8.231 Physics of Solids I — Fall 2017
Recitation 9

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1 Time Reversal Symmetry

1.1 Basic Properties

By definition, time reversal symmetry (TR) changes the arrow of time. Thus it will leave position operator unchanged and reverse the momentum operator:

$$T\hat{x}T^{-1} = \hat{x}, \quad T\hat{p}T^{-1} = -\hat{p}. \tag{1}$$

This immediately implies that T is anti-unitary:

$$TiT^{-1} = \frac{1}{\hbar}T[x,p]T^{-1} = \frac{1}{\hbar}[x,-p] = -\frac{1}{\hbar}[x,p] = -i. \tag{2}$$

The most general form of an anti-unitary linear operator is $T = UK$, where U is unitary and K is the complex conjugation. The form of U is actually highly restricted by noting that physically, applying T twice to any state should result in the same state, with potentially an additional phase factor: $T^2 = e^{i\phi}I$. This implies

$$T^2 = UKUK = UU^* = U(U^T)^{-1} = e^{i\phi}I, \tag{3}$$

where we have used the factor that $K^2 = I$ and $UU^\dagger = I$. Then

$$\begin{cases} U = e^{i\phi}U^T, \\ U^T = Ue^{i\phi}. \end{cases} \Rightarrow U = e^{i\phi}Ue^{i\phi} = e^{2i\phi}U, \tag{4}$$

which can only be satisfied when $e^{i\phi} = \pm 1$. Thus

$$T^2 = \pm I. \tag{5}$$

The sign depends on the spin of the particle. $T^2 = I$ for integer spin particles and $T^2 = -I$ for half-integer spin particles. We will only consider spinless particles in the following for simplicity.

1.2 TR Symmetry in Bloch Bands

Consider tight-binding approximation. Denote $\hat{c}_i$ as the electron annihilation operator on site i. By definition, we have $T\hat{c}_iT^{-1} = \hat{c}_i$. Its effect in Bloch electrons can be computed as

$$T\hat{c}_iT^{-1} = T\left(\frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_j}\hat{c}_{\mathbf{k}}\right)T^{-1} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j}T\hat{c}_{\mathbf{k}}T^{-1} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_j}\hat{c}_{\mathbf{k}}. \tag{6}$$

It is not hard to see that this equation can only be satisfied if

$$T\hat{c}_{\mathbf{k}}T^{-1} = \hat{c}_{-\mathbf{k}}. \tag{7}$$

With this, let us derive the effect of T on the Bloch Hamiltonian $H(\mathbf{k})$. Suppose the full Hamiltonian has TR symmetry $T\hat{H}T^{-1} = H$. Then

$$\begin{aligned} T\hat{H}T^{-1} =& T\left(\sum_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} H(\mathbf{k})\hat{c}_{\mathbf{k}}\right)T^{-1} = T\left(\sum_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} T^{-1}TH(\mathbf{k})T^{-1}T\hat{c}_{\mathbf{k}}\right)T^{-1} \\ =& \sum_{\mathbf{k}} \hat{c}^\dagger_{-\mathbf{k}} TH(\mathbf{k})T^{-1}\hat{c}_{-\mathbf{k}} = \sum_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} H(\mathbf{k})\hat{c}_{\mathbf{k}}, \end{aligned} \tag{8}$$

where we have inserted $T^{-1}T = I$. This equation can only be satisfies when

$$TH(\mathbf{k})T^{-1} = H(-\mathbf{k}). \tag{9}$$

2 Local Stability of Dirac Fermions in Graphene

As an application of what we have developed so far, we will demonstrate that the Dirac fermion in the graphene is protected by the TR symmetry and the inversion symmetry.

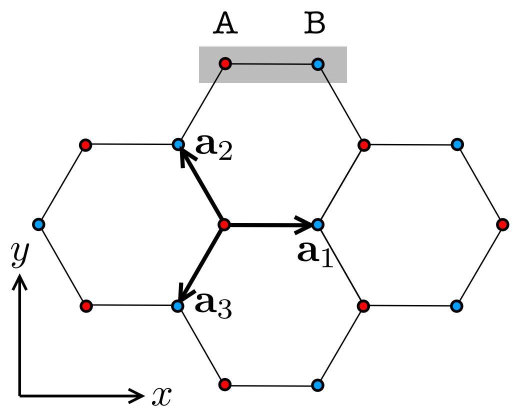

Figure 1: Geometry of graphene.

