Chern insulators

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1 The field theory of graphene

1.1 Tight-binding model

Let's start from the tight-binding model of graphene. A Chern insulator is by no means required to be realized in a graphene, but the model of graphene helps us to see how Dirac cone appears and how emergent Dirac electrons appear in a condensed matter system.

The lattice structure of graphene is shown in Figure 1 on page 2. Note that there are three bonds per unit cell (Figure 1 on page 2(c)), and the tight-binding Hamiltonian is

$$H = -t\sum_{\boldsymbol{i}}(c^\dagger_{\boldsymbol{i}\mathrm{A}}c_{\boldsymbol{i}\mathrm{B}} + c^\dagger_{\boldsymbol{i}+\hat{\boldsymbol{x}},\mathrm{A}}c_{\boldsymbol{i}\mathrm{B}} + c^\dagger_{\boldsymbol{i}+\hat{\boldsymbol{y}},\mathrm{A}}c_{\boldsymbol{i}\mathrm{B}}) + \mathrm{h.c.} \tag{1}$$

Here $\boldsymbol{i}$ labels unit cells and not atoms. The Fourier transformation is

$$c^\dagger_{\boldsymbol{i}n} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_{\boldsymbol{i}}}c^\dagger_{\boldsymbol{k}n}, \quad \boldsymbol{R}_{\boldsymbol{i}} = i_x\boldsymbol{a}_1 + i_y\boldsymbol{a}_2, \tag{2}$$

and following the standard procedure to solve tight-binding models, we have

$$H = -t\sum_{\boldsymbol{k}}(1 + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1} + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2})c^\dagger_{\boldsymbol{k}\mathrm{A}}c_{\boldsymbol{k}\mathrm{B}} + \mathrm{h.c.} \tag{3}$$

Diagonalization of this Hamiltonian gives the familiar graphene band structure, and at K abd K' points in Figure 1 on page 2(b), we have energy minimum and linear dispersion, the so-called Dirac cones.

1.2 Effective theories at K

Now we derive the effective theory of (3) near K points. We rewrite it into

$$H = -t\sum_{\boldsymbol{k}} \Psi^\dagger_{\boldsymbol{k}} \begin{pmatrix} 0 & f(\boldsymbol{k}) \\ f^*(\boldsymbol{k}) & 0 \end{pmatrix} \Psi_{\boldsymbol{k}}, \quad f(\boldsymbol{k}) = 1 + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1} + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2}, \quad \Psi_{\boldsymbol{k}} = (c_{\boldsymbol{k}\mathrm{A}}, c_{\boldsymbol{k}\mathrm{B}}). \tag{4}$$

Let's do Taylor expansion of $f(\boldsymbol{k})$ around, for example, the rightmost point in Figure 1 on page 2(b), that is

$$\boldsymbol{K} = \left(\frac{4\pi}{3\sqrt{3}a}, 0\right). \tag{5}$$

It gives

$$\begin{aligned} f(\boldsymbol{K}+\boldsymbol{k}) &= 1 + \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3} - \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1} + \mathrm{e}^{\mathrm{i}\frac{2\pi}{3} - \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2} \\ &= 1 + \left(-\frac{1}{2} - \frac{\sqrt{3}}{2}\mathrm{i}\right)(1 - \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1 + \cdots) + \left(-\frac{1}{2} + \frac{\sqrt{3}}{2}\mathrm{i}\right)(1 - \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2 + \cdots) \\ &= -\frac{3}{2}ak_x + \mathrm{i}\frac{3}{2}ak_y, \end{aligned} \tag{6}$$

and therefore we get the effective theory around the Dirac cone:

$$H = v\sum_{\boldsymbol{k}} \Psi^\dagger_{\boldsymbol{K}+\boldsymbol{k}} \begin{pmatrix} 0 & ak_x - \mathrm{i}ak_y \\ ak_x + \mathrm{i}ak_y & 0 \end{pmatrix} \Psi_{\boldsymbol{K}+\boldsymbol{k}}, \quad v = \frac{3}{2}t. \tag{7}$$

