Report Problems

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Through these problems, we explore the *graphene and its topological band structure*.

I. WANNIER STATES AND TIGHT-BINDING SYSTEM [1]

For electrons in periodic potential the Bloch states diagonalize the single-particle hamitonian H_0, that is,

$$H_0 = \sum_{\boldsymbol{k}} \epsilon_k \hat{a}^\dagger_{\boldsymbol{k}} \hat{a}_{\boldsymbol{k}}, \tag{1}$$

where $\hat{a}_{\boldsymbol{k}}$ and $\hat{a}^\dagger_{\boldsymbol{k}}$ are the annihilation and creation operators for an electron in a Bloch state indexed by the wave vector $\boldsymbol{k}$. Let us see this problem in the real space indexed by the atomic site $\boldsymbol{R}_i$ as opposed to $\boldsymbol{k}$. To this end, it is helpful to introduce the so-called *Wannier states*, for which the annihilation and creation operators, $\hat{a}_i$ and $\hat{a}^\dagger_i$ are respectively defined by

$$\hat{a}_i = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i} \hat{a}_{\boldsymbol{k}} \tag{2}$$

$$\hat{a}^\dagger_i = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} \hat{a}^\dagger_{\boldsymbol{k}}, \tag{3}$$

where N is the number of the atomic sites. The inverse of each expression reads

$$\hat{a}_{\boldsymbol{k}} = \frac{1}{\sqrt{N}} \sum_{i} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} \hat{a}_i \tag{4}$$

$$\hat{a}^\dagger_{\boldsymbol{k}} = \frac{1}{\sqrt{N}} \sum_{i} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i} \hat{a}^\dagger_i. \tag{5}$$

With these expressions the Hamiltonian Eq. (1) becomes

$$H_0 = \frac{1}{N} \sum_{ij} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} \epsilon_k \hat{a}^\dagger_i \hat{a}_j = \sum_{ij} \hat{a}^\dagger_i t_{ij} \hat{a}_j, \tag{6}$$

where we have defined the *hopping matrix* t_{ij} as

$$t_{ij} = \frac{1}{N} \sum_{\boldsymbol{k}} \epsilon_k e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)}. \tag{7}$$

Equation (6) is called *tight-binding Hamiltonian* and describes electrons hopping from one lattice site i to the other j, whose strength is dictated by the hopping matrix element t_{ij} in Eq. (7). You can see that when $\epsilon_k = \text{const.}$, that is, single-particle Hamiltonian H_0 merely represents isolated atom and index $\boldsymbol{k}$ is irrelevant, then $t_{ij} = \delta_{ij}$ and there are no hopping. The dispersion $\epsilon_k \neq \text{const.}$ is thus pertinent to realize the inter-atomic hopping.

II. 2D SQUARE LATTICE - A TOY MODEL [1]

As an concrete example let us take a 2D square lattice with the lattice constant a.

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Problem 1

(1) By setting $t_{ij} = -t$ for i and j being nearest neighbors and zero otherwise, show that the tight binding Hamiltonian Eq. (6) can be diagonalized in terms of Bloch states and becomes

$$H_0 = \sum_{k_x,k_y} \left[-2t\left(\cos(k_x a) + \cos(k_y a)\right)\right] \hat{a}^\dagger_{k_x,k_y} \hat{a}_{k_x,k_y}. \tag{8}$$

The energy suface in Brillouin zone spanned by k_x and k_y with $-\frac{\pi}{a} \leq k_x \leq \frac{\pi}{a}$ and $-\frac{\pi}{a} \leq k_y \leq \frac{\pi}{a}$ is shown in Fig. 1.

