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Edge states in graphene-like systems

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ABSTRACT

The edges of graphene and graphene like systems can host localized states with evanescent wave function with properties radically different from those of the Dirac electrons in bulk. This happens in a variety of situations, that are reviewed here. First, zigzag edges host a set of localized non-dispersive state at the Dirac energy. At half filling, it is expected that these states are prone to ferromagnetic instability, causing a very interesting type of edge ferromagnetism. Second, graphene under the influence of external perturbations can host a variety of topological insulating phases, including the conventional quantum Hall effect, the quantum anomalous Hall (QAH) and the quantum spin Hall phase, in all of which phases conduction can only take place through topologically protected edge states. Here we provide an unified vision of the properties of all these edge states, examined under the light of the same one orbital tight-binding model. We consider the combined action of interactions, spin–orbit coupling and magnetic field, which produces a wealth of different physical phenomena. We briefly address what has been actually observed experimentally.

1. Introduction

Graphene has been the most studied material of the last decade. Its extraordinary electronic and mechanical properties came as a great surprise: the existence of stable two dimensional crystals was customarily dismissed, and surfaces had been identified as the source of reduction of electronic mobility, due to defects and adsorbate trapping. The age of graphene was initiated by the observation of the field effect transistors [1], and more strikingly the quantum Hall effect [2,3], a phenomena that had only been observed in high mobility semiconductor heterostructures [4].

Graphene is a two dimensional lattice of carbon atoms that form a honeycomb lattice, that can also be described as a triangular lattice with a two atom basis, displayed with different colors in Fig. 1. This makes of the graphene honeycomb lattice a bipartite lattice, a fact that strongly influences its electronic properties. The electronic properties of graphene can be described in terms of a very elegant and simple picture [5,6] by means of the Dirac equation. Close to the Fermi energy, electrons in graphene behave as two dimensional relativistic massless particles, the so-called Dirac electrons. The energy bands are linear, $E_{\pm} = \pm\hbar v_F|\vec{k}|$, so that the three dimensional plot of these two dimensional bands produces the so-called Dirac cones. The Brillouin zone associated to the honeycomb lattice is also hexagonal, and has a copy of these Dirac bands, located at the corners of the hexagon. Only two of these so-called valleys are actually non-equivalent. As a result, electrons in graphene have an additional isospin, the valley.

All these properties are also expected for a wider class of material systems, the graphene-like materials, that can also be described in terms of electrons moving in a honeycomb lattice with just one orbital per site. An incomplete list of graphene-like materials includes Silicene [7], Germanene [8], Stanene [9], metallic organic framework [10], hydrogenated Bi(1 1 1) [11], and artificial graphene lattices [12].

The purpose of this paper is to review what is known about the fate of the Dirac electrons at the edges, the boundaries of these otherwise endless two dimensional crystals. In some instances Dirac electrons simply scatter at the edges but, very often, graphene hosts edge states, i.e., states whose wave function are evanescent in the direction perpendicular to the edge, and itinerant in the parallel direction. Their energies are at, or close to, the Dirac point, and very often their wave functions have peculiar properties, such as sublattice polarization, spin polarization or net spin current, just to mention a few. Edge states are particularly important when graphene is driven into what nowadays are known as topological insulator phases [14]. Historically, the first example of this phase is associated to the quantum Hall effect (QHE) [4], observed in high mobility two dimensional electron gases in semiconductor heterostructures. In these systems, application of a sufficiently large

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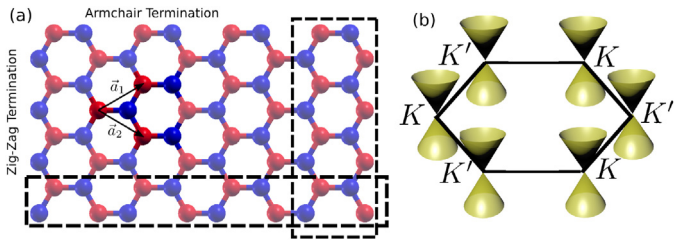

Fig. 1. (a) Honeycomb lattice showing two types of edge, zigzag and armchair. The two triangular sublattices, *A* and *B*, are displayed with fake color, red and blue. The vectors of the Bravais lattice are also shown. (b) Brillouin zone associated to the honeycomb lattice, including the plot of the two energy bands forming Dirac cones in the neighborhood of *K* and *K′* points (see text). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

magnetic field produces a discrete spectrum of Landau levels (LL) in the bulk states. This leads to an insulating state when the Fermi energy lies in between the LL. Importantly, in that situation the edges host chiral (or unidirectional) states that are ideal quantum conductors [15,16], and are responsible for the perfect quantization of the Hall conductance [4].

Soon after the discovery of the QHE, it was shown by Thouless and coworkers (TKNN [17]) that the Hall conductance could be expressed, using the conventional linear response theory, in terms of a topological invariant [17,18], the so-called Chern number $\mathcal{C}$, associated to the Berry curvature of wave functions of the bulk states.

The prediction of other insulating phases with quantized edge transport due to topological order without a net magnetic field is one of the greatest successes of modern condensed matter theory. This includes the quantum spin Hall (QSH) [19,20], and the quantum anomalous Hall (QAH) phases, proposed in a seminal paper by Haldane [21] where he showed how spinless fermions moving in a honeycomb lattice exposed to a periodic magnetic field with no net flux would display quantized Hall conductance, with topologically protected edge states.

