Engineering of Dirac cones in two-dimensional crystals

Gilles Montambaux

Laboratoire de Physique des Solides, Université Paris-Sud, bat 510, 91405- Orsay, France

We consider several examples of 2D crystals where the low energy properties can be described with a 2 x 2 Hamiltonian with a spectrum exhibiting several Dirac cones. These cones are characterized by a linear dispersion relation, and by a topological number, or "charge", related to a Berry phase associated to the spinorial structure of the wave function. For example, the graphene spectrum has a pair of Dirac cones with opposite Berry phases ($\pm\pi$). We study under which conditions these Dirac cones can be manipulated, created or suppressed, through a modification of band parameters, under the condition of conservation of the total "charge". We have considered several different cases:

We have shown that a single pair of Dirac points with *opposite* "charges" merge always at a symmetric point G/2 of the reciprocal space, where G is a reciprocal lattice vector. In the specific case of graphene, this situation is reached by a modification of one among the three hopping parameters between nearest neighbors. At the topological transition, the spectrum has the remarkable property to be linear in one direction and quadratic in the other direction (*semi-Dirac point*). We derive a universal Hamiltonian that describes the vicinity of the transition, characterized by three parameters, a mass, a velocity and a driving parameter Δ whose values are related to the band parameters of any 2D crystal with time-reversal and inversion symmetries. This model describes continuously the coupling between valleys associated with the two Dirac points, when approaching the transition $\Delta = 0$. We find a general scaling law for the energy levels which evolve continuously from a square-root to a linear dependence, with a new dependence at the transition (the *semi-Dirac* point).

A pair of Dirac points with *same* charge can also merge into a single point with double charge 2π, characterized by a gapless quadratic spectrum. This transition occurs in twisted graphene bilayers. This merging belongs to a different universality class, and the scaling behavior of the Landau levels is different from the previous case.

The case of strained bilayer is particularly interesting since the spectrum exhibits a pair of four Dirac points. Under strain, these four Dirac points can be manipulated and may disappear. Different types of merging can occur, either the merging of two Dirac points with opposite charges, or the merging of three Dirac points ($\pi, \pi, -\pi$) into a single one (π) (fig. c).

In each case, we obtain the Landau levels spectrum and we calculate the number of zero energy modes, and compare the exact spectrum with its semiclassical approximation. Finally, we discuss several other physical systems where such motion and merging of Dirac points can occur like the organic salt (BEDT-TTF)2 I3 and optical lattices of cold atoms. More exotic examples can be found in the Hofstadter spectra for various lattices in a strong magnetic field.

Collaborators: F. Piéchon, J.-N. Fuchs, M.-O. Goerbig, R. de Gail, P. Delplace, P. Dietl