Topological gap states of semiconducting armchair graphene ribbons

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In semiconducting armchair graphene ribbons a tensile strain can induce pairs of topological gap states with opposite energies. Near the critical value of the deformation potential these kink and antikink states become almost degenerate with zero energy and have a fractional charge of one-half. Such a semiconducting armchair ribbon represents a one-dimensional topological insulator with nearly zero energy end states. Using data collapse of numerical results we find that the shape of the kink displays an anomalous power-law dependence on the width of the local lattice deformation. We suggest that these gap states may be probed in optical measurements. However, “metallic” armchair graphene ribbons with a gap induced by many-electron interactions have no gap states and are not topological insulators.

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FIG. 1: (a) Armchair ribbon with length \( L_x \) and transverse width \( L_y \). A and B denote carbon atoms. In the stripe region tensile strain that has reflective symmetry about the \( x \) axis is applied along the ribbon direction. (b) In the stripe region the pseudospin density \( \Sigma(y) \) of a gap state rotates about the \( y \) axis with only \( x \) and \( z \) components. It represents a kink. Outside the stripe region the length of the pseudospin goes slowly to zero.

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Introduction.- Recently a rapid progress has been made in the fabrication of armchair graphene ribbons[1, 2]. They have a great potential for spintronic applications, where electronic many-body interactions may play a significant role[3, 4]. Armchair ribbons may also provide numerous interesting issues in fundamental physics, such as topological objects. By perturbing the graphene lattice and the tunneling coupling constants one can give rise to effective gauge and scalar fields[5] that generate solitonic objects[6, 7]. Generation mechanism of gap and vortices is at the center of the study of graphene material[8, 9, 10, 11, 12, 13].

According to tight-binding calculations an armchair ribbon has a gap and is semiconducting when the transverse width is \( L_x = (3M + 1)a_0 \) or \( 3Ma_0 \), where \( a_0 \) is the unit cell length and \( M \) is an integer. But when \( L_x = (3M + 2)a_0 \) the armchair ribbon has no gap and is metallic. However, the inclusion of many-electron interactions produces a gap[6]. It is unclear whether these armchair ribbons are topological insulators.

In polyacetylene a fermion mass potential produces a gap, and a twist in this scalar potential produces a zero energy soliton with mixed chirality and fermion fractionalization[9, 10, 12, 13]. Similarly, a chiral gauge field can simulate the effects of armchair edges and can open a gap. However, the Berry phase is absent in armchair ribbons (this can be shown by integrating the tight-binding wavefunction over the Brillouin zone). It is thus unclear whether zero energy solitons can exist in such a case, i.e., whether the armchair ribbon represents a one-dimensional topological insulator[14]. The purpose of the present paper is to find a distortion of the chiral gauge field that will produce a kink, antikink, soliton, and charge fractionalization, as the twist of a scalar potential does in polyacetylene.

Topological properties can be displayed in the variation of the pseudospin. Graphene armchair ribbons consist of A-carbon and B-carbon atoms, see Fig. 1. The sublattice spin is defined so that when an A-carbon atom is occupied its value is ’up’ and when a B-carbon atom is occupied it is ’down’ (massless fermions can either have their sublattice spin pointing along their direction of wave vector or opposed to it). The valley spin can be defined similarly. In an armchair ribbon the sublattice and valley degree of freedom mix, and their spins can be put together using 4 × 4 pseudospin matrices[18]

\[
\tilde{\Sigma} = I \otimes \tilde{\sigma}, \tag{1}
\]

where \( \tilde{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \) are Pauli spin matrices. We define the pseudospin density \( \tilde{\Sigma}(y) = \Psi^* (\vec{r}) \tilde{\Sigma} \Psi (\vec{r}) \), where \( \Psi (\vec{r}) \) is an eigenstate of the Hamiltonian. A quantum state with finite occupation probabilities only on A-carbon (’up spin’) atoms to the left of the stripe and only on B-carbon (’down spin’) atoms to the right would constitute a topological object called a kink.

