TFY4210, Quantum theory of many-particle systems, 2016: Solution to tutorial 4

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

(a) Multiplying with $\chi_n^*(\boldsymbol{r})$ from the left and integrating over \boldsymbol{r} gives

$$\int d^3r \, \chi_n^*(\boldsymbol{r})(h_a + \Delta u(\boldsymbol{r}))\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon(\boldsymbol{k}) \int d^3r \, \chi_n^*(\boldsymbol{r})\phi_{\boldsymbol{k}}(\boldsymbol{r}). \tag{1}$$

Now act with h_a on $\chi_n^*(\mathbf{r})$ to its left.¹ Since h_a is hermitian, the eigenvalue ε_n is real, so this gives

$$\int d^3r \,\chi_n^*(\boldsymbol{r})(\varepsilon_n + \Delta u(\boldsymbol{r}))\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon(\boldsymbol{k}) \int d^3r \,\chi_n^*(\boldsymbol{r})\phi_{\boldsymbol{k}}(\boldsymbol{r}).$$
(2)

Rearranging now gives the desired result.

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

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \sum_{\boldsymbol{R}} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{R})} g(\boldsymbol{r}-\boldsymbol{R}) \equiv e^{i\boldsymbol{k}\cdot\boldsymbol{r}} v_{\boldsymbol{k}}(\boldsymbol{r}).$$
(3)

We have

$$v_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R}) = \sum_{\boldsymbol{R}'} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{R}-\boldsymbol{R}')} g(\boldsymbol{r}+\boldsymbol{R}-\boldsymbol{R}')$$

$$= \sum_{\boldsymbol{R}''} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{R}'')} g(\boldsymbol{r}-\boldsymbol{R}'') = \sum_{\boldsymbol{R}'} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{R}')} g(\boldsymbol{r}-\boldsymbol{R}') = v_{\boldsymbol{k}}(\boldsymbol{r}).$$
(4)

In these expressions \mathbf{R}' runs over the set of lattice vectors in the system and we introduced $\mathbf{R}'' = \mathbf{R}' - \mathbf{R}$. Because of the periodic boundary conditions, the sums over \mathbf{R}'' and \mathbf{R}' in the last line are identical as the shift by \mathbf{R} in the summation variable merely shuffles the terms in the sum.

(c) The result follows by inserting $\phi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} g(\mathbf{r}-\mathbf{R}) \approx \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c_n \chi_n(\mathbf{r}-\mathbf{R})$ into that equation for $\varepsilon(\mathbf{k})$ which has the same same label n, cancelling the common factor c_n on the rhs and lhs, and solving for $\varepsilon(\mathbf{k})$.

$$\int d^3r \, \Phi_1^* \hat{O} \Phi_2 = \int d^3r \, (\hat{O}^{\dagger} \Phi_1)^* \Phi_2,$$

where in the second expression, as indicated by the parentheses, \hat{O}^{\dagger} acts only on Φ_1 .

¹I.e. we are using the definition of the adjoint,

(d) We have

$$t_{n,RR'} = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} \varepsilon_n(\mathbf{k})$$
$$= \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} \left[\varepsilon_n + \sum_{\mathbf{R}''} e^{i\mathbf{k} \cdot \mathbf{R}''} f_n(\mathbf{R}'') \right]$$
(5)

where $f_n(\mathbf{R}) = \int d^3r \ \chi_n^*(\mathbf{r}) \Delta u(\mathbf{r}) \chi_n(\mathbf{r} - \mathbf{R})$. Doing the \mathbf{k} summations using $\frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} = \delta_{\mathbf{R},0}$ gives

$$t_{n,\mathbf{R}\mathbf{R}'} = \varepsilon_n \delta_{\mathbf{R},\mathbf{R}'} + \sum_{\mathbf{R}''} f_n(\mathbf{R}'') \delta_{\mathbf{R}'',\mathbf{R}'-\mathbf{R}} = \varepsilon_n \delta_{\mathbf{R},\mathbf{R}'} + f_n(\mathbf{R}'-\mathbf{R})$$
$$= \varepsilon_n \delta_{\mathbf{R},\mathbf{R}'} + \int d^3 r \ \chi_n^*(\mathbf{r}) \Delta u(\mathbf{r}) \chi_n(\mathbf{r} - (\mathbf{R}'-\mathbf{R})).$$
(6)