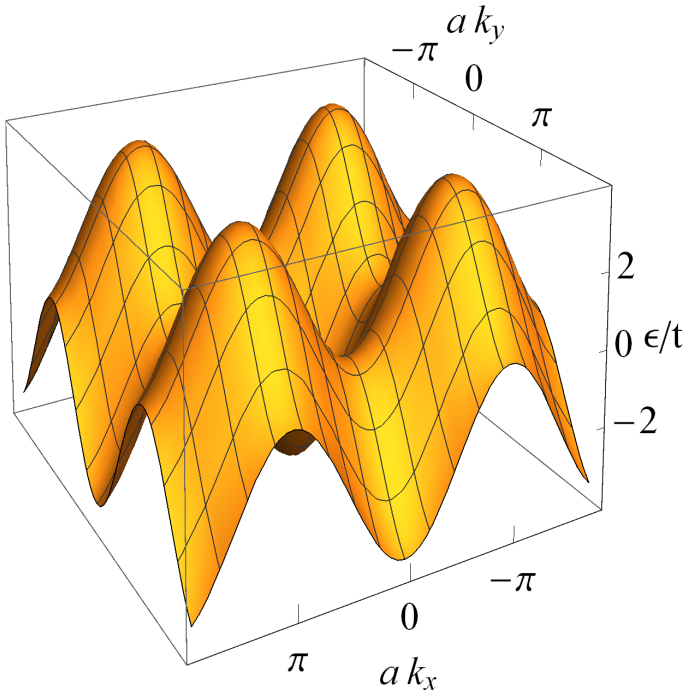

FIG. 1: Energy suface $\epsilon/t = -2\left(\cos(k_x a) + \cos(k_y a)\right)$ of an electron in the 2D square lattice dipicted in Brillouin zone spanned by k_x and k_y.

III. 2D HEXAGONAL LATTICE - *GRAPHENE* [1, 2]

Graphene is a single layer of graphite with 2D hexagonal lattice of carbon atoms. Graphene shows a number of interesting physics which basically originate from its band structure. From each carbon atom, $2s$, $2p_x$, and $2p_y$ orbits hybridize and they form the so-called σ-band as sp^2 *hybrids*. On the other hand, p_z orbits do not participate this hybridization and form the so-called π-band. Usually, the Fermi energy lays in the π-band and most of the interesting properties of graphene can thus be attributed to electrons in the π-band, which show a linear dispersion and behave like 2D Dirac fermions. Hereby we study this peculiar band dispersion with tight-binging approach.

The unit-cell of the graphene contains two atoms and spanned by two vectors

$$\boldsymbol{a}_1 = \left(\frac{\sqrt{3}}{2}a, \frac{1}{2}a\right), \tag{9}$$

$$\boldsymbol{a}_2 = \left(\frac{\sqrt{3}}{2}a, -\frac{1}{2}a\right), \tag{10}$$

$$\tag{11}$$

as shown in Fig. 2. By setting $t_{ij} = -t$ for i and j being nearest neighbors and zero otherwise, the *monatomic* tight-binding Hamiltonian Eq. (6) can be modified into the the *bi-atomic* nearest neighbor tight-binding Hamiltonian

