Solid State Physics

Homework Ch2 No.2, Due on Mar 25th, Friday

1. (a) From the relation between the Wannier function and the Bloch eigenstates: $f_n(\mathbf{R},\mathbf{r}) = \frac{1}{v_0}\int d^3\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}}\Psi_{n\mathbf{k}}(\mathbf{r})$, show that $\int f_n^*(\mathbf{R},\mathbf{r}) f_{n'}(\mathbf{R}',\mathbf{r}) d^3\mathbf{r} \propto \delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}$, where the orthogonality of the Bloch states $\Psi_{n\mathbf{k}}(\mathbf{r})$ can be applied.
(b) In particular, find the proper normalization factor so that $\int f_n^*(\mathbf{R},\mathbf{r}) f_{n'}(\mathbf{R}',\mathbf{r}) d^3\mathbf{r} = \delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}$.

2. Problem No.2 in Chapter 10 of "Solid State Physics" by Ashcroft/Mermin, "Tight-Binding p-Bands in Cubic Crystals". Questions (a)-(d).

3. Consider a one-dimensional lattice Hamiltonian $H = -\frac{1}{2}\nabla_x^2 + U(x)$, with $U(x) = -V_0\cos^2(k_0 x)$, where the constant $V_0 > 0$ denotes the amplitude of periodic lattice potential and $k_0 = \pi/a$, with a the lattice constant. For simplicity, here we take that the mass $m = 1$ and $\hbar = 1$. Thus the recoil energy reads $E_R = \hbar^2 k_0^2/2m = k_0^2/2$. The Bloch states of the Hamiltonian can be solved by plane-wave expansion

$$\Psi_k = \sum_l c_l e^{ikx + i\frac{2l\pi}{a}x}, \tag{1}$$

where $-k_0 \le k < k_0$ and l sums over all integers. Note that $2l\pi/a$ is a just reciprocal lattice vector.
(a) Find the secular equation for the coefficients c_l.
(b) Numerically solve the Bloch energy $\mathcal{E}_k$ for the lowest band under certain value of V_0, e.g. $V_0 = 3E_R$, and plot $\mathcal{E}_k$ as a function of k. This can be done by taking a cut-off l_0 for the summation of l, namely, l sums over for $l = -l_0$ to $l = l_0$. For simplicity, you can take $a = 1$ so that $k_0 = \pi$ and then $E_R = \pi^2/2$. For $V_0 = 3E_R$, you can see that by taking $l_0 = 5$, the numerically solved $\mathcal{E}_k$ of the lowest band is already very close to the exact solution (that's to say, if you increase the value of the cut-off l_0 the solution almost does not change). In your calculation and plot, you can take say 30 values of k within $[-k_0, k_0]$, namely, let $k = -\pi, -14\pi/(15), ..., 14\pi/(15), \pi$.

The following two are NOT homework problems, but you are encouraged to work out.

4. For the problem 3, find the Wannier function $f(x, R)$ for $R = 0$ of the lowest band. On the other hand, expand the potential $U(x)$ around $x = 0$ and keep the harmonic term, i.e. up to x^2. Solve the lowest eigen-function $\phi_0(x)$ for the harmonic potential. Then calculate the overlapping integral $\langle f(x, R = 0)|\phi_0(x)\rangle$ and compare it with unity. In particular, check the cases with $V_0 = 10E_R$ and $V_0 = 1.0E_R$.

5. *1D optical Raman lattice.*–An optical lattice for atoms is formed by standing wave laser which can provide a periodic trapping potential for neutral atoms. The atoms moving in the optical lattice is similar to the electrons moving in the periodic crystal potential. Optical lattice is a crucial platform for quantum simulation. We consider an optical Raman lattice, which was proposed recently and widely studied in theory and experiment. Particularly, for the 1D regime with spin-1/2 atoms. The Hamiltonian is given below

$$H(x) = \frac{p_x^2}{2m} - V_0\cos^2 k_0 x + M_0 \sin k_0 x \sigma_x + \frac{\delta}{2}\sigma_z, \tag{2}$$

where the second term is a spin-independent lattice potential of amplitude V_0, and the third term gives a so-called *Raman lattice potential* with amplitude M_0, which can induce spin-flip hopping transition. You may find that at each site of the spin-independent lattice, the Raman lattice potential vanishes. Accordingly, the Raman lattice potential is anti-symmetric with respect to each site of the spin-independent lattice (you can verify this by plotting the potentials). The term

$\frac{\delta}{2}\sigma_z$ denotes the Zeeman energy splitting. Consider the lowest s-band model, the tight-binding Hamiltonian with nearest-neighboring hopping takes the form

$$H_{\rm TB} = -\sum_{\langle i,j\rangle,\sigma=\uparrow,\downarrow} t_0^{ij}|\varphi_{i\sigma}\rangle\langle\varphi_{j\sigma}| + \sum_{\langle i,j\rangle}(t_{\rm so}^{ij}|\varphi_{j\uparrow}\rangle\langle\varphi_{j+1\downarrow}| + \text{h.c.}) + \sum_i \frac{\delta}{2}(|\varphi_{i\uparrow}\rangle\langle\varphi_{i\uparrow}| - |\varphi_{i\downarrow}\rangle\langle\varphi_{i\downarrow}|), \quad (3)$$