The QSH phase was proposed by Kane and Mele [19,20]. They found that intrinsic spin–orbit coupling would open a gap in graphene with non-trivial topological order that would come accompanied by spin filtered [19] edge states robust with respect to time reversal perturbations. Interestingly, the description of electrons with spin–orbit coupling in graphene was mathematically identical to two independent copies of the Haldane model, one per spin. They also introduced a Z_2 topological classification [20] of time-reversal invariant two dimensional systems, analogous to the TKNN classification of quantum Hall states.

Subsequent computational work [22,23] showed that the magnitude of the intrinsic spin–orbit coupling in graphene was so small that would render the observation of the QSH phase almost impossible. However, there are graphene-like materials, such as silicene and other group IV honeycomb crystals, for which the Kane Mele model applies [24] and for which these predictions are relevant. More importantly, there is quite strong experimental evidence that the QSH phase has been observed both in HgTe quantum wells [25] and inverted InAs/GaSb quantum wells [26], both theoretically predicted to be QSH insulators [27,28]

The role of Coulomb interactions can also affect dramatically the properties of some of these edge states, in particular, whenever edge states produce a large density of states at the Fermi energy, that makes them prone to Stoner instabilities. This is the case of zigzag edge states for which ferromagnetic order is expected [29–38]. The interplay between this magnetism, spin–orbit interactions [39–42] and the quantum Hall phases [43] is a very fascinating area of research that we also review here.

Apart from the previous examples, interfacial effects can also create topologically protected states. Some examples are driven by domain boundaries between gapped graphene [44,45], local electric edge fields [46,47] or interfaces between antiferromagnetic graphene and a superconductor [48].

The rest of this review is organized as follows. In Section 2 we review the tight-binding model that describes both the 2D and edge states in graphene, including the spin–orbit coupling and coupling to the magnetic field, responsible of the quantum spin Hall and quantum Hall phases. In Section 3 we review the properties of the zigzag edge states, including their connection with the bipartite character of the honeycomb lattice as well as the ferromagnetic order associated to Coulomb interactions. In Sections 4, 5 and 6 we review the quantum Hall, quantum anomalous Hall and quantum spin Hall edge states, respectively. In Section 7 we review the effect of Coulomb interactions on the spin-filtered edge states in graphene. In Section 8 we briefly review the experimental situation and in Section 9 we wrap up with some general conclusions.

2. Tight binding model for graphene and graphene-like materials

A material is said to be graphene-like if its quantum states can be described in terms of a tight-binding model that describes electrons hopping in a honeycomb lattice with a single state per site. In the case of graphene, Silicene, etc., the site would be a group *IV* atom, and the state would be p_z orbital. Within this model, electrons can hop to their first neighbor atoms, with a hopping amplitude *t*, that takes a value of $t \simeq 2.7$ eV [5] in the case of graphene. The tight-binding approach can also include the effect of magnetic fields by means of the so-called Peierls substitution. Basically, the effect of the magnetic field consists on multiplying by a phase the hopping integrals $t_{\alpha,\beta} \rightarrow t_{\alpha,\beta} e^{i\phi_{\alpha,\beta}}$ where

$$\phi_{\alpha,\beta} = \frac{e}{\hbar} \int_{\alpha}^{\beta} \vec{A} \cdot d\vec{r} \tag{1}$$

and $\vec{A}$ is the vector potential applied to the system.

2.1. Bloch and Dirac Hamiltonians

The honeycomb lattice of bulk graphene can be treated as two interpenetrating triangular lattices, that we label as *A* and *B* and assign them the red and blue color in Fig. 1. Thus, the honeycomb lattice is a triangular lattice with two atoms per unit cell that naturally leads, within the simple TB model, to a Bloch Hamiltonian of dimension two:

$$\mathcal{H}_0(\vec{k}) = \begin{pmatrix} \frac{\Delta}{2} & tf(\vec{k}) \\ tf^*(\vec{k}) & -\frac{\Delta}{2} \end{pmatrix} \tag{2}$$

where *t* is the first neighbor hopping, Δ is the so-called mass term that is present whenever there is a sublattice symmetry breaking perturbation and it is assumed to vanish in the case of freestanding graphene, $f(\vec{k}) = 1 + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2}$ is the form factor associated to first neighbor hopping in the honeycomb lattice, and $\vec{a}_1 = \frac{a}{2}\left(\sqrt{3}, 1\right)$, $\vec{a}_2 = \frac{a}{2}(\sqrt{3}, -1)$ where *a* is the unit cell spacing, which coincides with the second neighbor distance and it satisfies the relation $a = \sqrt{3} a_{CC}$ with the first neighbor distance. The resulting energy bands, $\epsilon_{\pm}(\vec{k}) = \pm\sqrt{|\Delta/2|^2 + |tf(\vec{k}|^2}$ are shown in Fig. 1b for the $\Delta = 0$ case relevant for graphene, and feature the so-called Dirac cones at the corners of the hexagonal Brillouin Zone. Valence and conduction band meet at the so-called Dirac point, which coincides with the Fermi energy at half filling. At this point we introduce the concept of sublattice as a pseudo spin degree of freedom. For