SFI5711 - Solid State Physics (2020)
List of exercises #2

1. Properties of Bloch electrons

(a) Use the Bloch theorem to show that the Eigenenergies of the Bloch wavefunction $\psi_{n,\mathbf{k}}$ obey the relationship $E_n(\mathbf{k}) = E_n(-\mathbf{k})$.

(b) Show the translation operator $T_{\mathbf{R}}$ [defined as $T_{\mathbf{R}}\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R})$] can be written as $\exp(R \cdot \nabla)$.

(c) The energy dispersion of a single non-degenerate band $E_n(\mathbf{k})$ is periodic in the reciprocal space. Therefore, its Fourier coefficients are non-vanishing only at the lattice sites R. Use this property and the result of item (b) to prove the Wannier theorem: $E_n(-i\nabla)\psi_{n,\mathbf{k}} = E_n(\mathbf{k})\psi_{n,\mathbf{k}}$.

2. Properties of Bloch electrons II

(a) Show that the electron mean velocity is given by $\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}E_n(\mathbf{k})$.

(*Hint*: Expand $E_n(\mathbf{k} + \mathbf{q})$ for $q \ll k$ up to 1st order. Now write down the Schrödinger equation for $u_{n,\mathbf{k}}(\mathbf{r})$, where $\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n,\mathbf{k}}(\mathbf{r})$. This equation is of type $H_{\mathbf{k}}u_{n,\mathbf{k}} = E_n(\mathbf{k})u_{n,\mathbf{k}}$. Now write $H_{\mathbf{k}+\mathbf{q}} = H_{\mathbf{k}} + \delta H$ and treat δH up to 1st order in perturbation theory to obtain $E_n(\mathbf{k}+\mathbf{q})$. Finally, compare this result with your expansion in q.)

(b) Show that the inverse of the effective mass tensor

$$\left(\mathbf{M}^{-1}\right)_{i,j} = \frac{1}{\hbar^2}\frac{\partial^2 E_n(\mathbf{k})}{\partial k_i \partial k_j} = \frac{1}{m}\left[\delta_{i,j} + \frac{1}{m}\sum_{n'\neq n}\frac{p_i^{n,n'}p_j^{n',n} + p_i^{n',n}p_j^{n,n'}}{E_{n'}(\mathbf{k}) - E_n(\mathbf{k})}\right],$$

where $p_j^{n',n} = \left\langle\psi_{n,\mathbf{k}}\left|\frac{\hbar}{i}\frac{\partial}{\partial x_j}\right|\psi_{n',\mathbf{k}}\right\rangle$.

(*Hint*: Repeat the same steps as in (a) but up to 2nd order. In the end, consider that there is no contribution in 1st order and define $E_n(\mathbf{k}+\mathbf{q}) = E_n(\mathbf{k}) + \frac{1}{2}\sum_{i,j}\left(M^{-1}\right)_{i,j}q_iq_j$.)

(c) Notice that $\mathbf{M}$ can be anysotropic. Give an example of a physical situation in which this is the case.

(d) Notice moreover that $\mathbf{M}$ can have positive and negative Eigenvalues. How do you interpret this result?

3. Dynamics of Bloch electrons

Although the crystal momentum $\hbar\mathbf{k}$ is not the electronic momentum $\mathbf{p}$, it follows simple dynamic equations. For instance, in the presence of a spatially uniform electric field $\mathbf{E}$ and a small magnetic field $\mathbf{B}$, it follows Lorentz equation:

$$\hbar\dot{\mathbf{k}} = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B}).$$

The purpose of this exercise is to guide you through the derivation of this expression. We start by considering the Hamiltonian of a single-electron in a Bloch state $|\psi_{n,\mathbf{k}}\rangle$.

$$H = \frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2 + U(\mathbf{r}) - e\phi,$$

where $U(\mathbf{r})$ is the lattice periodic potential, and ϕ and $\mathbf{A}$ are the scalar and vector potential, respectively. (Recall $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\frac{\partial}{\partial t}\mathbf{A} - \nabla\phi$).