Recall the Bloch Hamiltonian for the graphene is

$$H(\mathbf{k}) = \begin{pmatrix} 0 & t\sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} \\ t\sum_i e^{-i\mathbf{k}\cdot\mathbf{a}_i} & 0 \end{pmatrix} = t\sum_i \left[\sigma_x \cos(\mathbf{k}\cdot\mathbf{a}_i) - \sigma_y \sin(\mathbf{k}\cdot\mathbf{a}_i)\right], \tag{10}$$

where t is the nearest neighbour (NN) hopping strength, $\mathbf{a}_i$, $i = 1, 2, 3$ are the NN vectors (Fig. 1), and σ_i, $i = x, y, z$ are Pauli matrices. The Hamiltonian is under the atomic orbitals on the A/B sublattice basis.

Suppose the electrons are spinless. In this case $T = K$. It is straightforward to check that

$$TH(\mathbf{k})T^{-1} = H^*(\mathbf{k}) = H(-\mathbf{k}). \tag{11}$$

Thus the model has TR symmetry.

Apart from this symmetry, the model also has inversion symmetry. For example, one can choose the inversion center to be at the center of the hexagon. Note that under the inversion, A/B sublattice becomes B/A sublattice. The effect of the inversion operator I is then

$$I\hat{c}_{i,A/B}I^{-1} = \hat{c}_{-i,B/A}. \tag{12}$$

Following the same recipe in Eq. (7) and (9), one can deduce $IHI^{-1} = H$ translates to

$$IH(\mathbf{k})I^{-1} = \sigma_x H(\mathbf{k})\sigma_x = H(-\mathbf{k}), \tag{13}$$

for Bloch Hamiltonians. It is also straightforward to check the model has inversion symmetry.

We claim that these two symmetries guarantee that the Dirac fermions at $\mathbf{K}/\mathbf{K}'$ points in the Brillouin zone is stable. To show this, consider a generic two-band Bloch Hamiltonian

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \tag{14}$$

with $\mathbf{d}(\mathbf{k}) \equiv (d_x(\mathbf{k}), d_y(\mathbf{k}), d_z(\mathbf{k}))$ and $\boldsymbol{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$. Suppose the Hamiltonian has both TR symmetry and inversion symmetry so that both Eq. (11) and (13) are satisfied. It is straightforward to show that these two equations imply the following restrictions on $\mathbf{d}(\mathbf{k})$:

$$d_x(-\mathbf{k}) = d_x(\mathbf{k}),\ d_y(-\mathbf{k}) = -d_y(\mathbf{k}),\ d_z(\mathbf{k}) = -d_z(\mathbf{k}) = 0. \tag{15}$$

That is to say, with both TR symmetry and inversion symmetry, there can be at most be two Pauli matrices in the Bloch Hamiltonian.

Then recall that the low energy Hamiltonians at $\mathbf{K}/\mathbf{K}'$ points are

$$H(\mathbf{K}/\mathbf{K}' + \boldsymbol{\kappa}) = v(\kappa_x\sigma_x \pm \kappa_y\sigma_y). \tag{16}$$

As long as these two symmetries are satisfied, there is no way to create a term like $m\sigma_z$ to open up a gap the Dirac fermion. All the small perturbations that satisfies the two symmetries[1], will at most move the position of the Dirac point away from $\mathbf{K}$ and $\mathbf{K}'$. For example,

$$H(\mathbf{K} + \boldsymbol{\kappa}) = v(\kappa_x\sigma_x \pm \kappa_y\sigma_y) + a_x\sigma_x + a_y\sigma_y, \tag{17}$$

only shifts the Dirac point at $\mathbf{K}$ to $\mathbf{K} - \mathbf{a}/v$, $\mathbf{a} \equiv (a_x, a_y)$. This finishes the proof.

In boron nitride, the Dirac fermion is gapped because the inversion symmetry is broken, as A and B sublattices are different atoms. It is also possible to open up the gap by breaking the TR symmetry. The model was first proposed by Haldane in 1988 [1]. It turns out that the Haldane model has much richer physics that is deeply connected the topology.

References

[1] F. D M Haldane. Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly". *Phys. Rev. Lett.*, 61(18):2015–2018, oct 1988.

[1] Large perturbations can indeed gap the Dirac fermion. For example, imagine the scenario when a/v is larger than the range of the crystal momentum so that $\mathbf{K} - \mathbf{a}/v$ is out of the Brillouin zone.