Systems of non-interacting electrons

We now turn to a brief discussion of noninteracting electrons, which we'll define here as electrons that do not interact among themselves. Of course this is a fictional scenario since in reality electrons interact with each other via the Coulomb interaction. Nevertheless, there are several reasons why it is still worth discussing systems in which interactions between the particles are artificially neglected. First, non-interacting systems are much simpler than interacting ones, so we address them first because "you have to learn to crawl before you can learn to walk." Second, common approaches to interacting systems include (i) various types of perturbation theory, where one perturbs around a non-interacting system, and (ii) various treatments based on approximating the interacting system with some version of a non-interacting one, in the sense of being described by a Hamiltonian which is quadratic in creation/annihilation operators; for both approaches it is clearly necessary to have a good understanding of the non-interacting case. Third, and quite remarkably, it turns out that as far as low-energy and low-temperature properties are concerned, many electronic systems do in fact behave as *if* they were composed of non-interacting or weakly interacting spin-1/2 charge-*e* fermions (called *Landau quasi-particles*); such systems are known as *Fermi liquids*.

In these notes we will consider two different systems of noninteracting electrons: electrons that are not subjected to any external potential (called the free electron gas), and electrons that are subjected to an external potential that is periodic in space (which describes electrons in a crystal). In the latter case we will limit our discussion to the so-called tight-binding model. (Later we will also consider a very simple¹ model that incorporates some of the interactions between electrons in a crystal, namely the so-called Hubbard model.)

1 The free electron gas

We consider free electrons living in a three-dimensional "box" of macroscopic size with lengths L_x , L_y , and L_z and volume $V = L_x L_y L_z$. As our single-particle basis we take the plane-wave states that are eigenfunctions of the single-particle Schrödinger equation in the box, i.e.

$$\phi_{\boldsymbol{k}\sigma}(\boldsymbol{r},s) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \delta_{s\sigma}.$$
(1)

We use periodic boundary conditions $[\phi_{k\sigma}(\mathbf{r} + L_x \hat{e}_x, s) = \phi_{k\sigma}(\mathbf{r}, s)$ and similarly for the y and z directions], so the allowed wavevectors must satisfy $e^{ik_x L_x} = e^{ik_y L_y} = e^{ik_z L_z} = 1$, which implies that they take the form

$$\boldsymbol{k} = 2\pi \left(\frac{n_x}{L_x} \hat{e}_x + \frac{n_y}{L_y} \hat{e}_y + \frac{n_z}{L_z} \hat{e}_z \right),$$
(2)

¹Simple to write down, but not to solve!

where n_x , n_y , and n_z are arbitrary integers.

The Hamiltonian is simply the kinetic energy operator:

$$\hat{H} = \sum_{\boldsymbol{k},\sigma} \frac{\hbar^2 k^2}{2m} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{k}\sigma}$$
(3)

which is already diagonal in the chosen basis, so the many-particle eigenfunctions are Slater determinants made up of the plane-wave states (1). The ground state of a system with Nelectrons is obtained by filling the N plane-wave states (1) with the lowest possible energy in a way that is consistent with the Pauli principle, i.e. no more than one electron per state $(\mathbf{k}\sigma)$. Since σ can take two values $\pm 1/2$, two electrons may have the same wavevector \mathbf{k} provided they have opposite values of σ . Since the single-particle energy $\hbar^2 k^2/2m$ is independent of σ and only depends on the magnitude of \mathbf{k} (i.e. not on its direction), the ground state is obtained by putting 2 electrons in all \mathbf{k} -states inside a sphere centered around the origin in \mathbf{k} -space whose radius k_F (called the **Fermi wavevector**) is such that there are exactly N/2allowed \mathbf{k} -vectors inside the sphere (here we have assumed that N is an even number). This sphere is called the **Fermi sphere**. The surface of this sphere is called the **Fermi surface**: it separates the occupied \mathbf{k} -states (inside the sphere) from the unoccupied \mathbf{k} -states (outside the sphere). We can express the ground state $|FS\rangle$ (where FS stands for Fermi sphere) in terms of creation operators acting on the vacuum state:

$$|\mathrm{FS}\rangle = \prod_{|\mathbf{k}| \le \mathbf{k}_{\mathrm{F}}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{\mathbf{k}\downarrow} |0\rangle.$$
(4)