The contribution to the tight-binding Hamiltonian H_0 from terms with $\mathbf{R} = \mathbf{R}'$ is

$$\sum_{n} \sum_{\mathbf{R},\mathbf{R}'} \sum_{\sigma} \tilde{\varepsilon}_{n} \delta_{\mathbf{R},\mathbf{R}'} c_{n\mathbf{R}\sigma}^{\dagger} c_{n\mathbf{R}'\sigma} = \sum_{n} \tilde{\varepsilon}_{n} \sum_{\mathbf{R}} \sum_{\sigma} c_{n\mathbf{R}\sigma}^{\dagger} c_{n\mathbf{R}\sigma} = \sum_{n} \tilde{\varepsilon}_{n} \hat{N}_{n}$$
(7)

where $\tilde{\varepsilon}_n = \varepsilon_n + \int d^3r \ \chi_n^*(\mathbf{r}) \Delta u(\mathbf{r}) \chi_n(\mathbf{r})$ and $\hat{N}_n = \sum_{\mathbf{R}} \sum_{\sigma} c_{n\mathbf{R}\sigma}^{\dagger} c_{n\mathbf{R}\sigma}$ is the total number operator for electrons in band n. Unless the total Hamiltonian of the problem contains any terms causing inter-band transitions, $\sum_n \tilde{\varepsilon}_n \hat{N}_n$ can be replaced by a constant (i.e. \hat{N}_n is replaced by the eigenvalue N_n , whose value is the constant total number of electrons in band n) which in turn can be neglected as it only gives a constant shift of the energy of the system. This gives

$$H_0 = \sum_{n} \sum_{\boldsymbol{R} \neq \boldsymbol{R}'} \sum_{\sigma} t_{n \boldsymbol{R} \boldsymbol{R}'} c_{n \boldsymbol{R} \sigma}^{\dagger} c_{n \boldsymbol{R}' \sigma}$$
(8)

which describes electrons hopping between different sites on a lattice. Thus H_0 can be interpreted as the *kinetic energy* operator for the electrons on the lattice. But note that the parameters $t_{n\mathbf{R}\mathbf{R}'}$ in H_0 arise from the contribution $\Delta u(\mathbf{r})$ to the *potential energy* (Coulomb interaction energy) between the electrons and the lattice ions.

2. Electrons on a square lattice.

(a) We introduce Fourier transformed operators $c_{k\sigma}$ by writing

$$c_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_j} c_{\boldsymbol{k}\sigma} \tag{9}$$

where r_j is the position vector for site j (the vector going from the origin to site j). Here periodic boundary conditions are imposed in both the x and y direction, giving

$$k_x = \frac{2\pi n_x}{L_x}, \quad k_y = \frac{2\pi n_y}{L_y} \tag{10}$$

where n_x , n_y are integers and where $L_x = N_x a$ and $L_y = N_y a$ are the lengths of the system in the x and y directions, with N_x (N_y) being the number of sites in the x (y) direction (so $N = N_x N_y$) and a being the lattice constant. In the following, let us measure distances in units of the lattice constant, so that we set a = 1. Then the wavevectors \mathbf{k} become dimensionless. By choosing $n_x = -N_x/2, \ldots, N_x/2 - 1$ and $n_y = -N_y/2, \ldots, N_y/2 - 1$, the N \mathbf{k} -vectors lie inside the 1st Brillouin zone (1BZ) of the square lattice, which is a square in \mathbf{k} -space centered at $\mathbf{k} = 0$, with sides of length 2π parallel to the x and y axes.

Inserting (9) into H gives

$$\hat{H} = -t \sum_{j,\sigma} \sum_{\delta=\hat{x},\hat{y}} (c_{j,\sigma}^{\dagger}c_{j+\hat{\delta},\sigma} + h.c.)$$

$$= -t \sum_{j,\sigma} \sum_{\delta=\hat{x},\hat{y}} \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} e^{-i\mathbf{k}\cdot\mathbf{r}_{j}} e^{i\mathbf{k}'\cdot(\mathbf{r}_{j}+\hat{\delta})} c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}'\sigma} + h.c.$$

$$= -t \sum_{\sigma} \sum_{\delta=\hat{x},\hat{y}} \sum_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}'\sigma} e^{i\mathbf{k}'\cdot\hat{\delta}} \underbrace{\frac{1}{N} \sum_{j} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_{j}}}_{\delta_{\mathbf{k}\mathbf{k}'}} + h.c.$$

$$= -t \sum_{\kappa\sigma} \sum_{\delta=\hat{x},\hat{y}} c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\hat{\delta}} + h.c.$$

$$= -t \sum_{\kappa\sigma} \sum_{\delta=\hat{x},\hat{y}} c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma} (e^{i\mathbf{k}\cdot\hat{\delta}} + e^{-i\mathbf{k}\cdot\hat{\delta}})$$

$$= -t \sum_{\kappa\sigma} \sum_{\delta=\hat{x},\hat{y}} \cos(\mathbf{k}\cdot\hat{\delta})c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}$$

$$= -2t \sum_{\kappa\sigma} \sum_{\hat{\delta}=\hat{x},\hat{y}} \cos(\mathbf{k}\cdot\hat{\delta})c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}$$

$$= -2t \sum_{\kappa\sigma} \sum_{\hat{\delta}=\hat{x},\hat{y}} \cos(\mathbf{k}\cdot\hat{\delta})c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}$$

