Solid State Physics 2 - Problem set 1

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1. Study the tight-binding model in the hexagonal/triangular lattice, assuming only nearest-neighbor hopping. I usually take the primitive vectors to be

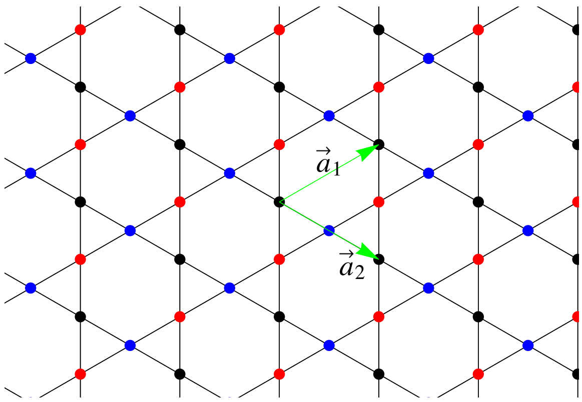
$$\boldsymbol{a}_1 = \frac{a}{2}(\sqrt{3}, 1), \qquad \boldsymbol{a}_2 = \frac{a}{2}(\sqrt{3}, -1) \tag{1}$$

   where a is the lattice spacing. But feel free to choose any other lattice vector you wish.

2. Study the tight-binding model in the Kagomé lattice, assuming nearest-neighbor interactions. The Bravais lattice is the hexagonal, with primitive vectors given by (1). Each unit cell contains 3 atoms in the basis, at positions

$$\boldsymbol{s}_1 = (0, 0), \qquad \boldsymbol{s}_2 = \boldsymbol{a}_2/2, \qquad \boldsymbol{s}_3 = (\boldsymbol{a}_2 - \boldsymbol{a}_1)/2 \tag{2}$$

   The Kagomé lattice is illustrated in the figure below, with $\boldsymbol{s}_1$, $\boldsymbol{s}_2$ e $\boldsymbol{s}_3$ represented by black, blue and red dots respectively.



3. Consider a particle moving in a one-dimensional lattice of spacing a, which we model by a Hamiltonian of the form

$$H = \frac{p^2}{2m} + U(x) \tag{3}$$

   where $U(x+a) = U(x)$ is the periodic potential produced by the atoms.

(a) Derive Bloch's theorem. That is, show that the eigenfunctions of this Hamiltonian may be written as

$$\psi_{k,\alpha} = e^{ikx} u_{k,\alpha}(x) \tag{4}$$

where α is a quantum number called the *band index*, $k \in [-\frac{\pi}{a}, \frac{\pi}{a}]$ and $u_{k,\alpha}(x+a) = u_{k,\alpha}(x)$ is a periodic function. Bloch's theorem says that if the potential is periodic, then so will $|\psi|^2$. But ψ itself is not, since it has a phase e^{ikx}.

(b) Consider now the **Wannier functions** defined as

$$\chi_{n,\alpha}(x) = \frac{1}{\sqrt{N}} \sum_k e^{ikx_n} \psi_{k,\alpha}(x) \tag{5}$$

where $x_n = an$ is the position of atom n in the one-dimensional lattice. The sum over k here is over all allowed values of k, which are quantized as

$$k = \frac{2\pi\ell}{Na}, \qquad \ell = -\frac{N}{2}, \ldots, \frac{N}{2}$$

The Bloch wavefunctions are completely delocalized (spread out through all space), whereas the Wannier functions are very localized within site n.

(c) Check that the Wannier functions satisfy $\chi_{n,\alpha}(x) = \chi_{0,\alpha}(x - x_n)$. This means we only really need to understand $\chi_{0,\alpha}$. The others are simply constructed by translations. Check also that the Wannier functions form an orthonormal basis set, provided of course this is also true for the Bloch functions.

(d) Have some fun with Wannier functions. In particular, find the Wannier functions when $u_{k,\alpha}(x) = \text{const}$. Make a plot of $\chi(x)$ in this case. It should look cute and localized.

