Trigonal distortion of topologically confined channels in bilayer Graphene.

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In this work we show that the trigonal warping of the electronic bands in bilayer graphene dramatically modifies the behavior of the topologically confined one-dimensional modes due to an inhomogeneous bias that changes sign across a channel. Up to four zero modes are present, depending on the orientation of the channel, these zero modes are related with a fractionalization of the topological charge due to the trigonal warping.

Intervallay transport and coherence in graphene-based systems is an appealing subject, due to both the intriguing physical phenomena that it entails and the great potential that it displays from an applied perspective. Among others, valley-dependent resistance effects and valley-filter devices, have been proposed in several contexts. 1,2 Importantly, basic theoretical estimates prove that such devices are well within current or soon to come technological capabilities.

Bilayer graphene (BLG), two coupled graphene layers, has an electronic structure remarkably different from graphene. Unlike single layer graphene (SLG) the electronic dispersion near the K points is parabolic and a gap can be induced by applying an external electric field perpendicular to the layers.

The coherence between carriers on each of the layers of BLG opens up an additional effect. It has been shown3,4 that biased BLG is characterized by non-trivial topological structure associated with the behavior of the pseudo-spin degree of freedom. This topological property leads to several fascinating predictions5–7. In particular it can be shown that confined gapless bands can be induced in BLG by applying an inhomogeneous bias that changes sign across a channel. In this way a one dimensional confined structure associated with the behavior of the pseudo-spin degeneracy of freedom is enhanced in wide domain walls however in such a case more branches can be found inside the gap. These other branches are localized within the domain wall and are of the same nature that the ones obtained in modelling a contact of two materials with inverted bands. They are present regardless of the trigonal warping.

A low energy reduced (dimensionless) Hamiltonian for the stacked AB bilayer, including the interaction responsible for the trigonal warping and an external field can be written as:8

$$\mathcal{H} = \varepsilon_0 \left( k^2 - sk_+ \right) - V$$

where $$\varepsilon_0 = (\gamma_3/\gamma_0)^2/2 \approx 4 \text{meV}$$, the units of k are $$k_0 = 2\gamma_3\gamma_1/(\sqrt{3a+h})$$, where we have used $$\gamma_0 = 3.16 \text{eV}$$, $$\gamma_1 = 0.39 \text{eV}$$, and $$\gamma_3 = 0.315 \text{eV}$$, and a = 0.246 nm is the lattice constant. Additionally we employed the artificial parameter s to include continuously the effect of trigonal warping from s = 0, where it is strictly absent, to s = 1 where it acquires its full value. The symbol $$k_\pm$$ stands for $$\xi k_x \pm ik_y$$, where $$\xi = 1$$ for $$\mathcal{H}$$ around K’ and $$\xi = -1$$ for K. We can also write the Hamiltonian in the following manner ready to assess topological invariants.

$$\mathcal{H} = \varepsilon_0 \mathbf{g}(k_x, k_y) \cdot \sigma,$$

where $$\mathbf{g}(k_x, k_y) = g_0(k_x, k_y) + sg_w(k_x, k_y)$$. In this equation $$g_0(k_x, k_y) = (k_x^2 - k_y^2, 2\xi k_x k_y, V)$$ and $$g_w(k_x, k_y) = (-k_x, k_y, 0)$$ where $$\sigma$$ are the Pauli matrices. $$g_w$$ is the part responsible for the trigonal warping. The topological invariant $$N_3$$ which determines K points is the winding number of the mapping of the sphere $$\sigma_2$$ around the K points to the 2-sphere of the unit vector $$\mathbf{g} = g/|g|$$ is:9

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The topological charge $N_3$ can be found with no difficulties from the equations given above. It turns out that $N_3 = \xi \text{sign}(V)$, independently of $s$. Despite this invariance the effects of trigonal warping are far from trivial. The trigonal warping splits the Fermi point, $K$ into four pockets: three Dirac points away from the $K$ point with charge $+\xi$ and the $K$ point with charge $-\xi$. A reversal of the bias voltage over a region of space is therefore associated with a change of $|\delta N_3| = 2$ for each valley and spin. This gives the minimum number of zero-energy left movers minus right movers, there should be then at least two branches per valley per spin that cross the Fermi-level.

The special case of $s = 0$ (neglecting the effects of trigonal warping) can be solved analytically in terms of hypergeometric functions. However, the inclusion of trigonal warping makes it more convenient to pursue a numerical approach.

The resulting eigenproblem can be solved independently for each value of $p_y$. For a given value of $p_y$ we discretize the axes across the wall and perform a numerical diagonalization of the resulting Hamiltonian. The results are listed in Fig. (2) for several values of the angle $\vartheta$ ($V_0 = 0.5$). It is evident that despite the severe deformation suffered by the bands, there are still two bands that cross the Fermi level in each case. The velocity is heavily distorted and the trigonal distortion induces local energy extrema that are not present in the isotropic case. The location and depth of those valleys formed by trigonal distortion depend strongly on the angle that the wall makes with the lattice.

We found that for an angle of $30^\circ$ ($90^\circ$ for the other branch) the distortion is maximum, and is more evident from Fig. (3) that one of the confined bands crosses three times the zero energy. There is an angle ($\sim 23^\circ(37^\circ)$) where two crossings also can be found making a total of three zero modes. The effect is enhanced by increasing the domain wall width. This interesting regularity can be found from the picture of fractionalization of Chern numbers. The integrand in eq. (3) (Berry Curvature) depends on the applied bias, the result is always the same but four well defined peaks can be found in the limit of small bias, one central dip with a contribution of $-1/2$ and three others with a $+1/2$ value each, farther from the center and narrower the lower the bias. The total value of the integral is still $+1$ and on the other side of the wall, the values are opposite.

The index theorem sets an inferior bound to the number of zero modes in $(N_3^a - N_3^b)$. If we sum the sign of the slopes at the crossings we obtain the number predicted by the theorem. Rotation of the domain wall breaks the symmetry between the two regions in such a way that the effective Chern numbers $(N_3^{a,b})$ take different values on both sides of the wall. For instance $(3 \times (+1/2)) - (-3 \times (-1/2) + 1/2)$ gives two, but the number three can
be obtained with \((3 \times (+1/2) + 1/2 - 1/2) - (3 \times (-1/2))\)
or shifting the \(\pm 1/2\) to the other side, and the four zero modes can be formed with \((3 \times (+1/2) + 1/2) - (3 \times (-1/2) - 1/2)\). Such reorganization of the topological charge on each side of the wall lead us to the proper number of zero modes. It is not possible to do a combination to obtain more than four zero modes with those fractions. These half integer contribution has been explored theoretically recently in several models.\(^{13,14}\)

There are three contributions to the appearance of these zero modes, at low bias, important to split the topological charge, second an angle of the domain wall around 30°(90°), breaking the symmetry, and a wide domain wall with a wide wave function and in turn a \(k\) vector more localized, the latter needed to take account of the slight splitting of the \(K\) point.

Another important effect that can be appreciated is the lack of electron-hole symmetry in the system except in the case \(\vartheta = 0^\circ\ (\sim 60^\circ)\). This effect is expected since the Hamiltonian in Eq. (11) fails to commute with the charge conjugation operator.

The propagating modes need to lie in the channel defined by the domain wall, otherwise their energy will be gapped. In Fig. 2 it is clear that the singularities associated with the distortion of the confined channels lie within the gap and they are well localized inside the domain wall, singularities are different for different angles as expected from the band structure, we expect an increase in the conductivity with respect to the isotropic case in the ballistic regime, due to the appearance of the extra zero mode.

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