear.

First, let us compute the disorder-averaged value $\overline{q}_A$ as a function of $E$. We count the left zigzag edge states in the energy interval $[E - \frac{\Delta E}{2}, E + \frac{\Delta E}{2}]$ and compute the average value $\overline{q}_A$. Fig. 9 displays this disorder-averaged value $\overline{q}_A$ as a function of $E$ for $d = 0$. For small values of $\Gamma$ we see that the value of $\overline{q}_A$ takes the minimum value for the midgap states (the energies of midgap states are in a small energy interval $[-\frac{\Delta E}{2}, \frac{\Delta E}{2}]$ around the Fermi energy $E_F = 0$). When both the left and right edge states are counted in each energy interval, the average value $\overline{q}_A$ is close to $1/2$, independent of $E$. For example, let us consider states near the gap edge $E = -\frac{\Delta E}{2}$. If one of them is localized on the left zigzag edge with edge charge $q_A \approx 1$ ($q_B \approx 0$), then there is also a state that is localized on the right edge with edge charge $q_B \approx 1$ ($q_A \approx 0$). The resulting mean value of $q_A$ is then $1/2$. Counting both the left and right edge states we find that states in the middle of the gap are mostly of type II while states near the gap edges are mostly of type I. At other energies type III states are distributed broadly between $E = 0$ and $\pm \Delta/2$.

Now we examine the distribution of these type I, II, and III states denoted by $P(q_A)$, which is the probability distribution function showing the number of the left and right gap-edge states that have a $q_A$ value in the interval $[q_A - \frac{\Delta q}{2}, q_A + \frac{\Delta q}{2}]$. As shown in Fig. 11, $P(q_A)$ is sharply peaked near $q_A = 1/2$ for small $\Gamma$ and $d = 0$. Let us explain qualitatively why $P(q_A)$ of gap-edge states is peaked at $q_A = 1/2$ in the weak disorder regime. This peak of $P(q_A)$ implies that there are numerous type II states in the gap in the presence of disorder. Two factors are important for this effect: (a) When $U \neq 0$ and $\Gamma = 0$...
FIG. 9: TDOS for disorder strength $\Gamma = 0.5t$. The number of disorder realization is $N_D = 800$, impurity concentration $n_{imp} = 0.01$, and range $d = 0$. The width and length of the ribbon are $w = 7.1\text{Å}$ and $L = 307.4\text{Å}$, respectively. The histogram energy interval is $\Delta E/t = 0.01$.

FIG. 10: Disorder-averaged value of $\overline{q}_A$ of the left edge states for the range $d = 0$. The parameters are $N_D = 1000$, $n_{imp} = 0.1$, $w = 7.1\text{Å}$, and $L = 125.4\text{Å}$. The histogram interval is $\delta E = 0.1\Delta$. Note that some states with energy outside of the energy gap are also included.

The band structure calculation shows that the states near the edges of the Brillouin zone $k = -\frac{\pi}{a_0}$ and $k = \frac{\pi}{a_0}$ are zigzag edge states, see Fig. 2. (b) A short-ranged disorder potential with $d \sim a_0$ couples these zigzag edge states $\phi_{R,\uparrow}$ and $\phi_{L,\uparrow}$ near $k = \frac{-\pi}{a_0}$ and $k = \frac{\pi}{a_0}$ since a significant wave vector transfer occurring in a backscattering is $|k - k'| \sim 1/a_0$\cite{21}. Moreover, when disorder is weak the DOS near the gap edges $E = \pm\Delta/2$ is sharply peaked. Because of this sharp peak, even a weak disorder potential can mix the type I left and right zigzag edge states and generate type II states with energy in the gap.

The disorder-averaged $\overline{q}_A$ and the distribution function $P(q_A)$ for $d = 2a_0$ are shown in Figs. 12 and 13. We see in Fig. 12 that for small values of $\Gamma$ and $E \approx 0$, the average value $\overline{q}_A$ of the left edge states is not as close to the quantized value $1/2$ as in the case of $d = 0$. Figure 13 shows the probability distribution function $P(q_A)$ for the left and right edge states combined. Note, near $q_A = 1/2$, this function is not as sharply peaked as the $d = 0$ case. This is because the strength of the disorder potential is not as strong as in the case of $d = 0$. 

FIG. 11: FIG. 11: Probability distribution of disorder-averaged $\overline{q}_A$ for the range $d = 0$ (normalized so that $\int_0^1 P(q_A)dq_A = 1$). Only the gap states are included in this analysis. The parameters are $N_D = 1000$, $n_{imp} = 0.1$, $w = 7.1\text{Å}$, and $L = 125.4\text{Å}$. The histogram interval is $\Delta q_A = 0.025$.

FIG. 12: As in Fig. 10 but for $d = 2a_0$.

FIG. 13: As in Fig. 11 but for $d = 2a_0$. 

