TFY4210, Quantum theory of many-particle systems, 2013: 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 $U(\mathbf{r})$ given by the sum of the potential energy from all atoms. The Schrödinger equation is

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

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

$$U(\boldsymbol{r}) = \sum_{\boldsymbol{R}} U_{\text{atom}}(\boldsymbol{r} - \boldsymbol{R})$$
⁽²⁾

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

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

which is the Hamiltonian for an electron that only feels the potential due to an atom located at the origin $\mathbf{R} = 0$. Let $\chi_n(\mathbf{r})$ and ε_n be the associated electronic eigenfunctions and energy levels for this atom, i.e. $H_a\chi_n(\mathbf{r}) = \varepsilon_n\chi_n(\mathbf{r})$. Furthermore, define $\Delta U = \sum_{\mathbf{R}\neq 0} U_{\text{atom}}(\mathbf{r}-\mathbf{R})$. Then (1) can be written

$$(H_a + \Delta U)\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon(\boldsymbol{k})\phi_{\boldsymbol{k}}(\boldsymbol{r}).$$
(4)

(a) By multiplying (4) with $\chi_n^*(\mathbf{r})$ from the left and integrating over \mathbf{r} , derive the following set of equations for $\varepsilon(\mathbf{k})$:

$$[\varepsilon(\boldsymbol{k}) - \varepsilon_n] \int d^3r \; \chi_n^*(\boldsymbol{r}) \phi_{\boldsymbol{k}}(\boldsymbol{r}) = \int d^3r \; \chi_n^*(\boldsymbol{r}) \Delta U \phi_{\boldsymbol{k}}(\boldsymbol{r}). \tag{5}$$

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

$$\phi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} g(\mathbf{r} - \mathbf{R}).$$
(6)

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

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

$$g(\mathbf{r}) = \sum_{n} c_n \chi_n(\mathbf{r}).$$
(7)

In the lectures we showed 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 $\varepsilon_n(\mathbf{k})$ for the nth energy band becomes

$$\varepsilon_n(\boldsymbol{k}) = \varepsilon_n + \frac{\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \int d^3r \ \chi_n^*(\boldsymbol{r}) \Delta U \chi_n(\boldsymbol{r} - \boldsymbol{R})}{\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \int d^3r \ \chi_n^*(\boldsymbol{r}) \chi_n(\boldsymbol{r} - \boldsymbol{R})}.$$
(8)

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 (8) is well approximated by the term $\mathbf{R} = 0$ only, which gives

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

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

$$H_0 = \sum_{n} \sum_{\boldsymbol{R}, \boldsymbol{R}'} \sum_{\sigma} t_{n, \boldsymbol{R}\boldsymbol{R}'} c^{\dagger}_{n\boldsymbol{R}\sigma} c_{n\boldsymbol{R}'\sigma}$$
(10)

where the hopping matrix element $t_{n,RR'}$ is given by

$$t_{n,\boldsymbol{R}\boldsymbol{R}'} = \frac{1}{N} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} \varepsilon_n(\boldsymbol{k}).$$
(11)

Use Eq. (9) to calculate the rhs of this expression.

2. A tight-binding model for electrons in a one-dimensional crystal.

Consider a tight-binding model of noninteracting electrons in a one-dimensional crystal with Hamiltonian given by

$$\hat{H} = -t \sum_{j,\sigma} (\hat{c}_{j,\sigma}^{\dagger} \hat{c}_{j+1,\sigma} + \text{h.c.}) + t' \sum_{j,\sigma} (\hat{c}_{j,\sigma}^{\dagger} \hat{c}_{j+2,\sigma} + \text{h.c.}).$$
(12)

Here the sum over j goes over the N sites of the system and periodic boundary conditions are imposed as usual. The first term on the rhs is the same as considered in the lectures. It describes hopping between nearest-neighbour sites in the one-dimensional lattice. The second term on the rhs describes hopping between next-nearest-neighbour sites. These two types of processes have amplitudes -t and t', respectively.

(a) Show that \hat{H} can be written on diagonal form as

$$\hat{H} = \sum_{k,\sigma} \varepsilon_k \hat{c}_{k\sigma}^{\dagger} \hat{c}_{k\sigma} \tag{13}$$

where the wavevector sum is over the 1st Brillouin zone $[-\pi,\pi\rangle$ and

$$\varepsilon_k = -2t\cos k + 2t'\cos 2k \tag{14}$$

(note that here we have for simplicity set the lattice constant a to 1, so the wavevectors become dimensionless).

In the remainder of the problem we take t to be a positive constant and we assume that the system is **half-filled**, i.e. the number of electrons N_e equals the number of sites N. We will consider the ground state of the Hamiltonian for different nonnegative values of t'. The notion of **Fermi points** will be used, so recall that a Fermi point of a one-dimensional system is a wavevector that separates a region of occupied wavevectors from a region of unoccupied wavevectors in the ground state of the system.

(b) Plot ε_k for t' = 0. What are the values of the Fermi points and occupied wavevectors in this case?

(c) Next consider t' to be positive and define the ratio r = t'/t (> 0). Show that there is a critical value r_c such that for $r < r_c$ the system has two Fermi points while for $r > r_c$ the system has four Fermi points. Derive the value of r_c .

(d) Plot ε_k for r = 0.4. What are the values of the Fermi points and occupied wavevectors in this case?

(e) Plot ε_k for r = 1. What are the values of the Fermi points and occupied wavevectors in this case?