We find that the tensile strain with reflective symmetry about the \( x \) axis can generate a pair of gap states

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The tensile strain will induce changes of C-C bonds along the ribbon direction, in addition to changes of the C-C bonds along other directions. In the effective mass approximation \[ V_f = \frac{eA_{1,0}v_F}{c} > 0 \] and has units of energy. Increasing \( V_f \) corresponds to weakening of the C-C bonds.

An eigenstate of the total Hamiltonian \( H_0 + V \) can be solved as a linear combination of the basis states \( \psi_{s,k}^\circ(\vec{r}) \) that are solutions of the Dirac Hamiltonian \( H_0 \) of the armchair ribbon: \( \Psi(\vec{r}) = \sum_{s,k} C_{s,k} \psi_{s,k}^\circ(\vec{r}) \), where \( C_{s,k} \) are the expansion coefficients of the lowest energy conduction subband \((s = 1)\) and highest energy valence subband \((s = -1)\). The momentum space interval \(-k_c \leq k_y \leq k_c\) is divided into \( N \) grid points (periodic boundary condition is used with \( k_c = \frac{\pi}{L_y} N \), where \( N \) is an odd number and \( L_y \) is the length of the ribbon). The results presented below are obtained by this method, or by a tight-binding calculation including many-electron interactions.

Kink, antikink, and soliton of semiconducting armchair ribbons.- We show that kink and antikink states can exist in the gap. We solve the effective mass Hamiltonian \( H_0 \) in the presence of the deformation potential \( V_f \) and find that the gap states \( \Psi_1 \) and \( \Psi_{-1} \) are present with opposite energies, see in Fig.2. The wave-function components of \( \Psi_1 \) and \( \Psi_{-1} \) are related through chiral operation: \( \Psi_1 = (\Psi_A, \Psi_B, \Psi_A', -\Psi_B')^T \), and \( \Psi_{-1} = (\Psi_A, -\Psi_B, \Psi_A', \Psi_B')^T \), where the \( A \) and \( B \)-components satisfy \( \Psi_A(y) = -\Psi_B(-y) \) and the overall phase factors are removed. The probability density of an antikink state \( \Psi_{-1} \) is shown in Fig.3(a). We have computed the angle \( \theta \) between the \( x \) axis and \( \Sigma(y) \), see Fig.3(b). (The \( y \) component of the pseudospin density is \( \Sigma(y) = 0 \).) The magnitude of the pseudospin density \( |\Sigma(y)| \) decays exponentially, see Fig.3(b). In this exponentially decaying region the angle is well approximated by \( \theta(y) = \pm v \tanh(\alpha y) \). Here the minus sign corresponds to the antikink state while the plus sign corresponds to the kink state. In the strong coupling region \( V_f > 2 \) eV the amplitude is \( v \approx \pi/2 \).

The energy of a kink is determined by the values of \( v \) and \( \alpha \), which are related to the physical properties of...
The kink, namely its amplitude and the inverse size. For \( V_f/V_c < 2 \) our numerical energies agree approximately with the analytical result

\[
E_{-1} = \frac{\Delta}{2} - \frac{8}{3} (\nu \xi)^v \quad \text{and} \quad E_1 = -\frac{\Delta}{2} + \frac{8}{3} (\nu \xi)^v.
\]

In Fig 3(c) the energy correction \( \frac{\Delta}{2} - \frac{8}{3} (\nu \xi)^v \) is shown and compared with the numerical result. The parameter \( \xi = 0.150eV\AA \) can be determined by fitting the analytical energy \( E \) to the numerical energy. The deviation between the numerical and the analytical energies is the largest near the critical value \( V_c = 2.51eV \), which is the maximum value of strength of the deformation potential \( V_c \approx t \). Using a tight-binding approach we include the effects not included in our model, and find more than two gap states.

