Free Electron Gas in Crystals with Unequal Dimensions

Advanced

- If we consider a crystal with dimensions L_x, L_y, L_z, it has the volume $V = L_x \cdot L_y \cdot L_z$.
  - All we have to do is to replace the periodic boundary conditions $\psi(x + L) = \psi(x)$ by:

$$\psi(x + L_x, y, z) \;=\; \psi(x, y + L_y, z) \;=\; \psi(x, y, z + L_z) \;=\; \psi(x, y, z)$$

- This leads to simple expressions for the allowed wave vectors $\mathbf{k}$:

$$k_x \;=\; 0, \quad \pm\frac{2\pi}{L_x}, \quad \pm\frac{4\pi}{L_x}, \quad \ldots$$

$$k_y \quad 0, \quad \pm\frac{2\pi}{L_y}, \quad \pm\frac{4\pi}{L_y}, \quad \ldots$$

$$k_z \quad 0, \quad \pm\frac{2\pi}{L_z}, \quad \pm\frac{4\pi}{L_z}, \quad ..$$

  - The pre-exponential factor, which was $(1/L)^{3/2}$, now changes to $(1/V)^{1/2}$.
- Since all relevant quantities are usually expressed as densities, i.e. divided by V, and the quantization of $\mathbf{k}$ is usually given up in favor of a continuous range of $\mathbf{k}$'s, we may just as well stick to the more simple description of a crystal with equal sides - the results are the same.