where $|\varphi_{i\sigma}\rangle$ denotes the Wanneir function at the site R_i of the spin-independent lattice and in the spin state σ. Here the spin-conserved hopping couplings t_0^{ij} are due to the spin-independent lattice potential, given by

$$t_0^{ij} = -\int dx \varphi_{i\sigma}(x)\left[\frac{\hbar^2 p_x^2}{2m} - V_0\cos^2 k_0 x\right]\varphi_{j\sigma}(x), \quad (4)$$

and the Raman-coupling driven spin-flip hopping coefficients $t_{\rm so}^{ij}$ are

$$t_{\rm so}^{ij} = \int dx \varphi_{i\uparrow}(x)\big(M_0\sin k_0 x\sigma_x\big)\varphi_{j\downarrow}(x). \quad (5)$$

(a) Since the wavefunctions $\varphi_{i\sigma}(x)$ are spin-independent (due to the spin-independent lattice) and satisfy $\varphi_{j\sigma}(x) = \phi_\sigma^{(0)}(x - x_j)$, show that $t_0^{ij} = -t_0$ is a constant in the whole lattice, with

$$t_0 = -\int dx \varphi_\sigma^{(0)}(x)\left[\frac{\hbar^2 p_x^2}{2m} - V_0\cos^2 k_0 x\right]\phi_\sigma^{(0)}(x - a). \quad (6)$$

(b) On the other hand, from the relative space antisymmetry of Raman lattice potential with respect to each lattice site, show that

$$t_{\rm so}^{j,j\pm1} = \pm(-1)^j t_{\rm so}, \quad (7)$$

with (pay attention to the subtle difference compared with Eq. (5))

$$t_{\rm so} = M_0\int dx \varphi_\sigma^{(0)}(x)\sin(k_0 x)\phi_\sigma^{(0)}(x - a). \quad (8)$$

(c) The staggered property of the spin-flip hopping can be absorbed by a gauge transformation that $|\varphi_{j\downarrow}\rangle \to -e^{i\pi x_j/a}|\varphi_{j\downarrow}\rangle$. Show that after this transformation the tight-binding model reads

$$\begin{aligned} H_{\rm TB} &= -t_0\sum_{\langle i,j\rangle}(|\varphi_{i\uparrow}\rangle\langle\varphi_{j\uparrow}| - |\varphi_{i\downarrow}\rangle\langle\varphi_{j\downarrow}|) + \sum_i \frac{\delta}{2}(|\varphi_{i\uparrow}\rangle\langle\varphi_{i\uparrow}| - |\varphi_{i\downarrow}\rangle\langle\varphi_{i\downarrow}|) \\ &+ \left[\sum_j t_{\rm so}(|\varphi_{j\uparrow}\rangle\langle\varphi_{j+1\downarrow}| - |\varphi_{j\uparrow}\rangle\langle\varphi_{j-1\downarrow}|) + \text{h.c.}\right]. \end{aligned} \quad (9)$$

It can be seen that the gauge transformation effectively reverses the sign of the hopping coefficient (in the first term) of spin-down states.

(d) The Bloch Hamiltonian by transforming $H_{\rm TB}$ to momentum space finally yields

$$\mathcal{H}(k_x) = (\frac{\delta}{2} - 2t_0\cos k_x a)\sigma_z + 2t_{\rm so}\sin k_x a\sigma_y. \quad (10)$$

This result is similar to the SSH model, but here the Pauli matrices describe the real spin, not the sublattice degree of freedom (here we have real spin-orbit coupling!), so the topological classification is indeed different. You can easily check that the nontrivial topological phase is obtained when $|\delta/2| < 2t_0$.

Solid State Physics

Homework Ch2 No.1, Due on Mar 18th, Friday

1. Problem No.1 in Ch8 of "Solid State Physics" by Ashcroft/Mermin, "Periodic potential in One Dimension". Questions (a)-(h). (Each subproblem counts 5 points)

2. Consider a one-dimensional lattice Hamiltonian $H = P_x^2/2m + U(x)$, with $U(x) = -V_a \cos^2(k_0 x)$, where the constant $V_a > 0$ denotes the amplitude of periodic lattice potential and k_0 denotes the periodicity. Assume that $V_a \ll E_R$, with $E_R = \hbar^2 k_0^2/2m$ called *recoil energy*. (Each subproblem counts 5 points)
   (a) Find the momentum component of $U_{\mathbf{K}}$, with $\mathbf{K} = K\hat{e}_x$.
   (b) Solve the energy $\mathcal{E}_{k_x}$ of the Bloch states ψ_{k_x} of the "lowest band" with momentum $|k_x| \ll k_0$ up to the order of V_a^2. The "lowest band" means that the energy of the states with momentum k_x without lattice potential (i.e. $V_a = 0$) should be $\mathcal{E}_{k_x}^{(0)} = \hbar^2 k_x^2/2m$.
   (c) The gap between the lowest and the second bands is opened at $k_x = \pm k_0$. Solve the magnitude of the gap up to the order of V_a and V_a^2, respectively.

3. (This is *not* a homework problem) Please read through the content in textbook (chapter 8) regarding the density of states (DOS), and the van Hove singularity and try to answer the questions given in lecture notes Ch2-2.