$$= \sum_{\kappa\sigma} \varepsilon_{\mathbf{k}}c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}$$
(11)

with

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y). \tag{12}$$

(b) Since H is diagonal in the $(\mathbf{k}\sigma)$ single-particle basis, the ground state for a given particle number N_e is obtained by filling the N_e single-particle states with lowest energy, with the restriction (from the Pauli principle) that each $(\mathbf{k}\sigma)$ can accommodate no more than 1 fermion. The energy $\varepsilon_{\mathbf{k}}$ of a $(\mathbf{k}\sigma)$ state only depends on \mathbf{k} , with the lowest-energy state at $\mathbf{k} = 0$. By plotting a contour plot of $\varepsilon_{\mathbf{k}}$ (i.e. a plot of constant-energy lines $\varepsilon_{\mathbf{k}} = c$ in \mathbf{k} -space, for various choices of c, see Fig. 1) one can convince oneself that the \mathbf{k} -states filled in the ground state make up a single connected region in the 1BZ (i.e. there are no "holes" of unfilled \mathbf{k} -states in the interior of this region). The Fermi "surface" is the boundary of this region of filled \mathbf{k} -states, such that all the \mathbf{k} -states on the Fermi surface have the same



Figure 1: Contour plot of $\varepsilon_{\mathbf{k}}$ in the 1st Brillouin zone.

energy ε_F (the Fermi energy). Thus the total number of electrons N_e can be expressed as

$$N_e = 2 \sum_{\substack{\boldsymbol{k} \\ \varepsilon_{\boldsymbol{k}} \leq \varepsilon_F}} 1 \tag{13}$$

where the factor 2 comes about because each occupied k has 2 electrons (one with spin up and one with spin down). In the thermodynamic limit we rewrite the sum as an integral as explained in the lectures, giving

$$N_e = 2 \frac{N_x}{2\pi} \frac{N_y}{2\pi} \int_{\varepsilon_k \le \varepsilon_F} dk_x dk_y.$$
(14)

Here the integral is $A_{\rm FS}$, the **k**-space area enclosed by the Fermi surface. Dividing by $N = N_x N_y$ we get that the density $n = N_e/N$ is given by

$$n = \frac{2}{(2\pi)^2} A_{\rm FS} = \frac{A_{\rm FS}}{2\pi^2}.$$
 (15)

Thus the proportionality constant is $1/(2\pi^2)$. Note that if we had not set the lattice constant a to 1, the quantity $A_{\rm FS}$ would have had dimension (length)⁻², and there would have been an additional factor a^2 in the proportionality constant.

(c) Note that the area of the 1BZ, denoted A_{1BZ} , is $(2\pi)^2$. Thus Eq. (15) can be written

$$\frac{A_{\rm FS}}{A_{\rm 1BZ}} = \frac{n}{2}.\tag{16}$$

(i) $n \ll 1$. Using Eq. (16) this corresponds to $A_{\rm FS} \ll A_{\rm 1BZ}$. Thus only **k**-states close to $\mathbf{k} = 0$ are filled. As seen from Fig. 1, in the vicinity of $\mathbf{k} = 0$ the equal-energy contours are approximately circular. Thus in this case the Fermi surface is approximately circular.

(ii) n = 1. This corresponds to $A_{\rm FS} = A_{1\rm BZ}/2$. From Fig. 1 one sees that the area inside the inscribed square (which is rotated by 45 degrees wrt the 1BZ) is exactly half the area of the Brillouin zone. Thus this square is the Fermi surface for n = 1.

(iii) n = 2. This corresponds to $A_{\rm FS} = A_{1\rm BZ}$. So all \mathbf{k} -states in the 1BZ are occupied. To understand what the Fermi surface looks like, it is helpful first to look at the case when n is a little less than 2, so that nearly all \mathbf{k} -states are occupied. From Fig. 1 one sees that the unoccupied states lie in the 4 corner regions of the 1BZ, where the equal-energy contours are approximately circular. Thus the Fermi surface consists of 4 quarter-circles, each one centered around a corner of the 1BZ. As $n \to 2$ the radius of these quarter-circles shrinks to 0. Thus for n = 2 the Fermi surface consists of the 4 corner points of the 1BZ. (Note, however, that these 4 corner \mathbf{k} -points are actually all equivalent, as they differ from each other by reciprocal lattice vectors.)

The Fermi surfaces for the cases (i), (ii), and (iii) are shown in red in Fig. 2 (the case of n a little less than 2 is also shown). The Fermi sea of occupied k-vectors in the ground state is the grey region enclosed by the Fermi surface, its area being given by (16).



Figure 2: Fermi surface (red curve) and Fermi sea (grey region) for $n \ll 1$ (upper left), n = 1 (upper right), n a little less than 2 (lower left), and n = 2 (lower right).