

**Homework#4 Solutions**

**Exercise (1). Phonon Thermal Conductivity**

(a)  $C' = 3nk_B$  where n is the density of atoms per unit volume. So

$$C' = 3nk_B = 3 \frac{N}{V_c} k_B = 3 \cdot \frac{2}{45 \times 10^{-30}} \cdot k_B = 1.84 \times 10^6 J/k$$

(b)  $K \approx C'v \frac{X}{3}$ ,  $X \approx v \cdot \tau = 7 \times 10^{-9} m$  for  $v = 7000 m/s$ ,  $\tau = 1 ps$ . So  $K = 30.0 W/m-k$  or  $0.3 W/cm-k$ .

**Exercise (2). Thermal Conductivity of Al**

a) For Al,

$$n_e = 18.06 \times 10^{22} /cm^3 = 18.06 \times 10^{28} /m^3, \sigma = 3.65 \times 10^5 /\Omega-cm \text{ (Table 3, Chapter 6, Kittel)}$$

so that,  $\tau = \frac{m\sigma}{neq^2} = \frac{(9.11 \times 10^{-31})(3.65 \times 10^7)}{(18.06 \times 10^{28})(1.6 \times 10^{-19})^2}$  or  $\tau = 0.72 \times 10^{-14} s = 7.2 fs$

b)  $C_{el} = \frac{1}{2} \pi^2 Nk_B T / T_F = 91.2 T \cdot V [J]$  (Eq. 36, Kittel Chapter 6)

for  $T_F = 13.49 \times 10^4 K$ ,  $V \rightarrow volume$

$$C'_{el} \text{ (specific heat capacity)} \equiv \frac{C_{el}}{V} = 91.2 T J/m^3 = 2.69 \times 10^4 J/m^3 @ 295K$$

c) So, since  $v = v_F = 2.02 \times 10^{28} cm/s = 2.02 \times 10^6 m/s$  (Al at RT)

$$K = \frac{1}{3} C'_{el} v^2 \tau \approx 2.63 \times 10^2 w/m-K$$

An accepted value for Thermal Conductivity is found in Kittel Chpater 5, Table 1.

$$K = 2.37 W/cm-K = 237 W/m-K \text{ for Al @ 300K. Our estimate using } \frac{1}{3} C'_{el} v^2 \tau \text{ is too}$$

high by 1.13 times/ This is caused largely by the inaccuracy of the Fermi

derivation used to derive heat capacity from  $\Delta U = U(T) - U(0)$ . In this derivation

we approximated  $\frac{dU(T)}{dT}$  by  $\frac{d\Delta U(T)}{dT}$ , which becomes increasingly inaccurate as T rises above zero K.

**Exercise (3)** Given  $\tau(U) = AU^{-S}$  and Maxwell-Boltzmann statistics,

$$\langle \tau \rangle = \frac{\langle v^2 \tau(v) \rangle}{\langle v^2 \rangle} = \frac{m}{3k_B T} \frac{\int v^2 \tau(v) f_o(v) v^2 dv}{\int f_o(v) v^2 dv} = \frac{2}{3k_B T} \frac{\int U^{3/2} \tau(U) f_o(U) dU}{\int U^{1/2} f_o(U) dU}$$

where  $f_o(u) = n \left( \frac{h^2}{2\pi m k_B T} \right)^{3/2} e^{-u/k_B T}$

$$\text{So } \langle \tau \rangle = \frac{2}{3k_B T} \frac{\int_0^\infty u^{3/2} A u^{-S} e^{-u/k_B T} dU}{\int_0^\infty u^{1/2} e^{-u/k_B T} dU}$$

$$U' = U/k_B T \Rightarrow dU = k_B T dU'$$

$$\langle \tau \rangle = \frac{2}{3k_B T} \frac{(k_B T)^{5/2} (k_B T)^{-S} \int_0^\infty A U'^{3/2-S} e^{-U'} dU'}{(k_B T)^{3/2} \int_0^\infty (U')^{1/2} e^{-U'} dU'}$$

Now recall definition  $\Gamma(z) = \int_0^\infty e^{-x} x^{z-1} dx$  .

$$\begin{aligned} \text{So } \langle \tau \rangle &= \frac{2A}{3k_B T} (k_B T)^{1-S} \frac{\Gamma(5/2 - S)}{\sqrt{\pi}/2} = \frac{4A}{3\sqrt{\pi} (k_B T)^S} \Gamma(5/2 - S) \\ &= \frac{4A}{3\sqrt{\pi} (k_B T)^S} \left(\frac{3}{2} - S\right) \Gamma\left(\frac{3}{2} - S\right) \quad (\text{by expansion of Gamma function}) \end{aligned}$$

**Exercise (4)** Boltzman transport eqn. In a uniform electric field

$$\frac{df}{dt} = -\frac{\partial f}{\partial v} \frac{d\vec{v}}{dt} - \frac{f - f_o}{\tau} = 0 \text{ in steady state}$$

$$\Rightarrow f - f_o = -q \frac{\vec{E}_o \tau}{m} \cdot \frac{\partial f}{\partial \vec{v}} = -\frac{q\tau \vec{E}_o}{m} \cdot \vec{\nabla}_v f$$