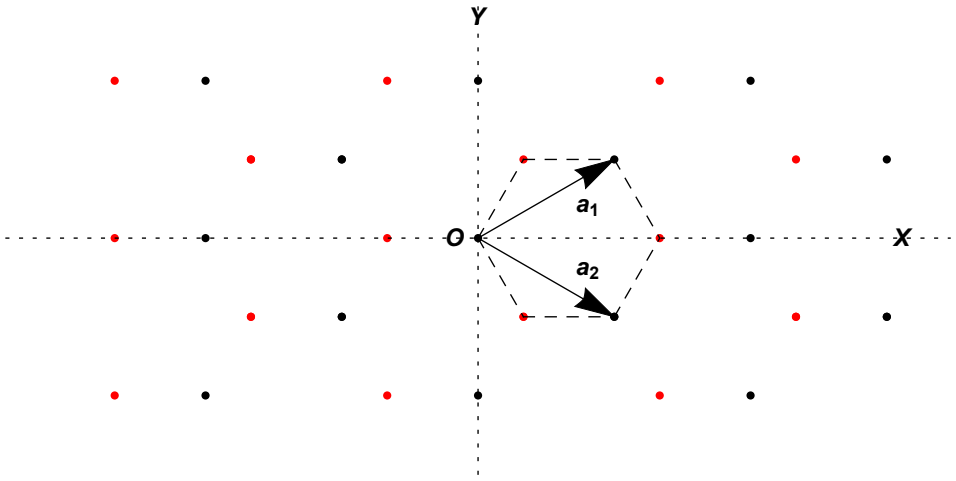

FIG. 2: 2D hexagonal lattice of carbon atoms. The black and red points show the inequivalent two atomic sites, A-site and B-site, respectively.

$$H = -t \sum_{\langle i,j \rangle} \left(\hat{a}^{\dagger}_{i,j} \left(b_{i,j} + b_{i+1,j+1} + b_{i+1,j-1} \right) + h.c. \right), \tag{12}$$

where $\hat{a}_{ij}$ ($\hat{b}_{ij}$) is the anninilation operator for the electron at (i,j) lattice point of A-site (B-site) and $\hat{a}^{\dagger}_{ij}$ ($\hat{b}^{\dagger}_{ij}$) is the corresponding creation operator.

Problem 2

(1) Show that the tight binding Hamiltonian Eq. (12) can be modified into

$$H = -t \sum_{k_x,k_y} \left[\hat{a}^{\dagger}_{k_x,k_y} \hat{b}^{\dagger}_{k_x,k_y} \right] \begin{bmatrix} 0 & f(k_x,k_y) \\ f(k_x,k_y)^* & 0 \end{bmatrix} \begin{bmatrix} \hat{a}_{k_x,k_y} \\ \hat{b}_{k_x,k_y} \end{bmatrix}, \tag{13}$$

where

$$f(k_x,k_y) = e^{-ik_x \frac{a}{\sqrt{3}}} + 2e^{ik_x \frac{a}{2\sqrt{3}}} \cos\left(\frac{k_y}{2}\right). \tag{14}$$

By applying the proper unitay transformation, the Hamiltonian Eq. (13) can be diagonalized. The energy surfaces are obtained as

$$\epsilon_k/t = \pm\sqrt{f(k_x,k_y) f(k_x,k_y)^*} = 1 + 4\cos\left(k_x \frac{\sqrt{3}a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_x a}{2}\right), \tag{15}$$

which are shown in Fig. 3.

IV. DIRAC CONE AND DIRAC MONOPOLE [2]

We are now in a position to see the connection between the band structure shown in Fig. 3 and the topology. The 2D hexagonal lattice in real space shown in Fig. 2 can be cast into the 2D hexagonal lattice in reciprocal space, that is, the Brillouin zone of the 2D hexagonal lattice, as shown in Fig. 4. We see that at $K = (k_x,k_y) = \frac{2\pi}{a}\left(0,-\frac{2}{3}\right)$ and $K' = (k_x,k_y) = \frac{2\pi}{a}\left(0,\frac{2}{3}\right)$ points in the Fig. 4, the two enery surfaces touch as shown in Fig. 3 (they look not touching but with higher resolution they are indeed touching).

