Professor: James Analitis

Physics 141A: Solid State Physics

Homework 4

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Question 1:

Include figure

The low temperrature specific heat of a metal can be described by the equation

$$c_v = \frac{\pi^2}{3} g(E_F) k_B^2 T + \frac{12\pi^4}{5} n k_B \left(\frac{T}{\Theta}\right)^3$$

1. Explain the physical origin of the two terms.
2. Using the free electron model, show that the density of states in three dimensions $g(E_F)$ is given by
$$g(E_F) = \frac{3}{2}\frac{n_e}{E_F}$$
where n_e is the carrier density.
3. In the Drude model we assumed that n_e electrons were solely responsible for the conductivity in a metal. If we follow this model and assume that the carrier density at high temperature (145 K) is denoted n_{HT} and the carrier density at low temperature is denoted n_{LT} (say at 125 K). Extimate the ration n_{LT}/n_{HT} from figure 1. Note that 10^4 Oe $= 1T$
4. The scattering time at high temperature is denoted τ_{HT} and the scattering rate at low temperature is denoted τ_{LT}. Estimate τ_{LT}/τ_{HT}.
5. Calculate the Fermi energy above and below the phase transition.
6. $BaFe_2As_2$ is a metal. Using your knowledge of patterns of properties in the periodic table, argue that most of the mobile electrons likely come from the Fe atoms.
7. If we want to add more electrons to $BaFe_2As_2$ we can replace its atoms with sp-called "dopants". What transition metal(s) would you choose to replace the Fe site to add electrons?

8. As more electrons δn are added, we expect the Sommerfeld coefficient $\frac{\pi^2}{3}g(E_F)k_B^2$ to increase. Define $c_v^0 = \frac{\pi^2}{3}g(E_{F0})k_B^2$ where E_{F0} is the Fermi energy when there are no dopants added. Show that c_v will approximately increase as

$$c_v \approx c_v^0 + \frac{\pi^2}{3}\frac{\delta n}{2}\frac{k_B^2 T}{E_{F0}}$$

9. Show that if $BaFe_2As_2$ was a two-dimensional, free electron metal, that the Sommerfeld coefficient would not be expected to increase when more electrons are added.

Solution:

1. The term proportional to T^1 is due to the electrons in the metal, while the term proportional to T^3 is due to lattice vibrations (phonons).

2. In the free electron model, with the metal assumed to be a box of volume $V = L^3$ and periodic boundary conditions, we have plane wavefunctions $e^{i\mathbf{k}\cdot\mathbf{r}}$ quantized as

$$\mathbf{k} = \frac{2\pi}{L}\mathbf{n} = \frac{2\pi}{L}(n_1, n_2, n_3),\ n_i \in \mathbb{N}$$

and energies described by

$$\epsilon(\mathbf{k}) = \frac{\hbar^2|\mathbf{k}|^2}{2m}$$

with m being the electron mass. Finally, we have the dispersion relation $\omega = v|\mathbf{k}|$.

Then, the total number electrons in the system is N and we have

$$N = \frac{2V}{(2\pi)^3}\int \mathbf{dk}\ n_F(\beta(\epsilon(\mathbf{k}) - \mu))$$

where μ is the chemical potential (the factor of 2 accounts for the two possible spins).

The total energy of the system is

$$E_{tot} = \frac{2V}{(2\pi)^3}\int \mathbf{dk}\ \epsilon(\mathbf{k}) \cdot n_F(\beta(\epsilon(\mathbf{k}) - \mu))$$

Using the fact that $\epsilon(\mathbf{k})$ only depends on $|\mathbf{k}| = :k$, we can switch from cartesian $\mathbf{k}$-coordinates to spherical coordinates as write

$$E_{tot} = \frac{2V}{(2\pi)^3} \cdot 4\pi \int_0^\infty dk\ \epsilon(k) \cdot n_F(\beta(\epsilon(k) - \mu))$$