As in lecture (and McMelvey) we approximate  $\vec{\nabla}_v f \cong \vec{\nabla}_v f_o$

So 
$$f \cong f_o - \frac{q\tau \vec{E}_o}{m} \cdot \vec{\nabla}_v f_o \equiv f_o - \vec{v}_o \cdot \vec{\nabla}_v f_o$$

once we define  $\vec{v}_o \equiv q\tau \vec{E}_o / m$

Now recall form of Taylor's series for increment, h

$$P(x + h) = P(x) + hP'(x) + \dots$$

By associating  $x \rightarrow \vec{v}, h \rightarrow -\vec{v}_o, P \rightarrow f_o$

We find 
$$f \cong f_o(\vec{v} - \vec{v}_o) = Ae^{-\frac{1}{2}m(\vec{v} - \vec{v}_o)^2 / k_B T}$$

The validity of this expression rests on accuracy of the Taylor expansion

$$f \cong f_o - \frac{q\tau \vec{E}_o}{m} \cdot \vec{\nabla} f_o$$

$$\vec{\nabla} f_o = \frac{mv}{k_B T} f_o \Rightarrow f \cong f_o - \frac{q\tau E_o}{m} \frac{mv}{k_B T} f_o$$

$$f = f_o \left(1 - v_o \frac{mv}{k_B T}\right)$$

Validity of Taylor expansion requires that  $f$  is small deviation from

$$f_o \Rightarrow v_o \frac{mv}{k_B T} \ll 1$$

$$v_o \frac{mv}{k_B T} \approx \frac{mv_o^2}{k_B T} < 1 \Rightarrow v_o \ll \sqrt{\frac{k_B T}{m}}$$

**Exercise (5)** Conductivity for energy independent mean-free-path

Define mean-free-path,  $\lambda = v \cdot \tau$  ; Apply Maxwell distribution

$$\sigma = \frac{ne^2 \langle \tau \rangle}{m} \quad \langle \tau \rangle = \frac{\langle \tau v^2 \rangle}{\langle v^2 \rangle} = \frac{\lambda \langle v \rangle}{\langle v^2 \rangle}$$

$$f_o = Ae^{-\frac{1}{2}mv^2/k_B T}$$

$$\begin{aligned} \langle v \rangle &= \int_0^{\infty} Ave^{-\frac{1}{2}mv^2/k_B T} v^2 dv = \int_0^{\infty} Av^4 e^{-\alpha v^2} dv \\ &= \frac{4}{8} \frac{3}{m} (k_B T)^2 \sqrt{\frac{\pi k_B T}{\frac{1}{2}m}} A = \frac{3\sqrt{2\pi}}{2} \left(\frac{k_B T}{m}\right)^{\frac{5}{2}} A = 3\sqrt{\frac{\pi}{2}} \left(\frac{k_B T}{m}\right)^{\frac{5}{2}} \cdot A \end{aligned}$$

$$\text{So } \langle \tau \rangle = \frac{\lambda \langle v \rangle}{\langle v^2 \rangle} = \frac{\lambda 2A(k_B T)^2 / m^2}{\frac{3A\sqrt{2\pi}}{2} \left(\frac{k_B T}{m}\right)^{\frac{5}{2}}} = \lambda \frac{4}{3} \sqrt{\frac{m}{2\pi k_B T}}$$

$$\langle \sigma \rangle = \frac{ne^2 \langle \tau \rangle}{m} = \frac{4}{3} \frac{\lambda ne^2}{\sqrt{2\pi m k_B T}}$$

Alternatively, could do integrals using  $\Gamma$  function

$$\text{Define } u = \frac{1}{2}mv^2 / kT \quad du = \frac{mv}{k_B T} dv$$

$$du = \frac{m}{k_B T} \sqrt{\frac{2uk_B T}{m}} dv$$

$$du = \sqrt{\frac{2um}{k_B T}} dv$$

$$\begin{aligned} \langle v^2 \rangle &= \int_0^{\infty} A \left(\frac{2uk_B T}{m}\right)^2 e^{-u} \sqrt{\frac{k_B T}{2um}} du \\ &= \int_0^{\infty} A \left(\frac{k_B T}{m}\right)^{\frac{5}{2}} (2u)^{\frac{3}{2}} e^{-u} du \end{aligned}$$

$$\int_0^{\infty} u^{\frac{3}{2}} e^{-u} du = \Gamma(5/2) = \Gamma\left(\frac{3}{2} + 1\right) = \frac{3}{2} \Gamma\left(\frac{3}{2}\right)$$

$$= \frac{3}{2} \Gamma\left(\frac{1}{2} + 1\right) = \frac{3}{4} \Gamma\left(\frac{1}{2}\right) = \frac{3\sqrt{\pi}}{4}$$

$$\text{So } \langle v^2 \rangle = A \left(\frac{k_B T}{m}\right)^{\frac{5}{2}} 2^{\frac{3}{2}} \cdot \frac{3\sqrt{\pi}}{4} = A \left(\frac{k_B T}{m}\right)^{\frac{5}{2}} \cdot 3\sqrt{\frac{\pi}{2}}$$

as derived with Gaussian integrals above