Let us now express the particle density n = N/V in terms of k_F . To do this, we write the particle number N as the ground-state expectation value of the total number operator \hat{N} :

$$N = \langle FS|\hat{N}|FS \rangle = \sum_{k,\sigma} \langle FS|\hat{n}_{k\sigma}|FS \rangle = \sum_{k,\sigma} \langle FS|n_{k\sigma}|FS \rangle = \sum_{k,\sigma} n_{k\sigma} = 2\sum_{k} \Theta(k_F - |k|), \quad (5)$$

where $\Theta(x)$ is the Heaviside step function, defined as $\Theta(x) = 1$ if x > 0, $\Theta(x) = 0$ if x < 0. For a system of macroscopic size, neighbouring **k**-states will be very close, since for each direction $\alpha = x, y, z$ the distance between adjacent allowed k values is $\Delta k_{\alpha} = 2\pi/L_{\alpha}$. Therefore the sum over **k** can be well approximated by an integral, as follows: Using that $(L_x/2\pi)\Delta k_x = 1$ etc., we have

$$\sum_{\mathbf{k}} = \frac{L_x}{2\pi} \frac{L_y}{2\pi} \frac{L_y}{2\pi} \sum_{\mathbf{k}} \Delta k_x \Delta k_x \Delta k_z = \frac{V}{(2\pi)^3} \sum_{\mathbf{k}} \Delta k_x \Delta k_y \Delta k_z \to \frac{V}{(2\pi)^3} \int dk_x dk_y dk_z.$$
(6)

The quantity $V/(2\pi)^3$ is thus the density of **k**-states in 3-dimensional **k**-space. Returning to the calculation of N, we note that since the integrand $\theta(k_F - |\mathbf{k}|)$ is spherically symmetric, it is preferable to use spherical coordinates in the integral. Thus we get

$$N = 2 \cdot \frac{V}{(2\pi)^3} \int_0^{2\pi} d\varphi \int_{-1}^1 d(\cos\theta) \int_0^{k_F} dk \, k^2 = 2 \cdot \frac{V}{(2\pi)^3} \cdot 2\pi \cdot 2 \cdot \frac{1}{3} k_F^3 = \frac{V k_F^3}{3\pi^2}, \tag{7}$$

and therefore

$$n = \frac{k_F^3}{3\pi^2}.\tag{8}$$

Next let us calculate the ground state energy E_0 . It can be expressed as the ground-state expectation value of the Hamiltonian:

$$E_{0} = \langle \mathrm{FS}|\hat{\mathrm{H}}|\mathrm{FS}\rangle = \sum_{\mathbf{k},\sigma} \frac{\hbar^{2}\mathbf{k}^{2}}{2\mathbf{m}} \langle \mathrm{FS}|\hat{\mathrm{n}}_{\mathbf{k}\sigma}|\mathrm{FS}\rangle = \sum_{\mathbf{k},\sigma} \frac{\hbar^{2}\mathbf{k}^{2}}{2\mathbf{m}} \langle \mathrm{FS}|\mathrm{n}_{\mathbf{k}\sigma}|\mathrm{FS}\rangle = \sum_{\mathbf{k},\sigma} \frac{\hbar^{2}\mathbf{k}^{2}}{2\mathbf{m}} \mathrm{n}_{\mathbf{k}\sigma}$$
$$= 2\sum_{\mathbf{k}} \frac{\hbar^{2}k^{2}}{2m} \Theta(k_{F} - |\mathbf{k}|) = 2\frac{\hbar^{2}}{2m} \frac{V}{(2\pi)^{3}} \int_{0}^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta) \int_{0}^{k_{F}} dk \, k^{2} \, k^{2}$$
$$= 2\frac{\hbar^{2}}{2m} \frac{V}{(2\pi)^{3}} \cdot 2\pi \cdot 2 \cdot \frac{1}{5} k_{F}^{5} = \frac{V}{5\pi^{2}} \frac{\hbar^{2}k_{F}^{5}}{2m}.$$
(9)

Let us introduce the **Fermi energy** $\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$, which is the energy of the electrons on the Fermi surface (i.e. ε_F is the energy of the most energetic electrons in the ground state). Invoking also Eq. (8) we then get

$$E_0 = \frac{3}{5} N \varepsilon_F. \tag{10}$$

Thus the *average* electron energy in the ground state of an electron gas is 3/5 of the energy of the *most energetic* electrons.

This discussion was for a three-dimensional electron gas. One can also consider the electron gas in two or one dimensions. In the 2D case the Fermi "sphere" of occupied k-states in the ground state will be a disk of radius k_F , and the Fermi "surface" will be the boundary (perimeter) of that disk. In the 1D case the Fermi "sphere" will be a line of length $2k_F$ (i.e. going from $k = -k_F$ to $k = +k_F$), and the Fermi "surface" is merely the two end-points $k = \pm k_F$ of that line (for this reason these points are also called the Fermi points in this 1D case).

