

Density of States

Derivation of $D(E)$ for the three-dimensional free electron gas

Basics

We start from the number of states inside a sphere with radius k in [phase space](#).

- The volume V of the sphere is $V = (4/3) \cdot \pi \cdot k^3$; the volume V_k of one unit cell (containing *two* states: spin up and spin down) is

$$V_k = \left(\frac{2\pi}{L} \right)^3$$

- This gives the total *number* of states, N_s , to be

$$N_s = 2 \cdot \frac{V}{V_k} = 2 \cdot \frac{4 \cdot \pi \cdot k^3 \cdot L^3}{3 \cdot 8 \cdot \pi^3} = \frac{k^3 \cdot L^3}{3\pi^2}$$

- For reasons that will become clear very soon, we will keep track of the *dimension* of what we get. The wave vector k has a dimension of $[k] = m^{-1}$; N_s thus is a dimensionless quantity - as it should be.

The density of states D is primarily a density on the energy scale, and only secondarily a density in space. The [definition](#) was

$$D = \frac{1}{V} \cdot \frac{dN_s}{dE} = \frac{1}{L^3} \cdot \frac{dN_s}{dE}$$

We thus must express the wave vector in terms of energy which we can do using the appropriate *dispersion relation*. For the free electron gas model we have

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

$$k = \pm \left(\frac{2 \cdot E \cdot m}{\hbar^2} \right)^{1/2}$$

- Insertion in the formula for N_s yields

$$N_s = \frac{L^3}{3\pi^2} \cdot \left(\frac{2 \cdot E \cdot m}{\hbar^2} \right)^{3/2} = \frac{L^3}{3\pi^2} \cdot \frac{(2m)^{3/2}}{\hbar^3} \cdot E^{3/2}$$

Dividing by L^3 and differentiating with respect to E gives the density of states D

$$D = \frac{1}{L^3} \cdot \frac{dN_s}{dE} = \frac{1}{2\pi^2} \cdot \left(\frac{2m}{\hbar^2} \right)^{3/2} \cdot E^{1/2}$$

- The dimension now is somewhat odd, we have (with [Plancks constant](#) $\hbar = h/2\pi = 6.5820 \cdot 10^{-19} \text{ eV}\cdot\text{s}$)

$$[D] = \text{kg}^{3/2} \cdot \text{eV}^{1/2} \cdot \text{eV}^{-3} \cdot \text{s}^{-3} = \text{kg}^{3/2} \cdot \text{eV}^{-5/2} \cdot \text{s}^{-3}$$

- while we would need $[D] = \text{m}^{-3} \cdot \text{eV}^{-1}$.

If we want to calculate numbers, we have to find the proper conversion. The problem came from the [dispersion relation](#) which gave the dimension of the energy as

- $[E] = \text{eV}^2 \cdot \text{s}^2 \cdot \text{m}^{-2} \cdot \text{kg}^{-1}$; which tells us that $\text{eV} \cdot \text{s}^2 \cdot \text{m}^{-2} \cdot \text{kg}^{-1} = 1$ must hold.
- This is indeed the case, of course, because the basic unit of energy, the Joule, is [defined](#) as $1 \text{ J} = 1 \text{ kg} \cdot \text{m}^2 \cdot \text{s}^{-2} = 6.24 \cdot 10^{18} \text{ eV}$.
- Substituting the **kg** in the dimension of **D** gives

$$1 \text{ kg} = 6.24 \cdot 10^{18} \text{ eV} \cdot \text{m}^{-2} \cdot \text{s}^2$$

$$1 \text{ kg}^{3/2} = 1.559 \cdot 10^{28} \text{ eV}^{3/2} \cdot \text{m}^{-3} \cdot \text{s}^3$$

Insertion into the dimensions for **D** gives the right dimension and yields for masses given in **kg**, length in **m** and energies in **eV**:

$$D = \frac{1.559 \cdot 10^{28}}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \cdot E^{1/2} \quad [\text{eV}^{-1} \cdot \text{m}^{-3}]$$

$$= 7.90 \cdot 10^{26} \cdot \left(\frac{2m}{\hbar^2} \right)^{3/2} \cdot E^{1/2} \quad [\text{eV}^{-1} \cdot \text{m}^{-3}]$$

Effective Density of States

In all practical calculations, the **effective** density of state N_{eff} is used instead of $D(E)$. N_{eff} is just a number, let's see how we can find this from the free electron gas model.