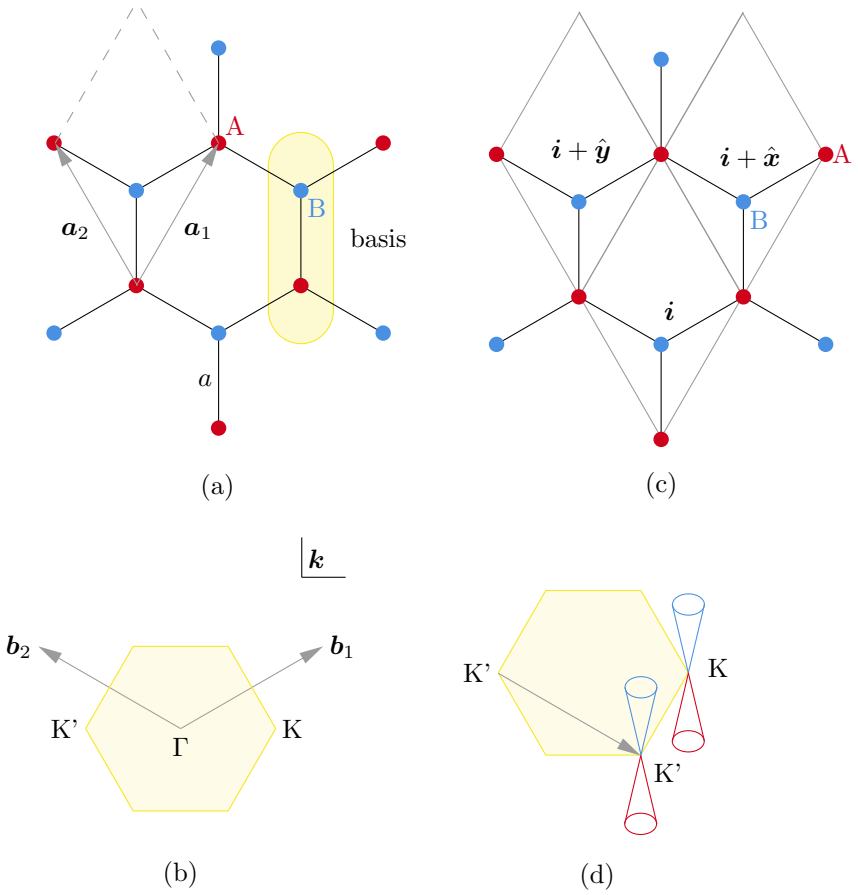

Figure 1: Tight-binding model of graphene (a) The real space lattice structure. The distance between nearest A atom and B atom is a. (b) The momentum space, with first Brillouin zone derived from the real space primitive lattice vectors. (c) Hopping in a unit cell and between unit cells. We have $|\boldsymbol{b}_1||\boldsymbol{a}_1|\cos 30^\circ = 2\pi \Rightarrow |\boldsymbol{b}_1| = 4\pi/3a$. (d) An effective theory of *all* (not just one) Dirac cones should cover two non-equivalent valleys (K and K') and two bands (corresponding to the A sublattice and the B sublattice).

The fact that there is no constant term in the above Hamiltonian also indicates that we are around a Dirac cone. Since we are not interested in the graphene system itself, and only use it as a platform to realize Dirac fermions, it doesn't bring any inconvenience to redefine $\Psi^\dagger_{\boldsymbol{K}+\boldsymbol{k}}$ as $\Psi^\dagger_{\boldsymbol{k}}$, and to rescale $\boldsymbol{k}$ so that $a\boldsymbol{k}$ becomes $\boldsymbol{k}$. The effective theory therefore becomes

$$H = v\sum_{\boldsymbol{k}} \Psi^\dagger_{\boldsymbol{k}}(k_x\sigma_x + k_y\sigma_y)\Psi_{\boldsymbol{k}}. \tag{8}$$

It should be (8) is only about K point in Figure 1 on page 2(b). It should be noted that the K' point is *not* connected to the K point with a $\boldsymbol{G}$ factor. Though in our free theory, there is no hopping between K and K', to find a complete theory about Dirac cones we still need to include K' (and we get a 4-component electron wave function, which may be seen as a Dirac electron). We therefore follow the procedure to derive (6), and replace $\boldsymbol{K}$ by $-\boldsymbol{K}$, and we get

$$f(-\boldsymbol{K}+\boldsymbol{k}) = \frac{3}{2}k_x a + \mathrm{i}\frac{3}{2}k_y a, \tag{9}$$

and therefore we need to change the sign of the k_x term in (8) for Γ' point and we get

$$H = v\sum_{\boldsymbol{k}} \Psi^\dagger_{\boldsymbol{k}}(-k_x\sigma_x + k_y\sigma_y)\Psi_{\boldsymbol{k}}. \tag{10}$$

Combining (8) and (10) together, we get

$$H = v\sum_{\boldsymbol{k}} \Psi^\dagger_{\boldsymbol{k}} \underbrace{\left(\mu^z\tau^x k_x + \tau^y k_y\right)}_{=:H_{\boldsymbol{k}}} \Psi_{\boldsymbol{k}}, \tag{11}$$

where

$$\mu^z = \mathrm{diag}(1,1,-1,-1), \quad \tau^x = \mathrm{diag}(\sigma^x,\sigma^x), \quad \tau^z = \mathrm{diag}(\sigma^z,\sigma^z). \tag{12}$$

Here we actually have two discrete degrees of freedom: The first degree of freedom is the position of valley (K or K'), and the second is the band index – or equivalently, the sublattice. (12) is under the basis

$$\{(\mathrm{K},\mathrm{A}),(\mathrm{K},\mathrm{B}),(\mathrm{K'},\mathrm{A}),(\mathrm{K'},\mathrm{B})\}.$$

So what's (11)?

So we find indeed Dirac electrons can be realized in a realistic model.

1.3 Symmetries

Before going on, let's first do a sketchy analysis of the Dirac electrons. Of course we have translational symmetry. We also have inversion symmetry: Under the inversion operation, sublattice A and sublattice B are exchanged, and $\boldsymbol{k}$ becomes $-\boldsymbol{k}$, which means K and K' are swapped, so because of the exchange of A and B, we have

$$\sigma^y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \longrightarrow \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix} = -\sigma^y,$$

and similarly

$$\sigma^x \longrightarrow \sigma^x,$$

and by the definition of τ^z and τ^x, exchange valley K and valley K' doesn't change their values, so finally we get

$$\tau^x \to \tau^x, \quad \tau^z \to -\tau^z. \tag{13}$$

On the other hand, swapping A and B doesn't change μ^z, but after K and K' are swapped, we get

$$\mu^z \to -\mu^z. \tag{14}$$

So we find the first quantization Hamiltonian $H_{\boldsymbol{k}}$ is invariant under spatial inversion: The sign of k and the sign of the matrices cancel.

Both translational symmetry and inversion symmetry are space group operations. (11) also has a non-space group symmetry: the time reversal symmetry.

1.4 Mass term