Density of States

Basics

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

- We start from the number of states inside a sphere with radius $\boldsymbol{k}$ 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 $\boldsymbol{k}$ has a dimension of $[k] = \mathrm{m}^{-1}$; 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 appopriate *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

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

- 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 $\hbar = h/2\pi = 6.5820 \cdot 10^{-19}$ *eV·s*)

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

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

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

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

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

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

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

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

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

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, lets see how we can this from the free electron gas model.

- Lets 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 fulll 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

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

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

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

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