Solution to Exercise 2.1-1 Free Electron Gas with Constant Boundary Conditions

Illustration

- Consider the free electron gas model but let the boundary conditions be: **$\psi(0) = \psi(L) = 0$**, i.e. we have fixed boundary conditions.
  - Derive the solution to the Schrödinger equation and the density of states for this case.
  - Show that the number of states is the same as for the periodic boundary conditions as given in the backbone.

- For the basic solution and the dispersion relation (energy vs. momentum / wave vector), due to the boundary conditions we now obtain

$$\psi(x, y, z) = A_{\underline{k}} \cdot \sin(k_x \cdot x) \cdot \sin(k_y \cdot y) \cdot \sin(k_z \cdot z)$$

$$E = \frac{\hbar^2 \cdot k^2}{2\,m}$$

  - Obviously, the boundary conditions **$\psi(x = 0) = \psi(x = L) = 0$** (and analogously so for ***y*** and ***z***) are satisfied by

$$k_x = \frac{n_x \cdot \pi}{L}$$

$$n_x = 1, 2, 3, \ldots$$

  - and analogously so for the ***y*** and ***z*** direction. The amplitude factor $A_{\underline{k}}$ follows from the condition that the probability to have the electron in the "box" equals 1:

$$1 = |A_{\underline{k}}|^2 \int_0^L \sin^2(k_x \cdot x)\, dx \int_0^L \sin^2(k_y \cdot y)\, dy \int_0^L \sin^2(k_z \cdot z)\, dz$$

  - Hence, here we have $|A_{\underline{k}}|^2 = (2/L)^3$, independent of $\underline{k}$.

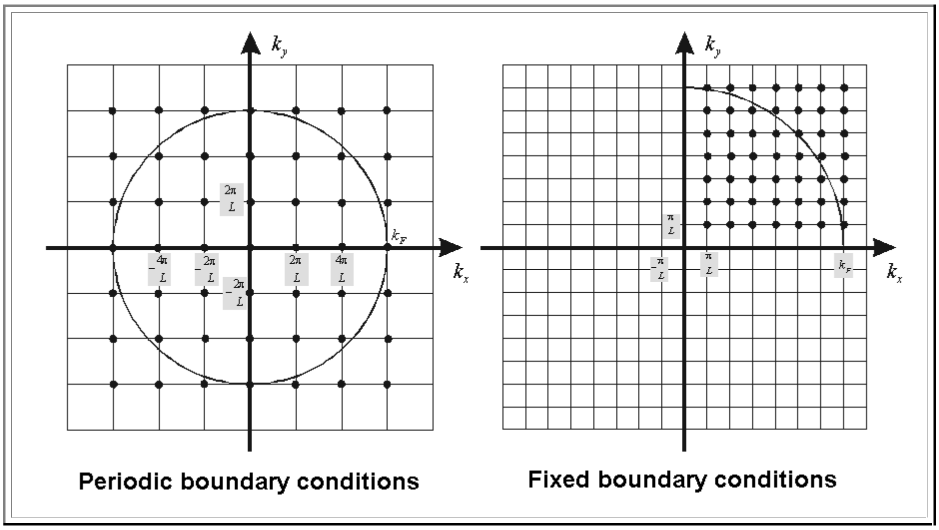
- The number of states $Z(\underline{k})$ up to a wave vector $\underline{k}$ is generally given by

$$Z(k) = \frac{\text{Volume of sphere with radius } E(k)}{\text{Volume of state}}$$

- For fixed boundary conditions we have

$$Z(k) = \frac{1}{8} \cdot \frac{4/3\,(\pi \cdot k)^3}{(\pi/L)^3} = \frac{(k \cdot L)^3}{6\pi^2}$$

- This is exactly what we would get for the periodic boundary conditions – thanks to the factor **1/8**.
  - Where does this factor come from? Easy – since the quantum numbers **n** are restricted to positive integers in this case, we can not count states in **7** of the **8** octants of the complete sphere and must divide the volume of the complete sphere by **8**.
  - This becomes clear if we look at a drawing of the possible states in phase space:



k_y
k_x
k_F
$\frac{2\pi}{L}$
$-\frac{4\pi}{L}$
$-\frac{2\pi}{L}$
$\frac{4\pi}{L}$
$\frac{\pi}{L}$
$-\frac{\pi}{L}$
Periodic boundary conditions
Fixed boundary conditions