

Electron DOS evaluation in the free electron model

We show here different methods to evaluate the electronic DOS according to the system dimensionality.

- 3 D

Method 1: We consider

$$\begin{aligned}
 D(E) &= g \frac{V}{(2\pi)^3} \int \delta(E - E(\vec{k})) d^3k = g \frac{V}{(2\pi)^3} \int \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) d^3k = \\
 &= g \frac{V}{(2\pi)^3} \int_{\mathbb{R}^+} \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) 4\pi k^2 dk = \quad \begin{array}{l} \text{Change of variables} \\ \frac{\hbar^2 k^2}{2m} = \alpha \rightarrow \frac{\hbar^2}{m} k dk = d\alpha \end{array} \\
 &= g \frac{V}{(2\pi)^3} 4\pi \int_{\mathbb{R}^+} \delta(E - \alpha) \sqrt{\alpha} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} d\alpha = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{E} \quad \dots \quad g=2
 \end{aligned}$$

Method 2:

$$\begin{aligned}
 D(E) &= g \frac{V}{(2\pi)^3} \int_{\text{shell}} dS_{\vec{k}} \frac{1}{|\nabla_{\vec{k}}(E(\vec{k}))|} = \quad \begin{array}{l} E(\vec{k}) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) \\ |\nabla_{\vec{k}}(E(\vec{k}))| = \frac{\hbar^2}{m} k \end{array} \\
 &= g \frac{V}{(2\pi)^3} \int_{\text{shell}} \frac{m}{\hbar^2} \frac{1}{k} dS_{\vec{k}} = \quad \begin{array}{l} \text{Notice that we are integrating over} \\ \text{a surface that is the boundary of a} \\ \text{sphere of fixed radius} \\ k^2 = \frac{2mE}{\hbar^2} \end{array} \\
 &= g \frac{V}{(2\pi)^3} \frac{m}{\hbar^2} \frac{1}{k} \int dS_{\vec{k}} = \quad \begin{array}{l} \text{Over this sphere the value of } 1/k \\ \text{is constant} \end{array} \\
 &= g \frac{V}{(2\pi)^3} \frac{m}{\hbar^2} \frac{1}{k} 4\pi k^2 = g \frac{V}{2\pi^2} \frac{m}{\hbar^2} \sqrt{\frac{2m}{\hbar^2}} \sqrt{E} = g \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{E} = \\
 &= \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{E}
 \end{aligned}$$

2D

$$\begin{aligned}
 D(E) &= g \frac{S}{(2\pi)^2} \int \delta(E - E(\vec{k})) d^2k = g \frac{S}{(2\pi)^2} \int_{\mathbb{R}^+} \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) 2\pi k dk = \left. \begin{array}{l} \frac{\hbar^2 k^2}{2m} = \beta \rightarrow \frac{\hbar^2}{m} k dk = d\beta \end{array} \right\} \\
 &= g \frac{S}{2\pi} \frac{m}{\hbar^2} \int_{\mathbb{R}^+} \delta(E - \beta) d\beta = g \frac{S}{2\pi} \frac{m}{\hbar^2} = \frac{S}{\pi} \frac{m}{\hbar^2}
 \end{aligned}$$

1D

$$\begin{aligned}
 D(E) &= g \frac{L}{2\pi} \int \delta(E - E(\vec{k})) dk = g \frac{L}{2\pi} \int_{\mathbb{R}^+} \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) dk = \left. \begin{array}{l} \gamma = \frac{\hbar^2 k^2}{2m} \\ d\gamma = \frac{\hbar^2}{m} k dk \end{array} \right\} \\
 &= g \frac{L}{2\pi} \frac{m}{\hbar^2} \sqrt{\frac{2m}{\hbar^2}} \int_{\mathbb{R}^+} \delta(E - \gamma) \frac{1}{\sqrt{\gamma}} d\gamma = g \frac{L}{2\pi} \sqrt{\frac{2m}{\hbar^2}} \frac{1}{\sqrt{E}} = \frac{L}{\pi} \sqrt{\frac{2m}{\hbar^2}} \frac{1}{\sqrt{E}} =
 \end{aligned}$$

0D

$$D(E) = g \delta(E - E_0)$$