2 Tight-binding model for electrons in a crystal

Consider a simple crystal, characterized by its atoms being arranged in an ordered way, such that their equilibrium positions are at the sites of a periodic lattice. In the so-called tight-binding model, each electron is taken to be in an orbital localized around a particular atom² and has a (small) amplitude for tunneling to a different orbital localized around a nearby atom. For simplicity let us assume that only one orbital per atom is relevant for this conduction and furthermore that the crystal is one-dimensional (1D).³ Consider therefore a 1D lattice with N sites.⁴ Let the operator $\hat{c}_{j\sigma}^{\dagger}$ create an electron in the orbital localized around site $j = 1, 2, \ldots, N$ with spin projection $\sigma = \pm 1/2$. We will use periodic boundary

²Technically, these orbitals are called Wannier orbitals. They form a complete orthonormal basis.

³For a general and careful discussion of the tight-binding model, see Ch. 10 of Ashcroft and Mermin, "Solid state physics", Thomson Learning, 1976.

⁴Please note that in this section N stands for the number of sites, while in the previous section N was the number of electrons, which in this section will be called N_{e}

conditions, i.e. $\hat{c}_{j+N,\sigma} = \hat{c}_{j,\sigma}$, which makes the system like a necklace, with the sites being "beads" evenly spaced along it. Let us consider the following Hamiltonian:

$$\hat{H} = -t \sum_{j,\sigma} (\hat{c}^{\dagger}_{j,\sigma} \hat{c}_{j+1,\sigma} + \text{h.c.})$$
(11)

where "h.c." means hermitian conjugate, i.e. the adjoint operator. This Hamiltonian is the kinetic energy operator associated with the electrons hopping between neighbouring sites on the 1D lattice. To see this, consider an electron with spin σ sitting on site ℓ and consider the process of this electron hopping to the site immediately to the right, which has label $\ell + 1$. So in the initial state this electron is on site ℓ while in the final state it has moved to site $\ell + 1$. Mathematically, the hopping can be described as a two-step process: First the electron with spin σ at site ℓ is annihilated, and then the electron with spin σ at site $\ell + 1$ is created. This is effected by the operator $\hat{c}^{\dagger}_{\ell+1,\sigma}\hat{c}_{\ell,\sigma}$. Its h.c. describes the hopping of an electron with spin σ from site $\ell + 1$ to site ℓ . The parameter t > 0 is called the hopping amplitude.⁵

We want to find the eigenstates and eigenvalues of \hat{H} . To this end, we introduce operators creating and annihilating electrons in definite k-states by writing

$$\hat{c}_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{ikr_j} \hat{c}_{k\sigma},\tag{12}$$

where

$$r_j = ja \tag{13}$$

is the position of site j in the lattice, where a is the distance between neighbouring sites (a is usually called the lattice constant). The total length of the system is L = Na. Periodic boundary conditions $\hat{c}_{j\sigma} = \hat{c}_{j+N,\sigma}$ imply that $e^{ikL} = 1$, i.e. the allowed wavevectors take the form $k = 2\pi m/L$ where m is an integer. Because we have (for each value of σ) N operators $\hat{c}_{j\sigma}$ (since $j = 1, 2, \ldots, N$), we also have N independent operators $\hat{c}_{k\sigma}$ corresponding to N inequivalent values of k. It is customary to choose these N k-values to be given by $m = -N/2, -N/2 + 1, \ldots, N/2 - 1$ (here we assumed that N is an even number). This gives $k = -\pi/a, -\pi/a + 2\pi/L, \ldots, \pi/a - 2\pi/L$, which in the limit $N \to \infty$ means that k lies in the region $[-\pi/a, \pi/a)$ which is called the 1st Brillouin zone for the 1D lattice. The inverse transformation is

$$\hat{c}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_{j} e^{-ikr_j} \hat{c}_{j\sigma}.$$
(14)

This can be seen by checking that the transformation and the inverse transformation "undo" each other, thus taking us back to where we started:

$$\hat{c}_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{ikja} \hat{c}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{ikja} \frac{1}{\sqrt{N}} \sum_{j'} e^{-ikj'a} \hat{c}_{j'\sigma}$$

$$= \sum_{j'} \hat{c}_{j'\sigma} \underbrace{\frac{1}{N} \sum_{k} e^{ik(j-j')a}}_{\delta_{jj'}(\text{see Appendix})} = \sum_{j'} \hat{c}_{j'\sigma} \delta_{jj'} = \hat{c}_{j\sigma}.$$
(15)

⁵For a more detailed discussion, see Sec. 3.1 in Nagaosa's "Quantum field theory in strongly correlated electronic systems" and Sec. 2.2 in "Condensed matter field theory" by Altland and Simons (p. 54-55). In our discussion we will just take t as a given parameter.

