Report Problems (*note: the parts corrected are in magenta*)

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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.

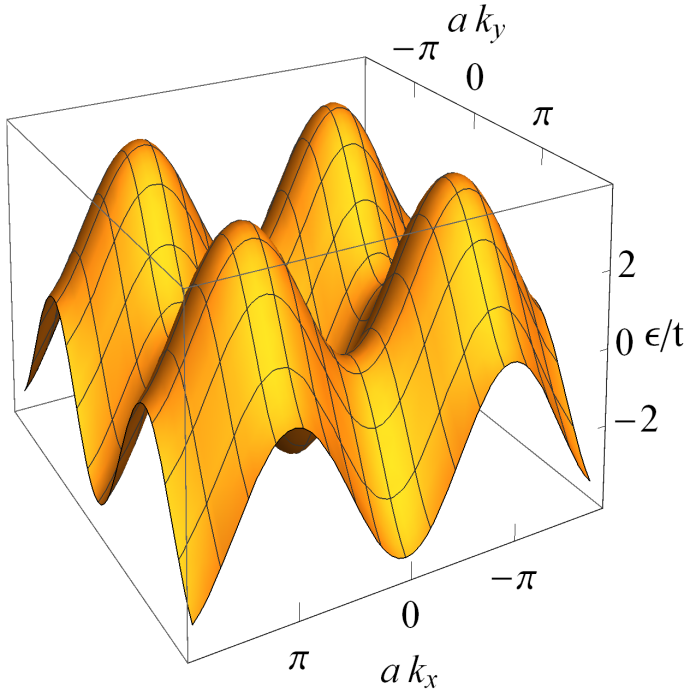

FIG. 1. Energy suface $\epsilon/t = -2\left(\cos(k_x a) + \cos(k_y a)\right)$ of an electron in the 2D square lattice dipicted in Brillouin zone spanned by k_x and k_y.

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

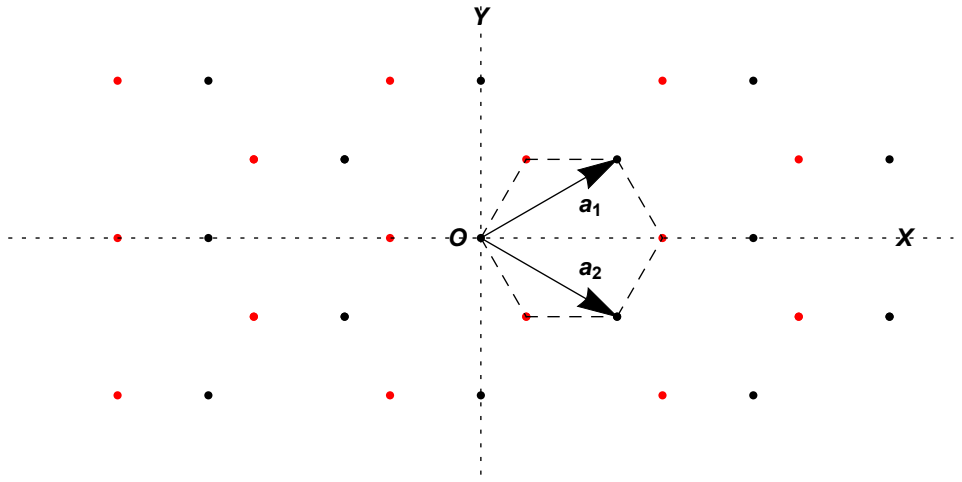

FIG. 2. 2D hexagonal lattice of carbon atoms. The black and red points show the inequivalent two atomic sites, A-site and B-site, respectively.

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

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

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

where

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

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

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

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).