4. The goal of this exercise is to show how one may derive the tight-binding Hamiltonian from Wannier functions. Consider the second-quantized version of the single-particle Hamiltonian (3):

$$\mathcal{H} = \int \mathrm{d}x \; \psi^\dagger(x) \Big[-\frac{\partial_x^2}{2m} + U(x) \Big] \psi(x) \tag{6}$$

where $\psi(x)$ is the annihilation operator for position n. The particles may be either Bosons or Fermions. The calculations will hold in both cases. Perform a change of variables from $\psi(x)$ to the discrete set of operators $b_{n,\alpha}$ according to

$$\psi(x) = \sum_{n,\alpha} \chi_{n,\alpha}(x) b_{n,\alpha} \tag{7}$$

where $\chi_{n,\alpha}$ are the Wannier functions defined in Eq. (5). Show that the Hamiltonian (6) may be written as

$$\mathcal{H} = -\sum_{n,m,\alpha,\beta} g_{\alpha,\beta}(n,m) b_{n,\alpha}^\dagger b_{m,\beta} \tag{8}$$

where

$$g_{\alpha,\beta}(n,m) = -\int \mathrm{d}x\ \chi_{n,\alpha}^*(x)\left[-\frac{\partial_x^2}{2m} + U(x)\right]\chi_{m,\beta}(x) \tag{9}$$

Since $U(x)$ is periodic and since $\chi_{n,\alpha}(x) = \chi_{0,\alpha}(x - x_n)$, we may write these transition amplitudes as

$$g_{\alpha,\beta}(n,m) = -\int \mathrm{d}x\ \chi_{0,\alpha}^*(x - x_n + x_m)\left[-\frac{\partial_x^2}{2m} + U(x)\right]\chi_{0,\beta}(x) \tag{10}$$

Hence $g_{\alpha,\beta}(n,m)$ depends only on the distance $x_n - x_m$. Moreover, it is related to the overlap of $H\chi_{0,\beta}(x)$ and $\chi_{0,\alpha}(x - x_n + x_m)$. The former is localized around $x = 0$, whereas the latter is localized around $x = x_n - x_m$. Consequently, the integral will only give a meaningful value when $x_n - x_m$ is small. This is how we justify choosing only nearest neighbors.

5. Consider a system described by two operators, a and b, which may be either Fermionic or Bosonic. Suppose that the Hamiltonian is given by

$$H = \epsilon(a^\dagger a + b^\dagger b) + g(a^\dagger b + b^\dagger a) \tag{11}$$

where ϵ and g are arbitrary parameters. Diagonalize this Hamiltonian by looking for new operators α and β which are linear combinations of a and b. Discuss the energy spectrum and the eigenvectors separately for Fermions and Bosons.

6. Consider now a system, similar to the previous problem, but with Hamiltonian

$$H = \epsilon(a^\dagger a + b^\dagger b) + g(a^\dagger b^\dagger + ba) \tag{12}$$

This Hamiltonian can be diagonalized by a **Bogoliubov transformation**. This type of problem appears often in problems such as superfluidity, superconductivity, quantum phase transitions and so on. The procedure must be done separately for Fermions and Bosons.

(a) Fermions: Introduce a new set of operators according to the transformation

$$\begin{aligned} a &= u\alpha - v\beta^\dagger \\ b &= u\beta + v\alpha^\dagger \end{aligned} \tag{13}$$

where u and v are complex numbers. Impose that α and β continue to satisfy the same algebra (i.e., the same commutation relations) as a and b. Discuss what constraints this imposes into u and v. Then insert the transformation (14) back into the Hamiltonian (12) and choose the coefficients u and v such that the terms proportional to $\alpha^\dagger\beta^\dagger$ and $\beta\alpha$ are zero. This is how you obtain a diagonal Hamiltonian. Find the corresponding energy eigenvalues of the system.

(b) Bosons: for Bosons, the Bogoliubov transformation comes out a little different

$$
\begin{aligned}
a &= u\alpha - v\beta^\dagger \\
b &= u\beta - v\alpha^\dagger
\end{aligned}
\tag{14}
$$