TFY4210, Quantum theory of many-particle systems, 2015: Tutorial 4

1. Band dispersion and hopping matrix element in the "tight-binding" description.

In the tight-binding description one considers a crystal composed of weakly coupled atoms. Consider the problem of an electron in a crystal subject to the periodic potential $u(\boldsymbol{r})$ given by the sum of the potential energy from all atoms. The Schrödinger equation is

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + u(\boldsymbol{r})\right\}\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon(\boldsymbol{k})\phi_{\boldsymbol{k}}(\boldsymbol{r}) \tag{1}$$

where $\boldsymbol{k}$ is in the 1st Brillouin zone. Here

$$u(\boldsymbol{r}) = \sum_{\boldsymbol{R}} u_{\text{atom}}(\boldsymbol{r} - \boldsymbol{R}) \tag{2}$$

where $u_{\text{atom}}(\boldsymbol{r})$ is the potential energy due to the atom centered at the lattice site located at position $\boldsymbol{R}$. Define

$$h_a(\boldsymbol{r}) = -\frac{\hbar^2}{2m}\nabla^2 + u_{\text{atom}}(\boldsymbol{r}) \tag{3}$$

which is the Hamiltonian for an electron that only feels the potential due to an atom located at the origin $\boldsymbol{R} = 0$. Let $\chi_n(\boldsymbol{r})$ and ε_n be the associated electronic eigenfunctions and energy levels for this atom, i.e. $h_a(\boldsymbol{r})\chi_n(\boldsymbol{r}) = \varepsilon_n\chi_n(\boldsymbol{r})$. Furthermore, define

$$\Delta u(\boldsymbol{r}) = \sum_{\boldsymbol{R}\neq 0} u_{\text{atom}}(\boldsymbol{r} - \boldsymbol{R}). \tag{4}$$

Then (1) can be written

$$(h_a(\boldsymbol{r}) + \Delta u(\boldsymbol{r}))\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon(\boldsymbol{k})\phi_{\boldsymbol{k}}(\boldsymbol{r}). \tag{5}$$

(a) By multiplying (5) with $\chi_n^*(\boldsymbol{r})$ from the left and integrating over $\boldsymbol{r}$, derive the following set of equations for $\varepsilon(\boldsymbol{k})$:

$$[\varepsilon(\boldsymbol{k}) - \varepsilon_n]\int d^3r\; \chi_n^*(\boldsymbol{r})\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \int d^3r\; \chi_n^*(\boldsymbol{r})\Delta u(\boldsymbol{r})\; \phi_{\boldsymbol{k}}(\boldsymbol{r}). \tag{6}$$

(b) We write $\phi_{\boldsymbol{k}}(\boldsymbol{r})$ as

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}g(\boldsymbol{r} - \boldsymbol{R}). \tag{7}$$

Show that this form satisfies Bloch's theorem, i.e. $\phi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}v_{\boldsymbol{k}}(\boldsymbol{r})$ where $v_{\boldsymbol{k}}(\boldsymbol{r})$ is periodic in the lattice, i.e. $v(\boldsymbol{r} + \boldsymbol{R}) = v(\boldsymbol{r})$ for an arbitrary lattice vector $\boldsymbol{R}$.

(c) The unknown function $g(\boldsymbol{r})$ can be expanded in the set of electronic eigenfunctions χ_n for the single-atom problem:

$$g(\boldsymbol{r}) = \sum_n c_n \chi_n(\boldsymbol{r}). \tag{8}$$

In the lectures we demonstrated that in the atomic limit, i.e. when the atoms in the crystal are so far apart that they are effectively decoupled from each other, only one term in the sum contributes to each solution, i.e. the solution labeled by n takes the form $c_n = 1$, $c_m = 0$ for $m \neq n$ (this is for nondegenerate atomic energy levels, which we assume here for simplicity). By using this an an approximation for the solution in the weakly coupled case, show that the expression for the energy dispersion $\varepsilon_n(\boldsymbol{k})$ for the nth energy band becomes

$$\varepsilon_n(\boldsymbol{k}) = \varepsilon_n + \frac{\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \int d^3r \, \chi_n^*(\boldsymbol{r}) \Delta u(\boldsymbol{r}) \, \chi_n(\boldsymbol{r} - \boldsymbol{R})}{\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \int d^3r \, \chi_n^*(\boldsymbol{r}) \chi_n(\boldsymbol{r} - \boldsymbol{R})}. \tag{9}$$

In the following we will assume that the overlap between the functions χ_n centered on different atoms is so small that the sum in the denominator in (9) is well approximated by the term $\boldsymbol{R} = 0$ only, which gives

$$\varepsilon_n(\boldsymbol{k}) = \varepsilon_n + \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \int d^3r \, \chi_n^*(\boldsymbol{r}) \Delta u(\boldsymbol{r}) \, \chi_n(\boldsymbol{r} - \boldsymbol{R}). \tag{10}$$

(d) The tight-binding representation of the Hamiltonian for a system of electrons in a crystal was derived in the lectures to be

$$H_0 = \sum_n \sum_{\boldsymbol{R},\boldsymbol{R}'} \sum_\sigma t_{n,\boldsymbol{R}\boldsymbol{R}'} c_{n\boldsymbol{R}\sigma}^\dagger c_{n\boldsymbol{R}'\sigma} \tag{11}$$

where the hopping matrix element $t_{n,\boldsymbol{R}\boldsymbol{R}'}$ is given by

$$t_{n,\boldsymbol{R}\boldsymbol{R}'} = \frac{1}{N} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} \varepsilon_n(\boldsymbol{k}). \tag{12}$$

Use Eq. (10) to calculate the rhs of this expression.

2. Electrons on a square lattice.

Consider the following Hamiltonian describing electrons hopping between nearest-neighbour sites on a two-dimensional square lattice:

$$H = -t \sum_{\langle i,j \rangle} \sum_\sigma (c_{j,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}). \tag{13}$$

Here $t > 0$ is the hopping amplitude, i and j are labels for the sites of the square lattice, and $\sigma = \pm 1/2$ labels the electron spin projection. The leftmost sum is over all pairs of nearest-neighbour sites (each such pair being counted once).

(a) Show that the Hamiltonian can be written on the diagonalized form

$$H = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{k},\sigma}, \tag{14}$$

where the sum over $\boldsymbol{k}$ runs over the 1st Brillouin zone of the square lattice. Give the dispersion relation $\varepsilon_{\boldsymbol{k}}$.

(b) Consider the density parameter $n = N_e/N$, where N_e is the number of electrons in the system and N is the number of sites. Show that in the ground state of the system (for a given number N_e of electrons), n is proportional to the $\boldsymbol{k}$-space area enclosed by the Fermi surface and find the proportionality constant.

(c) Sketch the Fermi surface for (i) $n \ll 1$, (ii) $n = 1$, and (iii) $n = 2$.