Note that $\hat{c}_{k+2\pi/a,\sigma} = \hat{c}_{k\sigma}$, which shows that wavevectors that differ by an integer multiple of $2\pi/a$ are equivalent to each other. This is of course consistent with our finding above that we could choose the N inequivalent values of k to all lie inside the 1st Brillouin zone, an interval of length $2\pi/a$. Using the anticommutation relations for the site-labeled operators, i.e.

$$\{c_{j\sigma}, c^{\dagger}_{j'\sigma'}\} = \delta_{jj'}\delta_{\sigma\sigma'}, \quad \{c_{j\sigma}, c_{j'\sigma'}\} = \{c^{\dagger}_{j\sigma}, c^{\dagger}_{j'\sigma'}\} = 0,$$
(16)

one finds that the wavevector-labeled operators satisfy the same kind of canonical anticommutation relations, i.e.

$$\{c_{k\sigma}, c_{k'\sigma'}^{\dagger}\} = \delta_{kk'}\delta_{\sigma\sigma'}, \quad \{c_{k\sigma}, c_{k'\sigma'}\} = \{c_{k\sigma}^{\dagger}, c_{k'\sigma'}^{\dagger}\} = 0.$$
(17)

Using the transformation (12) the sum $\sum_{j} \hat{c}_{j\sigma}^{\dagger} \hat{c}_{j+1,\sigma}$ appearing in \hat{H} becomes

$$\sum_{j} \hat{c}_{j\sigma}^{\dagger} \hat{c}_{j+1,\sigma} = \frac{1}{N} \sum_{j} \sum_{k,k'} e^{-ikja} e^{ik'(j+1)a} \hat{c}_{k\sigma}^{\dagger} \hat{c}_{k'\sigma}$$
$$= \sum_{k,k'} \hat{c}_{k,\sigma}^{\dagger} \hat{c}_{k'\sigma} e^{ik'a} \underbrace{\frac{1}{N} \sum_{j} e^{-i(k-k')ja}}_{\delta_{kk'}(\text{see Appendix})}$$
$$= \sum_{k} e^{ika} \hat{c}_{k\sigma}^{\dagger} \hat{c}_{k\sigma}.$$
(18)

Thus

$$\hat{H} = -t \sum_{k,\sigma} (e^{ika} \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma} + \text{h.c.}) = -t \sum_{k,\sigma} (e^{ika} + e^{-ika}) \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma}, \qquad (19)$$

i.e.

$$\hat{H} = \sum_{k\sigma} \varepsilon_k \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma}, \qquad (20)$$

where the energy function ε_k , often called the *dispersion relation*, is given by

$$\varepsilon_k = -2t\cos ka. \tag{21}$$

Eq. (20) gives \hat{H} as a linear combination of number operators $\hat{n}_{k\sigma} = \hat{c}^{\dagger}_{k\sigma}\hat{c}_{k\sigma}$. The eigenstates and eigenvalues of \hat{H} can then be read off easily. An arbitrary eigenstate $|A\rangle$ of \hat{H} is specified by giving its occupation numbers $n^{(A)}_{k,\sigma}$ (= 0 or 1) for all the single-particle state (k,σ) . The associated eigenvalue E_a is given by

$$E_a = \sum_{k\sigma \in A} \varepsilon_k \tag{22}$$

where the sum runs over those (k, σ) states that are occupied in $|A\rangle$ (i.e. have $n_{k\sigma}^{(A)} = 1$).

Typically we are interested in a system which contains some fixed number of electrons N_e (note that we must have $N_e \leq 2N$ due to the Pauli principle). The occupation numbers $n_{k,\sigma}$ of an eigenstate with N_e electrons therefore satisfies the constraint

$$\sum_{k,\sigma} n_{k,\sigma} = N_e. \tag{23}$$

The ground state of such a system is obtained by filling those $N_e(k, \sigma)$ states that have the smallest energy ε_k . Each k-state can be occupied by two electrons, one having $\sigma = +1/2$ (spin \uparrow) and the other having $\sigma = -1/2$ (spin \downarrow). As ε_k has a minimum at k = 0 and grows monotonically as k moves away from 0 inside the 1st Brillouin zone, the k-states that will be filled are the $N_e/2$ states closest to k = 0, which will enclose a region from $k = -k_F$ to $k = +k_F$ where k_F is the Fermi wavevector. Thus the ground state can again be written on the form (4), and the relationship between the particle density n and k_F can be worked out in a similar way as for the continuum electron gas (and so can the relationship between the ground state energy E_0 and k_F).

