Noninteracting electrons

We next turn to a discussion of noninteracting electrons, which we'll define here as electrons that do not interact among themselves.¹ Of course this is strictly speaking a fictional scenario. Nevertheless, there are several reasons why it is still worth discussing systems in which interactions between the electrons are neglected.

- 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." Mathematically, they are described by Hamiltonians that are quadratic ("bilinear") in creation and annihilation operators, i.e. linear combinations of terms like $c^{\dagger}_{\alpha}c_{\beta}$. Such Hamiltonians are either "automatically" diagonal (i.e. given as a linear combination of number operators $c^{\dagger}_{\alpha}c_{\alpha}$) in an appropriately chosen basis (the noninteracting electron gas discussed below is an example) or they can be brought on such diagonal form ("be diagonalized") by transforming to a suitable basis. In contrast, electron-electron interactions are represented by terms in the Hamiltonian of the "quartic" form $c^{\dagger}_{\alpha}c^{\dagger}_{\beta}c_{\gamma}c_{\delta}$, which are much more complicated beasts altogether.
- Two common approaches to interacting systems include (i) various types of **perturbation theory**, where one perturbs around a non-interacting system, and (ii) various types of **mean field theory**, in which one attempts to approximate the interacting system with a non-interacting one, by trying to identify and take into account the most important quartic terms and approximate them with "effective" quadratic terms (since the resulting effective Hamiltonian is quadratic it can be diagonalized in standard ways, thus leading to a solvable theory).
- Quite remarkably, it turns out that as far as various 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 and the theory behind them (developed by Landau in its original form) is called **Fermi liquid theory**.

Thus for the problems which can be analyzed using these theories and approaches, it is clearly useful to understand the properties of noninteracting electrons. We will first consider the simplest example of noninteracting electrons: the free electron gas, i.e. electrons not subjected to any spatially varying external potential.

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 $\Omega = L_x L_y L_z$. As our single-particle basis we take the

¹The definition of "noninteracting" used here is the same as the one used in "Solid state physics" by Ashcroft & Mermin: Electrons are called "noninteracting" if they do not interact with each other. Noninteracting electrons may or may not be "free." Electrons are called free unless they are subjected to an external spatially varying potential (given by a single-particle operator U).

plane-wave states that are eigenfunctions of the single-particle Schrödinger equation in the box, i.e.

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

where n_x , n_y , and n_z are arbitrary integers.

The Hamiltonian is just 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)

Due to its diagonal nature, i.e. the fact that it is simply a linear combination of number operators $\hat{n}_{\boldsymbol{k}\sigma} = \hat{c}^{\dagger}_{\boldsymbol{k}\sigma}\hat{c}_{\boldsymbol{k}\sigma}$, its eigenstates and eigenvalues can be read off easily. An arbitrary eigenstate $|A\rangle$ of \hat{H} is specified by giving its occupation numbers $n^{(A)}_{\boldsymbol{k}\sigma}$ (= 0 or 1) for all single-particle states (\boldsymbol{k}, σ). The eigenstate can be written

$$|A\rangle = \prod_{\boldsymbol{k},\sigma} (c^{\dagger}_{\boldsymbol{k}\sigma})^{n^{(A)}_{\boldsymbol{k},\sigma}} |0\rangle \tag{4}$$

where $|0\rangle$ is the state with no electrons (vacuum state). The associated eigenvalue $E^{(A)}$ is given by

$$E^{(A)} = \sum_{\boldsymbol{k},\sigma} \frac{\hbar^2 k^2}{2m} n^{(A)}_{\boldsymbol{k}\sigma}.$$
(5)

If the system has N electrons, the occupation numbers must satisfy

$$\sum_{\boldsymbol{k},\sigma} n_{\boldsymbol{k}\sigma}^{(A)} = N.$$
(6)