VII. VARIANCE OF FRACTIONAL CHARGE

The previous result suggests that the midgap states may display quantization of fractional charge. The energy dependence of the average value $q_A$ suggests that if an electron with spin $\sigma$ is added into or removed from a midgap state in the energy interval $\left[-\frac{\delta E}{2}, \frac{\delta E}{2}\right]$, it can become fractionalized into two $1/2$ charges located on opposite zigzag edges. However, to qualify for charge fractionalization the variance of $q_A$ due to disorder must be negligible. We perform disorder averaging to compute the variance of $q_A$. The variances $(q_A - \frac{1}{2})^2$ for $d = 0$ and $2a_0$ are shown in Figs. 14 and 15, respectively. It is independent of the energy interval $\delta E$ for sufficiently small $\delta E$. The variance is minimum for the midgap states.

![FIG. 14: Variance as a function of $E$ for $d = 0$. The parameters are $N_D = 1000$, $n_{imp} = 0.1$, $w = 7.1\text{Å}$, and $L = 125.4\text{Å}$. $\delta E = 0.1\Delta$.](image1)

![FIG. 15: Variance as a function of $E$ for $d = 2a_0$. Other parameters are the same as in Fig. 14.](image2)

FIG. 14: Variance as a function of $E$ for $d = 0$. The parameters are $N_D = 1000$, $n_{imp} = 0.1$, $w = 7.1\text{Å}$, and $L = 125.4\text{Å}$. $\delta E = 0.1\Delta$.

FIG. 15: Variance as a function of $E$ for $d = 2a_0$. Other parameters are the same as in Fig. 14.

![FIG. 16: Variance at $E = 0$ as a function of $\Gamma$ at $n_{imp} = 0.1$ for $d = 0$ and $2a_0$ (dotted line is a guide to the eye). Other parameters are the same as in Fig. 14.](image3)

![FIG. 17: Variance at $E = 0$ as a function of $U$ at $n_{imp} = 0.1$ for $d = 0$ and $2a_0$ (dotted line is a guide to the eye). The value of $\Gamma$ is $0.3t$. Other parameters are the same as in Fig. 14.](image4)

FIG. 16: Variance at $E = 0$ as a function of $\Gamma$ at $n_{imp} = 0.1$ for $d = 0$ and $2a_0$ (dotted line is a guide to the eye). Other parameters are the same as in Fig. 14.

FIG. 17: Variance at $E = 0$ as a function of $U$ at $n_{imp} = 0.1$ for $d = 0$ and $2a_0$ (dotted line is a guide to the eye). The value of $\Gamma$ is $0.3t$. Other parameters are the same as in Fig. 14.

The results of Figs. 16 and 17 suggest that the variance tends to decrease further when $\Gamma$ is reduced below $\Gamma = 0.1t$. In the weak disorder regime the variance of the $1/2$ fractional charge is smaller for $d = 0$ than that of $d = 2a_0$. However, when $\kappa > 0.1$ the opposite is true.

The results of Figs. 14 and 15 show that the charge variance of the midgap states is small in the weak disorder regime $\kappa = 0.33\Gamma/U \ll 1$ (with $\sqrt{n_{imp}} = 0.33$). The variance reduces rapidly as $\Gamma$ decreases: for $d = 0$ its magnitude is reduced to 0.004 at $\Gamma = 0.1t$. In the weak disorder regime the variance of the $1/2$ fractional charge is smaller for $d = 0$ than that of $d = 2a_0$. However, when $\kappa > 0.1$ the opposite is true.

The results of Figs. 16 and 17 suggest that the variance tend to decrease further when $\Gamma$ is reduced below $\Gamma = 0.1t$ (note that reducing the value of $n_{imp}$ has similar effects of reducing $\Gamma$). However, there will be fewer midgap states in the histogram interval. To circumvent this problem a larger value of the ribbon length $L$ is needed to include more midgap states in the histogram energy interval (we have verified numerically that there are indeed more midgap states when the length is increased to $L = 307.4\text{Å}$). However, disorder averaging and computing the variance for such a system is computationally demanding. Nonetheless, our numerical work indicates that, when disorder is weaker than on-site repulsion, the charge fractionalization of the midgap state is robust. We believe that the accuracy of quantization of fractional charge in the limit $\kappa \to 0$ is related to the presence of...
particle-hole symmetry of the underlying band structure in the absence of disorder (particle-hole symmetry also plays an important role in polyacetylene\cite{7}). We do not expect that the quantization of fractional charge is precise for long-ranged disorder potentials with $d \gg a_0$ since the coupling between non-edge states can be substantial (see the argument given in Sec. 5).

VIII. SUMMARY

We have investigated the properties of the gap-edge states of half-filled interacting disordered zigzag graphene nanoribbons. In disorder-free GNRs antiferromagnetic coupling between well separated zigzag edges is detrimental to formation of fractional edge charges. However, disorder may increase the coupling between the edges, and this may favor the formation of midgap states with a fractional edge charge.