Near the maximum value of strength of the deformation potential \( V_c \), two nearly zero energy kink and antikink gap states \( \Psi_1 \) and \( \Psi_{-1} \) exist, see Fig 2(b). We will call these kink and antikink solutions. Their probability densities are similar to the one shown in Fig 3(a). These modes are nonchiral. The usual charge counting argument gives that the sum of the charges of the two gap states is one, implying that each has a fractional charge of one half. In fact, they are similar to the nearly degenerate end states of a one-dimensional topological insulator with a finite length, despite that the Berry phase is zero in the unperturbed semiconducting armchair ribbon.

**Anomalous scaling.**- We find that the field \( \theta(y) \) satisfies near \( y = 0 \) the following finite-size scaling relation as a function of the width \( w \) and the momentum cutoff \( k_c \)

\[
\frac{\theta(y)}{\chi^{\beta}} = -A\tilde{y},
\]

where \( \tilde{y} = \frac{yk_c}{2\pi} \) is the dimensionless coordinate and \( \chi = \frac{w}{\xi v} \) is the dimensionless width. From our data collapse, shown in Fig 3(d), and the scaling relation Eq (6) we find that the slope of \( \theta(y) \) displays an anomalous dependence on the width \( w \):

\[
\nu \alpha = A(V_f)k_c\frac{w k_c}{2\pi \xi v} \chi^{\beta}
\]

with the numerical value of \( \beta = 0.203 \). The anomalous exponent \( \beta = 0.27 \) may also be measured experimentally near \( V_f = 2eV \), where the amplitude is \( v \approx \pi/2 \). The value of the slope \( \nu \alpha \) can be determined from the measured values of the kink and antikink energies, given by Eq (6). Then a plot of the slope \( \nu \alpha \) as a function of the width \( w \) would determine the exponent. Also we find that the constant \( A \) increases as the strength of the deformation potential increases. However, as the transverse length \( L_x \) increases, \( A \) is approximately unchanged.

**Metallic armchair ribbon.**- The inclusion of many-electron interactions produces a gap in a metallic armchair ribbon \( \Psi_0 \). To assess qualitatively the interplay between the chiral vector potential and many-electron interactions we model it in a half-filled Hubbard model of a honeycomb lattice. Applying the unrestricted Hartee-Fock method near \( V_f = V_c \), where the C-C bonds are cut, we find a significant gap when the on-site interaction \( U \) is sufficiently large but no gap states (localized states). This is because the on-site interaction \( U \) shifts zero-energy states into the energy continuum where wavefunctions become delocalized. The Kekule-like distortion, described by \( \gamma \Delta \), also produces a gap in the metallic armchair ribbon. However, adding a chiral vector potential to it does not generate gap states. The metallic armchair ribbon is thus not a topological insulator. In contrast, gap states exist for the semiconducting armchair ribbon when \( U \) is not too large.

**Discussions and summary.**- The optical transition from a kink \( \Psi_1 \) to antikink \( \Psi_{-1} \) has a substantial optical strength \( \left| \langle \Psi_1 | j_y | \Psi_{-1} \rangle \right|^2 \) when photons are polarized along the armchair ribbon (\( j_y \) is the current operator). It decreases as \( V_f \) increases. However, when photons are polarized along the transverse direction of the ribbon it is zero since \( \left| \langle \Psi_1 | j_x | \Psi_{-1} \rangle \right|^2 = 0 \). The Coulomb self-energy and vertex corrections renormalize the bare transition energy upwards about 15%. Optical resonant oscillations between \( \Psi_1 \) and \( \Psi_{-1} \) would be also interesting to observe near \( V_f \).

We have investigated gap states of semiconducting armchair ribbons within an effective mass Hamiltonian.
model, supplementing it with a tight-binding calculation including many-electron interactions. A chiral deformation can form kink and antikink pairs with opposite energies. Although the Dirac singularity at zero energy is destroyed by the gap the zero energy solitons, with a fractional charge of one half, can exist at the critical value of the deformation potential. Semiconducting armchair ribbons can thus represent a one-dimensional topological insulator. In contrast "metallic" armchair ribbons can thus be used to identify the local density of states of the topological gap states. Fractionally charged fermions can also exhibit non-Abelian braiding statistics.

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