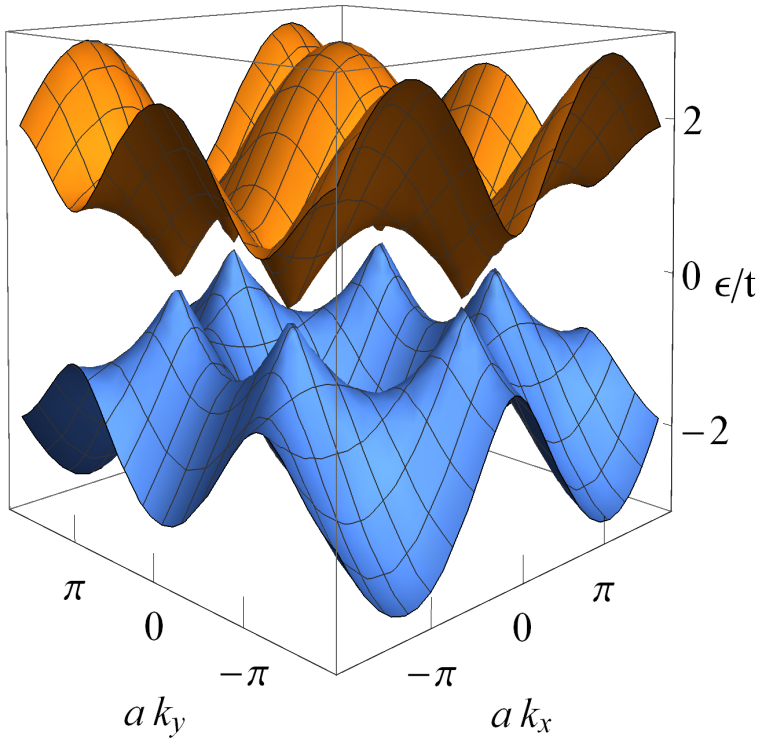

FIG. 3. Energy suface $\epsilon_k/t = \pm\sqrt{f(k_x,k_y)f(k_x,k_y)^*} = \pm\sqrt{1+4\cos\left(k_x\frac{\sqrt{3}a}{2}\right)\cos\left(\frac{k_y a}{2}\right)+4\cos^2\left(\frac{k_x a}{2}\right)}$ of an electron in the 2D hexagonal lattice dipicted in Brillouin zone spanned by k_x and k_y.

Problem 3

(1) By expanding Eq. (12) around the K' point, where $k_x = \tilde{k}_x$ and $k_y = \frac{4\pi}{3a} + \tilde{k}_y$, show that the tight binding Hamiltonian Eq. (12) can be approximated as

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

where

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

(2) By expanding Eq. (12), on the other hand, around the K point, where $k_x = \tilde{k}_x$ and $k_y = -\frac{4\pi}{3a} + \tilde{k}_y$, show that the tight binding Hamiltonian Eq. (12) can be approximated as

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

Now let us seek the connection between electrons at K and K' point of graphene 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. Now, the relation

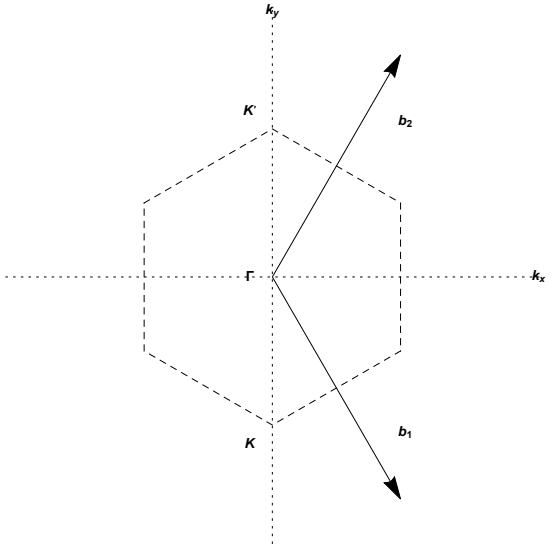

FIG. 4. 2D hexagonal lattice in reciprocal space.

between the single-particle Hamiltonian $\mathcal{H}_{\mathrm{D}'}$ in Eq. (16) and the second quantized Hamilotionian H'_{D} is [1]

$$H'_{\mathrm{D}} = \sum_{\tilde{k}_x,\tilde{k}_y} \begin{bmatrix} \hat{a}^\dagger_{\tilde{k}_x,\tilde{k}_y} & \hat{b}^\dagger_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix} \mathcal{H}'_{\mathrm{D}} \begin{bmatrix} \hat{a}_{\tilde{k}_x,\tilde{k}_y} \\ \hat{b}_{\tilde{k}_x,\tilde{k}_y} \end{bmatrix}, \tag{19}$$

we have

$$\mathcal{H}'_{\mathrm{D}} = -\hbar v \left(\sigma_x \tilde{k}_y - \sigma_y \tilde{k}_x \right) \tag{20}$$

for electron in K point. Let us perform an unitary transformation

$$\begin{aligned} \mathcal{H}'_{\mathrm{D}} \to \mathcal{H}_{\mathrm{K}'} &= e^{i\frac{\pi}{4}\sigma_z} \mathcal{H}_{\mathrm{D}} e^{-i\frac{\pi}{4}\sigma_z} \\ &= -\hbar v \left(\underbrace{e^{i\frac{\pi}{4}\sigma_z} \sigma_x e^{-i\frac{\pi}{4}\sigma_z}}_{-\sigma_y} \tilde{k}_y - \underbrace{e^{i\frac{\pi}{4}\sigma_z} \sigma_y e^{-i\frac{\pi}{4}\sigma_z}}_{\sigma_x} \tilde{k}_x \right) \\ &= \hbar v \left(\sigma_y \tilde{k}_y + \sigma_x \tilde{k}_x \right) \\ &= \hbar v \boldsymbol{\sigma} \cdot \tilde{\boldsymbol{k}}. \end{aligned} \tag{21}$$

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

This Hamiltonian is 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' point 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

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

[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).