Lecture 4.1

Electrons: Symbol e^-

Last time, good model of heat capacity: correct temperature dependence and good experimental fit for many materials, but not metals. Electrons are important!

Not yet considered how electrons can move through the material.

Electron behaviour governs some of the most important properites of materials, namely electrical and thermal.

Look at two simple models

1. Drude model (circa 1900) Classical kinetic theory of an electron gas
2. Sommerfeld model Quantum electron gas

In both of these, we neglect the lattice. In PH-307, you combine lattice and electron behaviour using concepts developed in PH-207.

Drude model

We **presume** some fraction of electrons in a metal are free to move throughout the crystal: we call these **conduction** electrons. (Find out how later.)

Treat these conduction electrons as a gas, confined to the crystal. Typical number density is $\sim 10^{20}\,\mathrm{cm}^{-3}$.

Assume

1. e^- don't interact with ions (This free e^- approximation is abandoned later)
2. e^- don't interact with each other except by collisions (Free electron approximation)

Equation of motion for electrons under the Drude model:

$$\ddot{\boldsymbol{x}} + \Gamma \dot{\boldsymbol{x}} = \boldsymbol{F}/m$$

where Γ is some damping (friction) term, $\boldsymbol{F}$ is some applied force, and m is the electron mass.

Usually, this is written as

$$\frac{d\boldsymbol{v}}{dt} + \frac{v}{\tau} = -eE/m$$

where $\boldsymbol{v} = \dot{\boldsymbol{x}}$, $\tau = \Gamma^{-1}$ is a damping time, e is the fundamental charge[3], and $\boldsymbol{E}$ is an external electric field.

(We will consider an external *magnetic* $\boldsymbol{B}$ field later.)

When no electric field applied, the average e^- velocity is zero.

Roughly, when there is a field $\boldsymbol{E}$ then electrons are accelerated $\boldsymbol{F} = -e\boldsymbol{E}$ and they collide with something after a time τ. We call τ the relaxation time.

DC Conductivity

To find the average, steady-state velocity of electrons under external electric field $\boldsymbol{E}$, we simply set the acceleration to zero:

$$\boldsymbol{v}_{\mathrm{av}} = \frac{-e\boldsymbol{E}\tau}{m}.$$

Consider a wire of cross-section area A with an electron density n and a drift velocity v_{av}.

In a time δt, e^- in a volume $A\,|\boldsymbol{v}_{\mathrm{av}}|\,\delta t$ pass any point.

Therefore, charge passing a point in time δt is

$$\delta Q = -enA\,|\boldsymbol{v}_{\mathrm{av}}|\,\delta t$$

so the current ($I = Q/t$) is

$$I = -enA\,|\boldsymbol{v}_{\mathrm{av}}|\,.$$

The current *density* is hence

$$\boldsymbol{j} = \boldsymbol{I}/A = -ne\boldsymbol{v}_{\mathrm{av}}$$

[3] $e = 1.602 \times 10^{-19}\,\mathrm{C}$ is the fundamental charge and, by convention, the charge on an electron is negative.

where we can think about current density being a flow in a particular direction, so it makes sense to keep the vectors.

Using the Drude model result for $\boldsymbol{v}_{\rm av}$ we get

$$\boldsymbol{j} = \frac{ne^2\tau}{m}\boldsymbol{E}.$$

The conductivity of a material is usually defined via Ohm's law, written as

$$\boldsymbol{j} = \sigma\boldsymbol{E}$$

and hence we identify the conductivity in the Drude model as

$$\sigma = \frac{ne^2\tau}{m}.$$

Comparison with experiment

Observed conductivities at room temperature give $\tau \sim 10^{-14}\ldots10^{-15}\,\rm s$.

Using typical thermal speeds for electrons

$$v_{\rm rms} \sim \sqrt{\frac{k_B T}{m}} \sim 7\times10^4\,\rm m/s$$

and typical lattice spacing $a \sim 10^{-10}\,\rm m$ this gives

$$\tau \sim 1.4\times10^{-15}\,\rm s$$

which suggests the model is sensible.

Note that τ is just a simple parameter that only roughly describes a very messy process.

Note: DC conductivity in metals works reasonably well, but there are many deviations from the Drude model. e.g. low temperature, or well-prepared samples (i.e. with large single crystals). for which we need to treat the electrons quantum mechanically.

AC conductivity

Proceed by using an oscillating electric field $\boldsymbol{E} = \boldsymbol{E}_0 e^{i\omega t}$ and assuming a harmonic solution for $\boldsymbol{v}(t)$.

Find

$$i\omega v_0 + v_0/\tau = -eE_0/m$$

and hence

$$v_0 = \frac{-eE_0\tau}{m}\frac{1}{1+i\omega\tau}.$$

The current density j is also oscillating $j = j_0 e^{i\omega t}$ and hence, using the definition $j=\sigma E$, we find

$$j_0 = -nev_0 = \frac{e^2 n\tau}{m}\frac{1}{1+i\omega\tau}E = \frac{\sigma_{\rm DC}}{1+i\omega\tau}E = \sigma_{\rm AC}E$$

where $\sigma_{\rm AC} = \sigma_{\rm DC}/(1+i\omega\tau)$.