- Let's just look at electrons in the conduction band; for holes everything is symmetrical as usual. We want to get an idea about the distribution of the electrons in the conduction band on the available energy states (given by $D(E)$).

We have in [full generality](#) for n_e = density of electrons in the conduction band

$$n_e = \int_{E_C}^{E^*} D(E') \cdot f(E', T) \cdot dE'$$

- With $f(E', E_F, T)$ = Fermi-Dirac distribution, and the integration running from the bottom of the conduction band to the top of the band at E^* , (or to infinity in practice). *The dash at the symbol for the energy, E' , just clarifies that the zero point of the energy scale is not yet the bottom of the conduction band.*
- Of course we use the Boltzmann approximation for the tail end of the Fermi distribution and obtain

$$n_e = \int_{E_C}^{\infty} D(E') \cdot \exp\left(-\frac{E' - E_F}{kT}\right) \cdot dE'$$

If we now take the bottom of the conduction band as the zero point of the energy scale for $D(E)$, we have $E = E' - E_C$ with E_C = energy of the conduction band. Insertion in the formula above gives

$$n_e = \exp\left(-\frac{E_C - E_F}{kT}\right) \cdot \int_0^{\infty} D(E) \cdot \exp\left(-\frac{E}{kT}\right) \cdot dE$$

Inserting the density of states from above with the abbreviation

$$N_0 = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2}$$

gives a final formula for computing

$$n_e = \exp\left(-\frac{E_C - E_F}{kT}\right) \cdot N_0 \cdot \int_0^{\infty} E^{1/2} \cdot \exp\left(-\frac{E}{kT}\right) \cdot dE$$

The definite integral $\int [E^{1/2} \cdot \exp(-E/kT)] dE$ can be found in integral tables; its value is $(1/2) \cdot (\pi^{1/2}) \cdot (kT)^{3/2}$.

Insertion, switching from \hbar to h , and some juggling of the terms gives the final result defining the effective density of states N_{eff}

$$n_e = 2 \cdot \left(\frac{2\pi \cdot m \cdot kT}{h^2} \right)^{3/2} \cdot \exp\left(-\frac{E_C - E_F}{kT}\right) =: N_{eff} \cdot \exp\left(-\frac{E_C - E_F}{kT}\right)$$

We now have the final result

$$N_{eff} = 2 \cdot \left(\frac{2\pi \cdot m \cdot kT}{h^2} \right)^{3/2}$$

And this is the formula we [used in the backbone](#).

What about numbers and the dimension? We have

$$[N_{eff}] = \text{kg}^{3/2} \cdot \text{eV}^{3/2} \cdot \text{eV}^{-3} \cdot \text{s}^{-3} = \text{kg}^{3/2} \cdot \text{eV}^{-3/2} \cdot \text{s}^{-3}$$

[From before](#) we have $1 \text{ kg}^{3/2} = 1.559 \cdot 10^{28} \text{ eV}^{3/2} \cdot \text{m}^{-3} \cdot \text{s}^3$. Inserting this finally gives (for masses given in **kg**, length in **m** and energies in **eV**):

$$\begin{aligned} N_{eff} &= 4.59 \cdot 10^{15} \cdot T^{3/2} \text{ cm}^{-3} \\ &= 2.384 \cdot 10^{19} \text{ cm}^{-3} \\ &= 2.384 \cdot 10^{25} \text{ m}^{-3} \quad (T = 300 \text{ K}) \end{aligned}$$

And those are very useful numbers – in particular, because they are quite close to the "real" (i.e. measured) values for **Si**.