(a) After an infinitesimal time $\mathrm{d}t$, the Bloch wavefunction evolves and becomes $\psi_n(\mathbf{k}')$ given by

$$\psi_n(\mathbf{k}') = e^{-\frac{i}{\hbar}H\mathrm{d}t}\psi_n(\mathbf{k}) \approx \left(1 - \frac{i}{\hbar}H\mathrm{d}t\right)\psi_n(\mathbf{k}).$$

Apply the translation operator $T_{\mathbf{R}}$ and show that

$$T_{\mathbf{R}}\psi_n(\mathbf{k}') = \left(1 - \frac{i}{\hbar}H\mathrm{d}t\right)T_{\mathbf{R}}\psi_n(\mathbf{k}) - \frac{i}{\hbar}[T_{\mathbf{R}}, H]\,\mathrm{d}t\psi_n(\mathbf{k}).$$

(b) Fixing $\mathbf{B}$ along the z-direction and using the Landau Gauge ($\mathbf{A} = Bx\hat{y}$), show that

$$[T_{\mathbf{R}}, H] = \left[e(\mathbf{E} + \mathbf{v} \times \mathbf{B})\cdot\mathbf{R} + \frac{e^2B^2}{2m}R_x^2\right]T_{\mathbf{R}}.$$

(c) By imposing the state $\psi_n (\mathbf{k}')$ to be a Bloch state and by making $\mathbf{k}' = \mathbf{k} + \dot{\mathbf{k}}dt$, show that, to leading order in $\mathbf{B}$, one obtains the Lorentz equation.

(d) Discuss physically why in Lorentz equation the crystal momentum $\mathbf{k}$, and not the electronic momentum, is present.

4. (Optional) Band dispersion near a Bragg plane

Using the results of the nearly free electron model, show that the constant-energy surfaces are perpendicular to the Bragg plane, i.e., the gradient $\nabla_{\mathbf{k}} E_{\mathbf{k}}$ calculated at the Bragg plane is parallel to it.

5. Kronig-Penney model

Consider the 1D model of an array of identical and equally spaced repulsive delta-peaked potentials given by

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U_0 a \sum_{n=-\infty}^{\infty} \delta (x - na).$$

Between two consecutive potentials, $na < x < (n+1)a$, the Eigenfunctions are superposition of plane waves

$$\psi (x) = A e^{iqx} + B e^{-iqx},$$

with free-particle dispersion $E_q = \frac{\hbar^2}{2m}q^2$. It is convenient to express A and B as $e^{\pm i\theta}$.

(a) Use Bloch theorem and the continuity conditions of $\psi (x)$ at $x = a$ to eliminate the constant θ and to show the following relationship between the crystal momentum k and the electron momentum q:

$$\cos ka = \cos qa + \frac{k_0}{q} \sin qa, \ \text{with } k_0 = \frac{mU_0 a}{\hbar^2}.$$

(b) Why does this relationship imply the existence of bands separated by gaps? Where in reciprocal space do the gaps open?

(c) In the case of a weak potential U_0, find an approximate analytical expression for the gaps.

(d) (Optional) For $k_0 a = 2$, make a "band plot" indicating the energy intervals [in units of $\hbar^2/\left(2ma^2\right)$] for which there is a gap or a band. You do not need to plot the band dispersion as function of k: just mark in the E_q axis where the bands and the gaps are.

6. van Hove singularities and Lifshitz transitions

The tight-binding model on the square lattice, considering nearest-neighbor hopping t only, yields the dispersion relation

$$E_{\mathbf{k}} = -2t \left(\cos k_x a + \cos k_y a\right).$$

Recall that the density of states is defined as

$$\rho (E) = 2 \times \int \frac{\mathrm{d}^2 k}{\left(2\pi\right)^2} \delta \left(E - E_{\mathbf{k}}\right),$$

where the integral is over the Brillouin zone: $-\frac{\pi}{a} < k_i \le \frac{\pi}{a}$.