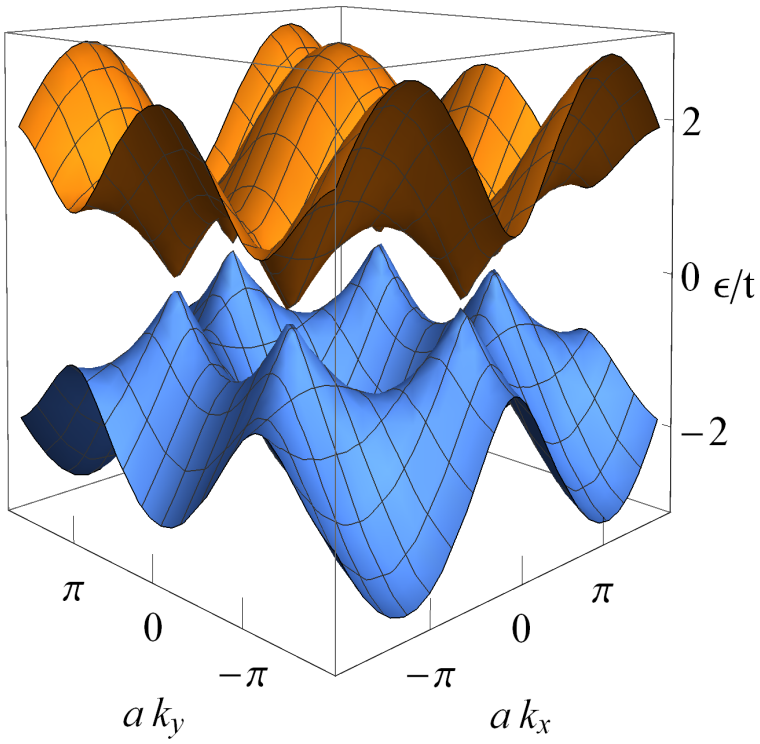

FIG. 3: Energy suface $\epsilon_k/t = \pm\sqrt{f(k_x,k_y)f(k_x,k_y)^*} = 1 + 4\cos\left(k_x\frac{\sqrt{3}a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_x a}{2}\right)$ of an electron in the 2D hexagonal lattice dipicted in Brillouin zone spanned by k_x and k_y.

Problem 3

(1) By expanding Eq. (12) around the K point, show that the tight binding Hamiltonian Eq. (12) can be approximated as

$$\begin{aligned} H_{\rm D} &= -\hbar v \sum_{\tilde{k}_x,\tilde{k}_y} \begin{bmatrix} \hat{a}^\dagger_{\tilde{k}_x,\tilde{k}_y} & \hat{b}^\dagger_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix} \begin{bmatrix} 0 & \tilde{k}_x - i\tilde{k}_y \\ \tilde{k}_x + i\tilde{k}_y & 0 \end{bmatrix} \begin{bmatrix} \hat{a}_{\tilde{k}_x,\tilde{k}_y} \\ \hat{b}_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix} \\ &= -\hbar v \sum_{\tilde{k}_x,\tilde{k}_y} \begin{bmatrix} \hat{a}^\dagger_{\tilde{k}_x,\tilde{k}_y} & \hat{b}^\dagger_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix} \left(\sigma_x\tilde{k}_x + \sigma_y\tilde{k}_y\right) \begin{bmatrix} \hat{a}_{\tilde{k}_x,\tilde{k}_y} \\ \hat{b}_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix}, \end{aligned} \tag{16}$$

where

$$v = \frac{\sqrt{3}at}{2\hbar}. \tag{17}$$

(2) By expanding Eq. (12), on the other hand, around the K' point, show that the tight binding Hamiltonian Eq. (12) can be approximated as

$$H_{\rm D} = \hbar v \sum_{\tilde{k}_x,\tilde{k}_y} \begin{bmatrix} \hat{a}^\dagger_{\tilde{k}_x,\tilde{k}_y} & \hat{b}^\dagger_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix} \left(\sigma_x\tilde{k}_x + \sigma_y\tilde{k}_y\right) \begin{bmatrix} \hat{a}_{\tilde{k}_x,\tilde{k}_y} \\ \hat{b}_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix}. \tag{18}$$

This Hamiltonian is formally equivalent to that for the massless Dirac particles. The *masslessness* manifests itself as the linear dispersion, that is, $H_{\rm D} \propto \tilde{k}_i$. The cones around K and K' points suppended by $\tilde{k}_x$ and $\tilde{k}_y$ as shown in Fig. 3 are called the *Dirac cones*.