Because the constraint (23) can be cumbersome to work with, for convenience one instead often uses a formulation in which the particle number can vary, and only the average number of particles is fixed. This involves replacing the Hamiltonian \hat{H} with the operator

$$\hat{K} = \hat{H} - \mu \hat{N} \tag{24}$$

(sometimes called the "Kamiltonian"), where \hat{N} is the total particle number operator and μ is the so-called chemical potential, which is chosen such that the average number of electrons equals the constant N_e , the actual number of electrons in the system of interest. If one considers such a system at thermal equilibrium at a temperature T, μ becomes a function of temperature, i.e. $\mu = \mu(T)$. For a given value of $\mu(T = 0)$, the ground state of the system is obtained as the eigenstate of \hat{K} with the smallest eigenvalue. As an example of this procedure, consider again the problem of electrons hopping on a 1D lattice. Using that

$$\hat{N} = \sum_{j,\sigma} \hat{c}^{\dagger}_{j\sigma} \hat{c}_{j\sigma} = \sum_{k,\sigma} \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma}$$
(25)

one finds

$$\hat{K} = \sum_{k,\sigma} (\varepsilon_k - \mu) \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma}.$$
(26)

We see that the only difference from (20) is the replacement $\varepsilon_k \to \varepsilon_k - \mu$. The smallest eigenvalue of \hat{K} is obtained by taking $n_{k,\sigma} = 1$ for those k with $\varepsilon_k - \mu < 0$ and $n_{k,\sigma} = 0$ for those k with $\varepsilon_k - \mu > 0$. In other words, all single-particle states (k, σ) with energy ε_k less than $\mu(T = 0)$ are occupied, while all states with higher energy are empty. This shows that the zero-temperature value of the chemical potential is equal to the Fermi energy ε_F of the system.

So far we have considered electrons hopping on a 1D lattice. Of course, electrons hopping on 2- or 3-dimensional lattices is at least as relevant, and it is straightforward to generalize the hopping Hamiltonian (11) to such higher-dimensional lattices. An example is considered in Exercise 1 for Week 16. In this course we limit ourselves to "hypercubic" lattices, i.e. a square lattice in two dimensions and a cubic lattice in three dimensions. Then the associated 1st Brillouin zone becomes a square in two dimensions and a cube in three dimensions, centered at the origin in k-space and with sides of length $2\pi/a$ parallel to the axes of the real-space lattice. Note that when discussing lattice problems like these, one very often chooses to measure distances in units of the lattice spacing a, thus setting a = 1. Then wavevectors become dimensionless, so the sides of the 1st Brillouin zone have length 2π (i.e. running from $-\pi$ to π in each of the D k-space directions for a D-dimensional lattice).

A Some frequently encountered k- and j-sums

In Sec. 2 we used that

$$\sum_{k} e^{ik(j-j')a} = N\delta_{jj'}, \qquad (27)$$

$$\sum_{j} e^{-i(k-k')ja} = N\delta_{kk'}, \qquad (28)$$

where $k = 2\pi m/L$ and $k' = 2\pi m'/L$, with m and m' integers that can take the values $-N/2, \ldots, N/2 - 1$ such that k and k' are in the 1st Brillouin zone $[-\pi/a, \pi/a\rangle$, and $j = 1, 2, \ldots N$.

Let us prove Eq. (27). If j = j' the exponential is 1, so the sum is $N \cdot 1 = N$. If $j \neq j'$, consider the summand which is

$$e^{ik(j-j')a} = e^{i\frac{2\pi}{Na}m(j-j')a} \equiv x^m$$
, where $x \equiv e^{i2\pi(j-j')/N}$. (29)

Since both j and j' can only take values between 1 and N, and we have assumed $j \neq j'$, we get 0 < |j - j'| < N, and therefore $x \neq 1$. We now rewrite the sum as

$$\sum_{k} e^{ik(j-j')a} = \sum_{m=-N/2}^{N/2-1} x^m = x^{-N/2} \sum_{m=0}^{N-1} x^m = x^{-N/2} \frac{1-x^N}{1-x},$$
(30)

where we used the formula for the sum of a geometric series. Since $x \neq 1$ the denominator 1-x is nonzero. Furthermore, $x^N = e^{i2\pi(j-j')} = 1$, so $1-x^N$ vanishes. This proves Eq. (27).

The proof of (28) is very similar and is therefore left to the reader.