(a) In the interval $-4t < E < 4t$, show that

$$\rho (E) = \frac{1}{\pi^2 a^2 t} K \left(1 - \left(\frac{E}{4t}\right)^2\right),$$

where $K (x)$ is the complete elliptical integral of 1st kind.

(b) Plot the density of states. Show there is a divergence at $E = 0$ (called van Hove singularity) and obtain an approximate expression for ρ around this energy.

(c) We now want to study the Fermi surface (for 2D models, the surface becomes a set of lines in which $E_{\mathbf{k}} = \mu$). Plot the Fermi surface for the cases in which $N = 0.5$, 0.9, 1.0 (half-filling, which corresponds to chemical potential $\mu = 0$), 1.1, and 1.5, where N is the number of electrons per unit cell. Notice that the Fermi topology changes from closed to open. This is called Lifshitz transition. (Notice you will have to compute the Fermi surface numerically.)

(d) The Lifshitz transition of the previous item is due to the existence of a saddle point in the band dispersion at $\mathbf{k}_0 = \left(\frac{\pi}{a}, 0\right)$ (and the symmetry-equivalent points). Make a three-dimensional plot of the band structure near this

point to verify the existence of a saddle point. Expand $E_\mathbf{k}$ around this point up to quadratic order in the appropriate coordinates $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$. Calculate the density of states associated related to this approximate form of the dispersion and show that it diverges at $E = 0$. Thus, the Lifshitz transition is closely related to the van Hove singularity found in item (b).

7. Graphene and carbon nanotubes

In graphene, carbon atoms occupy the sites of a honeycomb lattice. Recall this lattice lattice can be described as triangular Bravais lattice with primitive vectors $\mathbf{a}_{1,2} = \frac{1}{2}\left(3, \pm\sqrt{3}\right) a$ plus a basis containing two atoms, A and B. Here, a is the distance between nearest-neighbor A-B atoms. Consider there is hopping only between nearest-neighbors, i.e., between the two atoms of the basis. The corresponding Tight-Binding model is

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(a_{i,\sigma}^\dagger b_{j,\sigma} + \text{h.c.} \right),$$

where $a_i^\dagger$ and a_i are the usual creation and annihilation operators of electrons at site i (related to an A atom) with spin projection σ. The definition for $b_{i,\sigma}$ is analogous for the B sites. Due to the existence of two atoms per unit cell, the problem can be suitably cast in a 2×2 matrix form. (Be aware that there are some situations in which the hopping between next-nearest-neighbors is important.)

(a) Calculate the tight-binding band dispersion of graphene. Make a three-dimensional plot of the band structure and show that it is composed of two bands that are completely gapped except at the two points $\mathbf{K} = \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right)$ and $\mathbf{K}' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right)$ (and the symmetry-equivalent points). Therefore, at half-filling (one electron per carbon atom), the Fermi surface is composed only by these two points, the so-called Dirac points.

(b) For $\mathbf{k} = \mathbf{K} + \mathbf{q}$, show that the band dispersion vanishes linearly with the momentum $\mathbf{q}$. Therefore near the Dirac points, it can be approximated by a cone. Show that, in terms of the 2×2 matrix representation, the kinetic energy can be written (up to an unimportant global phase factor) as the massless Dirac Hamiltonian:

$$H = v_F \mathbf{q} \cdot \boldsymbol{\sigma},$$

with $v_F = \frac{3}{2}ta$, and $\boldsymbol{\sigma}$ being the Pauli matrices.

