Fermi Quantities

By: Albert Liu

We now apply quantum mechanics for the first time. Since we are concerned with non-relativistic particles, we use the time independent Schrodinger equation with zero potential ($V(x, y, z) = 0$):

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) = E\psi(x,y,z) \tag{1}$$

Since we will be examining the general properties of electrons in metals, the shape of our metal is not important (as long as it's big). We use a cube of side length L for convenience. As usual, we need boundary conditions to be able to solve (1). These boundary conditions must mean the electron is confined to our metal cube, and cannot affect the *bulk* properties of the metal (away from the surface). One possibility would be to have the wavefunction go to zero at the cube surface. This is not a good choice however, since this method gives standing wave solutions that aren't suitable for analyzing the motion of the electrons. A better choice is the **Born-von Karman boundary conditions** (a.k.a. periodic boundary conditions), which require:

$$\begin{aligned}\psi(x+L,y,z) &= \psi(x,y,z)\\ \psi(x,y+L,z) &= \psi(x,y,z)\\ \psi(x,y,z+L) &= \psi(x,y,z)\end{aligned} \tag{2}$$

In a way, we have removed the effect of the surface all together, since an electron exiting one face will essentially enter from the opposite face. This satisfies both conditions that our boundary conditions were supposed to satisfy. A solution to the Schrodinger equation that can satisfy these boundary conditions is the well known plane wave:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}} \tag{3}$$

with energy:

$$E(k) = \frac{\hbar^2 k^2}{2m} \tag{4}$$

Recalling the momentum operator $\hat{p} = i\hbar\nabla$, we find this solution is a momentum eigenstate:

$$\hat{p}\psi_{\mathbf{k}}(\mathbf{r}) = \hbar\mathbf{k}\frac{1}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}} \tag{5}$$

with momentum eigenvalue:

$$\mathbf{p} = \hbar\mathbf{k} \tag{6}$$

We now examine the effect of the boundary conditions on the wavefunction. Plugging $\psi_{\mathbf{k}}(\mathbf{r})$ into the boundary conditions:

$$\begin{aligned}\frac{1}{\sqrt{V}}e^{i(k_x x+k_y y+k_z z)} &= \frac{1}{\sqrt{V}}e^{i(k_x(x+L)+k_y y+k_z z)} \\ &= \frac{1}{\sqrt{V}}e^{i(k_x x+k_y(y+L)+k_z z)} \\ &= \frac{1}{\sqrt{V}}e^{i(k_x x+k_y y+k_z(z+L))} \end{aligned} \tag{7}$$

This gives the condition:

$$1 = e^{ik_x L} = e^{ik_y L} = e^{ik_z L} \tag{8}$$

We have thus quantized the wavevector components by:

$$k_x = \frac{2n_x\pi}{L} \quad k_y = \frac{2n_y\pi}{L} \quad k_z = \frac{2n_z\pi}{L} \tag{9}$$

where n_x, n_y, n_z are any integers. If we imagine every possible k vector as a point in **k-space** (k_x, k_y, k_z), we will obtain a grid of points with spacing $\Delta k = \frac{2\pi}{L}$. In k-space, each possible k vector thus occupies a volume $\left(\frac{2\pi}{L}\right)^3$.

We now consider N electrons in the metal volume $V = L^3$. Because of the Pauli exclusion principle for fermions, no two electrons can occupy the same quantum state at the same time. We must remember that electrons have an intrinsic spin (up or down). Two electrons can thus occupy each value of $\mathbf{k} = (k_x, k_y, k_z)$ simultaneously, resulting in $2\left(\frac{L}{2\pi}\right)^3$ modes per unit k-space volume. At absolute zero temperature, all N electrons will fill the k states starting from the lowest energy. Since energy is proportional to k^2, they will fill states from the origin outwards, and for large N the filled states will resemble a sphere in k-space. For a sphere of radius k_0, the number of states $\mathcal{N}$ the sphere will enclose is:

$$\mathcal{N} = 2\left(\frac{L}{2\pi}\right)^3 \frac{4}{3}\pi k_0^3 = \frac{V}{3\pi^2}k_0^3 \tag{10}$$

For N electrons, the modes will occupy a sphere in k-space with radius k_F:

$$N = \frac{V}{3\pi^2}k_F^3 \rightarrow k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}} \tag{11}$$

We call k_F the **Fermi wavevector**, and the surface of this sphere is called the **Fermi surface**. We can also define the **Fermi energy** E_F, **Fermi momentum** p_F, **Fermi velocity** v_F, and **Fermi temperature** T_F:

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} \qquad p_F = \hbar k_F = \hbar\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} \tag{12}$$

$$v_F = \frac{p_F}{m} = \frac{\hbar}{m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} \qquad T_F = \frac{E_F}{k_B} = \frac{\hbar^2}{2mk_B}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} \tag{13}$$

We can also generalize these Fermi quantities to 2D and 1D metals as well. In 2D, k-space will be two dimensional as well, with the same spacing between k states $\Delta k = \frac{2\pi}{L}$. With $2\left(\frac{L}{2\pi}\right)^2$ modes per unit k-space area, the N occupied modes at absolute zero will resemble a circle of radius k_F:

$$N = 2\left(\frac{L}{2\pi}\right)^2 \pi k_F^2 \rightarrow k_F = \sqrt{\frac{2N\pi}{A}} \tag{14}$$

with the associated Fermi energy, Fermi momentum, Fermi velocity, and Fermi temperature:

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2 N\pi}{Am} \qquad p_F = \hbar k_F = \hbar\sqrt{\frac{2N\pi}{A}} \tag{15}$$

$$v_F = \frac{p_F}{m} = \frac{\hbar}{m}\sqrt{\frac{2N\pi}{A}} \qquad T_F = \frac{E_F}{k_B} = \frac{\hbar^2 N\pi}{Amk_B} \tag{16}$$

In 1D, we again have the same k state spacing $\Delta k = \frac{2\pi}{L}$. N electrons will thus occupy N k states, which will cover a k length:

$$k_0 = \frac{1}{2} N \frac{2\pi}{L} \tag{17}$$

where the factor of $\frac{1}{2}$ comes from the spin degeneracy. Since the k states can take on negative values of k and fill from the origin outwards, we divide k_0 by two to find the maximum magnitude k_F:

$$k_F = \frac{k_0}{2} = \frac{N\pi}{2L} \tag{18}$$

The other Fermi quantities are thus:

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2 N^2 \pi^2}{8mL^2} \qquad p_F = \hbar k_F = \frac{\hbar N\pi}{2L} \tag{19}$$

$$v_F = \frac{p_F}{m} = \frac{\hbar N\pi}{2Lm} \qquad T_F = \frac{E_F}{k_B} = \frac{\hbar^2 N^2 \pi^2}{8mL^2 k_B} \tag{20}$$