Now let us seek the connection between the Dirac cone and the Dirac monopole, the later of which we have learned in the Lecture. To see this connection, we shall reverse the usual *second quantization* procedure, that is, from the second quantized Hamiltonian to the single-particle Hamiltonian. Since the relation between the single-particle Hamiltonian

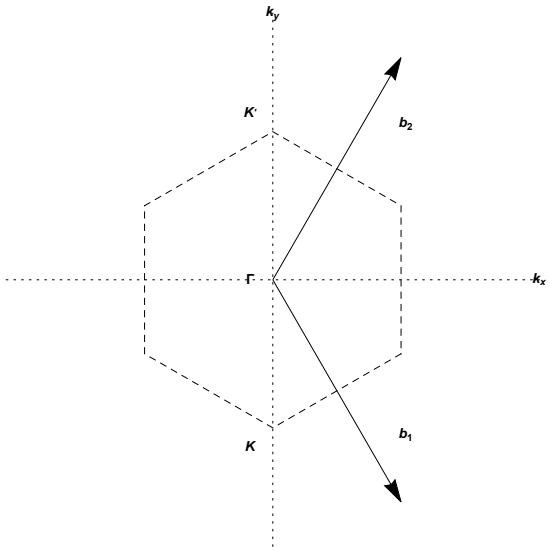

FIG. 4: 2D hexagonal lattice in reciprocal space.

$\mathcal{H}_{\rm D}$ and the second quantized Hamilotionian $H_{\rm D}$ is [1]

$$H_{\rm D} = \sum_{\tilde{k}_x,\tilde{k}_y} \left[\hat{a}^\dagger_{\tilde{k}_x,\tilde{k}_y}\ \hat{b}^\dagger_{\tilde{k}_x,\tilde{k}_y}\right] \mathcal{H}_{\rm D} \begin{bmatrix} \hat{a}_{\tilde{k}_x,\tilde{k}_y} \\ \hat{b}_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix}, \tag{19}$$

we have

$$\begin{aligned} \mathcal{H}_{\rm D} &= -\hbar v \left(\sigma_x \tilde{k}_x + \sigma_y \tilde{k}_y\right) \\ &= -\hbar v \boldsymbol{\sigma}\cdot\tilde{\boldsymbol{k}} \end{aligned} \tag{20}$$

for K Dirac particle and

$$\begin{aligned} \mathcal{H}_{\rm D} &= \hbar v \left(\sigma_x \tilde{k}_x + \sigma_y \tilde{k}_y\right) \\ &= \hbar v \boldsymbol{\sigma}\cdot\tilde{\boldsymbol{k}} \end{aligned} \tag{21}$$

for K' Dirac particle. These Hamiltonians are formally equivalent to the one we encountered in the Lecture [Eq. (8) in the Lecture 3: *Path integral for spin*], that is,

$$H = \hbar\gamma\boldsymbol{\sigma}\cdot\boldsymbol{B}. \tag{22}$$

Thus the Dirac electrons moving adiabatically around the K and K' points in the Brillouin zone are formally equivalent to a charged particle moving adiabatically around the Dirac monopole!

Following the argument we have delineated in the Lecture [the Lecture 4: *Berry phase and Dirac monopole*], going around, e.g., K' point in the Brillouin zone an electron acquires the Berry phase

$$\gamma = \pi. \tag{23}$$

It can be shown, from the argument of symmetry, that the Berry curvature is only finite at $(\tilde{k}_x, \tilde{k}_y) = (0,0)$, that is exactly at the K and K' points and

$$\boldsymbol{\Omega} = \begin{bmatrix} 0 \\ 0 \\ \pi\delta(\tilde{k}_x,\tilde{k}_y) \end{bmatrix}. \tag{24}$$

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[1] A. Altland and B. D. Simons, *Condensed Matter Field Theory*, 2nd ed. (Cambridge University Press, Cambridge, 2010).
[2] T. Ando, J. Phys. Soc. Jan. **74**, 777 (2005).