The many-particle eigenfunctions are Slater determinants made up of the plane-wave states (1) that are occupied. The ground state of a system with N electrons is obtained by filling the N plane-wave states 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/2 allowed \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

k-states (inside the sphere) from the unoccupied k-states (outside the sphere). These things are illustrated in Fig. 1. We can express the ground state $|FS\rangle$ (where FS stands for Fermi sphere) in terms of creation operators acting on the vacuum state:

$$|\mathrm{FS}\rangle = \prod_{|\mathbf{k}| \le \mathbf{k}_{\mathrm{F}}} \hat{\mathbf{c}}_{\mathbf{k}\uparrow}^{\dagger} \hat{\mathbf{c}}_{\mathbf{k}\downarrow}^{\dagger} |0\rangle.$$
(7)

Let us now express the particle density $n = N/\Omega$ 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} :

$$N = \langle FS|\hat{N}|FS\rangle = \sum_{k,\sigma} \langle FS|\hat{n}_{k\sigma}|FS\rangle = \sum_{k,\sigma} \langle FS|n_{k\sigma}|FS\rangle = \sum_{k,\sigma} n_{k\sigma} = 2\sum_{k} \Theta(k_F - |k|), \quad (8)$$

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

$$\sum_{\mathbf{k}} = \frac{L_x}{2\pi} \frac{L_y}{2\pi} \frac{L_y}{2\pi} \sum_{\mathbf{k}} \Delta k_x \Delta k_x \Delta k_z = \frac{\Omega}{(2\pi)^3} \sum_{\mathbf{k}} \Delta k_x \Delta k_y \Delta k_z \to \frac{\Omega}{(2\pi)^3} \int dk_x dk_y dk_z.$$
(9)

The quantity $\Omega/(2\pi)^3$ 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

$$N = 2 \cdot \frac{\Omega}{(2\pi)^3} \int_0^{2\pi} d\varphi \int_{-1}^1 d(\cos\theta) \int_0^{k_F} dk \, k^2 = 2 \cdot \frac{\Omega}{(2\pi)^3} \cdot 2\pi \cdot 2 \cdot \frac{1}{3} k_F^3 = \frac{\Omega k_F^3}{3\pi^2}, \tag{10}$$

and therefore

$$n = \frac{k_F^3}{3\pi^2}.\tag{11}$$

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

$$E_{0} = \langle \mathrm{FS}|\hat{\mathrm{H}}|\mathrm{FS}\rangle = \sum_{\mathbf{k},\sigma} \frac{\hbar^{2}\mathbf{k}^{2}}{2\mathbf{m}} \langle \mathrm{FS}|\hat{\mathrm{n}}_{\mathbf{k}\sigma}|\mathrm{FS}\rangle = \sum_{\mathbf{k},\sigma} \frac{\hbar^{2}\mathbf{k}^{2}}{2\mathbf{m}} \langle \mathrm{FS}|\mathrm{n}_{\mathbf{k}\sigma}|\mathrm{FS}\rangle = \sum_{\mathbf{k},\sigma} \frac{\hbar^{2}\mathbf{k}^{2}}{2\mathbf{m}} \mathrm{n}_{\mathbf{k}\sigma}$$
$$= 2\sum_{\mathbf{k}} \frac{\hbar^{2}k^{2}}{2m} \Theta(k_{F} - |\mathbf{k}|) = 2\frac{\hbar^{2}}{2m} \frac{\Omega}{(2\pi)^{3}} \int_{0}^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta) \int_{0}^{k_{F}} dk \, k^{2} \, k^{2}$$
$$= 2\frac{\hbar^{2}}{2m} \frac{\Omega}{(2\pi)^{3}} \cdot 2\pi \cdot 2 \cdot \frac{1}{5} k_{F}^{5} = \frac{\Omega}{5\pi^{2}} \frac{\hbar^{2}k_{F}^{5}}{2m}.$$
(12)

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. (11) we then get

$$E_0 = \frac{3}{5} N \varepsilon_F. \tag{13}$$



Figure 1: Fermi spheres, Fermi surfaces, and Fermi wavevectors in 3, 2, and 1 dimensions.

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

We have here discussed 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). These things are illustrated in Fig. 1.