(c) (Optional) Using the band structure that we just calculated, we can also study carbon nanotubes. They are formed by rolling the graphene sheet into a cylinder, overlapping two sites separated by an arbitrary lattice vector c. There are several ways of rolling a nanotube, depending on the vector c. By imposing periodic boundary conditions, this leads to the quantization condition by an arbitrary lattice vector $\mathbf{R}$. There are several ways of rolling a nanotube, depending on the vector $\mathbf{R}$. By imposing periodic boundary conditions, this leads to the quantization condition

$$\mathbf{R} \cdot \mathbf{k} = 2\pi m, \text{ with } m \in \mathbb{Z}.$$

The band structure of the carbon nanotube is then the one calculated in item (a) subject to the appropriate quantization of $\mathbf{k}$. Show that the zig-zag nanotube, with $\mathbf{R} = n\left(\mathbf{a}_1 - \mathbf{a}_2\right)$, is a metal if n is a multiple of 3, and an insulator otherwise. Show also that the armchair nanotube, with $\mathbf{R} = n\left(2\mathbf{a}_1 - \mathbf{a}_2\right)$, is a metal for any value of n.

8. (Optional) Tight-binding model for the iron pnictides

The single-orbital Tight-Binding model on a square lattice is often used to describe the cuprates (such as La_2CuO_4). Here we will discuss the simplest tight-binding model that describes another class of high-temperature superconductors: the iron pnictides (such as BaFe_2As_2). They can also be modeled on the square lattice, but unlike the cuprates, a single-orbital is not enough. The reason is that while Cu is on a $3d^9$ electronic configuration, with one empty $d_{x^2-y^2}$ orbital, Fe is on the $3d^6$ configuration. The simplest approach considers hopping between two of the five 3d orbitals, namely, d_{xz} and d_{yz}:

$$H = -\sum_{i,j,\sigma} \sum_{m,n} t_{m,n}^{i,j} a_{m,i,\sigma}^\dagger a_{n,j,\sigma}.$$

Here, the indices i and j refers to sites of the square lattice, whereas m and n refers to the two orbitals of interest. Due to the symmetry of the d_{xz} and d_{yz} orbitals, the hopping may be different along $\hat{x}$ and $\hat{y}$ directions. For nearest neighbors it follows that $t_{m,m}^{\langle i,j \rangle} = t_1$ if $\mathbf{R}_j = \mathbf{R}_i \pm a\hat{x}$ and $m = d_{xz}$, or $\mathbf{R}_j = \mathbf{R}_i \pm a\hat{y}$ and $m = d_{yz}$; $t_{m,m}^{\langle i,j \rangle} = t_2$ if $\mathbf{R}_j = \mathbf{R}_i \pm a\hat{y}$ and $m = d_{xz}$, or $\mathbf{R}_j = \mathbf{R}_i \pm a\hat{x}$ and $m = d_{yz}$. There is no nearest-neighbor hopping for electrons in different orbitals: $t_{m,n}^{\langle i,j \rangle} = 0$, for $n \neq m$. For next-nearest neighbors, it follows that $t_{m,m}^{\langle\langle i,j \rangle\rangle} = t_3$ for any orbital m and

any next-nearest-neighbor site j; and $t_{m,n}^{\langle\langle i,j\rangle\rangle} = \pm t_4$ for $m \neq n$ with the $+$ $(-)$ sign referring to hoppings along the diagonal (anti-diagonal), i.e., for $\mathbf{R}_j = \mathbf{R}_i \pm a\,(1,1)$ $(\mathbf{R}_j = \mathbf{R}_i \pm a\,(1,-1))$.

(a) Calculate the band dispersion.

(b) Using $t_1 = -0.33\,\mathrm{eV}$, $t_2 = 0.385\,\mathrm{eV}$, $t_3 = -0.234\,\mathrm{eV}$, $t_4 = 0.26\,\mathrm{eV}$, plot the Fermi surface in the 1st Brillouin zone for the chemical potential $\mu = 0.55\,\mathrm{eV}$ (half-filling).

(c) Plot the band dispersion across the highly symmetric directions $\mathbf{k} = k\,(1,0)$ and $\mathbf{k} = k\,(1,1)$.

(d) Analyzing the concavity of the band dispersion in item (c), classify each pocket of the Fermi surface of item (b) in electron-like or hole-like depending on whether the corresponding band disperses downwards or upwards, respectively.