Optical properties

Derive Maxwell's wave equation with $\boldsymbol{j} \neq 0$:

$$\nabla\times E = -\frac{\partial B}{\partial t}\,;\ \nabla\times B = \mu_0\epsilon_0\frac{\partial E}{\partial t} + \mu_0 j$$

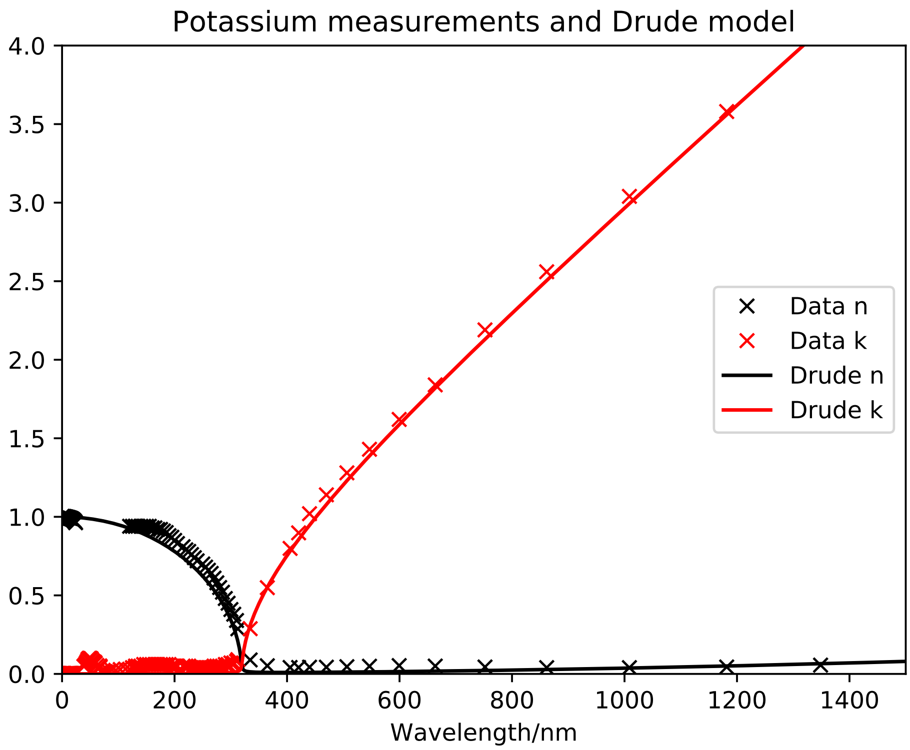
to find

$$\nabla^2 E = \frac{\omega^2}{c^2}\left(1+\frac{i\sigma}{\epsilon_0\omega}\right)E$$

where we have used $j=\sigma E$. See this as a wave propagating in a medium with a complex refractive index.

Drude model for Potassium

```
import numpy as np
import matplotlib.pyplot as plt
pi = np.pi

data = np.genfromtxt("other/Spectrum_K_from_HOCS.txt")

h = 6.63e-34; c = 299792458; q = 1.602e-19; epsilon0 = 8.85e-12; m = 9.1e-31

tau = 2.4e-14
num = 2.4e28/2.2 # best fit by hand

sigmaDC = num*q**2*tau/m
sigmaAC = lambda omega: sigmaDC/(1-1j*omega*tau)
epsilon = lambda omega: 1 + 1j*sigmaAC(omega)/(omega*epsilon0)
nomega = lambda omega: np.real(np.sqrt(epsilon(omega)))
komega = lambda omega: np.imag(np.sqrt(epsilon(omega)))
n = lambda l: nomega(2*pi*c/l); k = lambda l: komega(2*pi*c/l)

l = h*c/(q*data[:,0])
plt.plot(l/1e-9,data[:,1],'kx', label='Data n')
plt.plot(l/1e-9,data[:,2],'rx', label='Data k')

l = np.linspace(l.min(),l.max(),100000)
plt.plot(l/1e-9,n(l),'k', label='Drude n')
plt.plot(l/1e-9,k(l),'r', label='Drude k')
plt.xlim([0,1500]); plt.ylim([0,4])
plt.xlabel('Wavelength/nm'); plt.legend(loc=7)
plt.title("Potassium measurements and Drude model")
plt.savefig("figs/Drude_K.pdf"); plt.close('all')
```



Heat Capacity

Classically, all we can call upon is the Equipartition Theorem: each quadratic degree of freedom contributes $(1/2)k_B T$ of energy.

Thus, the electrons should give a constant contribution to the specific heat capacity:

$$C_{\text{elec}}^{\text{Clas}} = \frac{3}{2}k_B n$$

per unit volume.

This does **not** agree with experiment!