Using a self-consistent Hartree-Fock mean field approach we find that the variance of the fractional charge of the midgap states is determined by the competition between the strength of disorder, impurity range, and on-site $U$. In weak disorder regime $\kappa \ll 1$ and for short-ranged potentials the charge variance of these midgap states is small and a well-defined quantized fractional charge of 1/2 can be formed. Our numerical result suggests that, in the weak disorder regime, the quantized fractional charge becomes more precise as the values of $\Gamma$, $n_{\text{imp}}$, and $d$ decrease. We believe that the accuracy of quantization of fractional charge in the weak disorder limit $\kappa \to 0$ is related to particle-hole symmetry of the underlying bandstructure in the absence of disorder. For longer range impurities the variance is larger and it decreases more slowly as $\kappa \to 0$.

Our work shows that the role of disorder is important in mitigating the effect of antiferromagnetic coupling on the midgap states. The coupling of the left and right edge states by a short-ranged potential is important for this effect. Other gap states with $E \neq 0$ have larger charge fluctuations than those of the midgap states. In addition, we find that numerous gap-edge states become spin-split and singly occupied (note that the Mott-Anderson insulator also has spin-split singly occupied states).

It will be interesting to develop a field theoretical model in the presence of disorder\cite{12, 13}. The calculation of the distribution of type I, II, and III gap states as a function of energy and disorder strength is desirable. There has been considerable experimental effort to measure edge states in ZGNRs. The measurement of the differential conductance in atomically precise ZGNRs\cite{34}, using a scanning tunneling microscopy\cite{35} may provide rich information on the distribution of edge charges.

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Appendix A: Magnetic properties of gap-edge states

Let us investigate how gap-edge states contribute to magnetic properties of ZGNRs. The edge magnetism decreases as $\Gamma$ changes. The quantitative analysis the magnetization at the $i$th site may be obtained by averaging over many disorder realizations. The disorder-averaged value of the site magnetization is defined by

$$\langle s_i \rangle_{\Gamma} = \langle \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle \rangle_{\Gamma},$$

where the overline indicates a disorder-averaged value. Note that type I, II, and III gap-edge states contribute to the occupation numbers $\langle n_{i\sigma} \rangle$, in addition to non-edge states, see Eq.(\ref{eq3}). However, the contribution from the gap-edge states is dominant.

![FIG. 18: Disorder-averaged spin value per edge site vs. $\Gamma$. The parameters are $d = 0$, $n_{\text{imp}} = 0.1$, $L = 125.4\text{Å}$, and $w = 7.1\text{Å}$. The number of disorder realization is $N_D = 10$.](image_url)

In Fig.18 the disorder-averaged value of the edge magnetization per site $\langle s_i \rangle_{\Gamma}$ is plotted as a function of the disorder parameter $\Gamma$. At $\Gamma = 0$ type I edge states contribute to a finite edge magnetization and the expectation value of the edge magnetization per site on the boundaries is $\langle s_i \rangle = \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle = \pm 0.24$. The value $\langle s_i \rangle$ decays into the ZGNR over several carbon-carbon distances. However, along the zigzag edges, $\langle s_i \rangle$ is uniform. The edge magnetization decreases with increasing $\Gamma$. Our results show that, in addition to the proliferation of type II gap-edge states (topological kinks), the partial spin polarization of the type I and III gap-edge states on each zigzag edge plays a role in this reduction. Note that the edge antiferromagnetism persists even in the presence of a substantial amount of disorder, albeit small.
Consider a graphene sublattice basis, consisting of two carbon atoms A and B. Suppose that the probability amplitude to find an electron on A and B atoms is $u_{1k}$ and $u_{2k}$, respectively. This can be represented as a spinor $\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$. Using this spinor, the components of the pseudospin matrices $\sigma_x, \sigma_y, \sigma_z$ are:

\[ Z = \sum_{i \in \text{occ}} \int_{B.Z.} \langle u_{ik}|\nabla_k u_{ik} \rangle \cdot dk, \]

where $|u_{ik}\rangle$ is the periodic part of the Bloch wave function of the $i$'th band and the sum is over the occupied bands.

A kink is a one-dimensional topological object with a phase change of $\pi$ when the position coordinate varies through the kink (the crucial feature is that it does not matter how the phase changes as the coordinate changes). In our case the phase is the angle of the pseudospin vector.

In graphene systems only a short-ranged disorder potential is effective in inducing localization. Depending on the electron energy, perfectly conducting channels may appear. These properties are in sharp contrast to those of ordinary one-dimensional localization theory.

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\[ Z = \sum_{i \in \text{occ}} \int_{B.Z.} \langle u_{ik}|\nabla_k u_{ik} \rangle \cdot dk, \]

where $|u_{ik}\rangle$ is the periodic part of the Bloch wave function of the $i$'th band and the sum is over the occupied bands.

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