Switching from k to ϵ using

$$k = \sqrt{\frac{2m\epsilon}{\hbar^2}} \implies dk = \sqrt{\frac{m}{2\epsilon\hbar^2}}d\epsilon$$

we have

$$\begin{aligned} E_{tot} &= \frac{2V}{2\pi^2}\int_0^\infty \left(\sqrt{\frac{m}{2\epsilon\hbar^2}}d\epsilon\right)\cdot\epsilon\cdot n_F(\beta(\epsilon-\mu)) \\ &= V\int_0^\infty d\epsilon\ \epsilon\cdot g(\epsilon)\cdot n_F(\beta(\epsilon-\mu)) \end{aligned}$$

where we have density of states

$$\begin{aligned} g(\epsilon)d\epsilon &= \frac{2}{(2\pi)^3}\cdot 4\pi k^2 dk \\ &= \frac{2}{(2\pi)^3}\cdot 4\pi\cdot\left(\frac{2m\epsilon}{\hbar^2}\right)\cdot\left(\sqrt{\frac{m}{2\epsilon\hbar^2}}d\epsilon\right) \\ &= \frac{(2m)^{3/2}}{2\pi^2\hbar^3}\epsilon^{1/2} \end{aligned}$$

Now recall that the Fermi Energy was

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

and

$$N = \frac{2V}{(2\pi)^3}\int \mathbf{dk}\ n_F(\beta(\epsilon(\mathbf{k})-\mu))$$

The Fermi-Energy is defined at $T=0$, and at absolute zero, the Fermi-Dirac Distribution $n_F(\beta(\epsilon-\mu))$ is a step function $\begin{cases}1,\ k\le k_F\\ 0,\ k>k_F\end{cases}$. Thus,

$$\begin{aligned} N &= \frac{2V}{(2\pi)^3}\int_{k\le k_F}\mathbf{dk} \\ \implies N &= \frac{2V}{(2\pi)^3}\cdot\left(\frac{4}{3}\pi k_F^3\right) \\ \implies k_F &= (3\pi^2 n)^{1/3},\quad n:=N/V \\ \implies E_F &= \frac{\hbar^2(3\pi^2 n)^{2/3}}{2m} \\ \implies \frac{(2m)^{3/2}}{\hbar^3} &= \frac{3\pi^2 n}{E_F^{2/3}} \end{aligned}$$

and substituting this into the expression for $g(\epsilon)$ we obtain

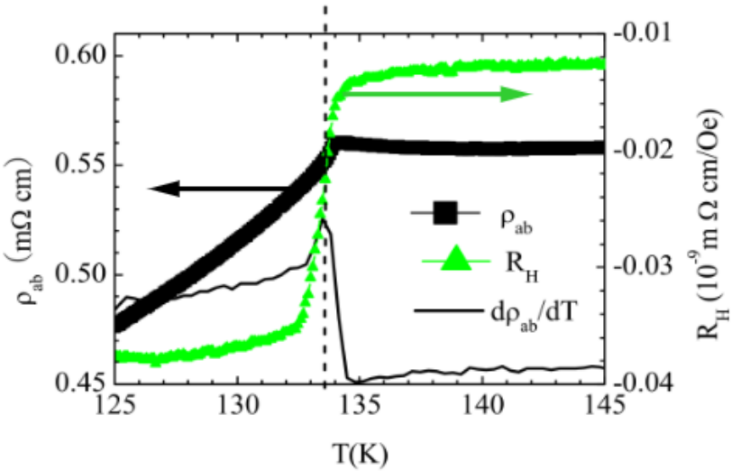
$$\boxed{g(\epsilon) = \frac{3n_e}{2E_F}\left(\frac{\epsilon}{E_F}\right)^{1/2}}$$

where $n = n_e =$ Carrier density

Therefore,

$$\boxed{g(E_F) = \frac{3n_e}{2E_F}}$$

3. We have carrier densities n_{HT}, n_{LT} at 145K and 125K respectively. In the Drude model, $R_H = (-1)/ne \implies n = (-1)/(e \cdot R_H)$



So, looking at the Figure above, we estimate

$$\begin{aligned}\frac{n_{LT}}{n_{HT}} &= \frac{(-1)}{e \cdot (R_H)_{LT}} \cdot \frac{e \cdot (R_H)_{HT}}{(-1)} \\ &= \frac{(R_H)_{HT}}{(R_H)_{LT}} \\ &= \frac{-0.012 \cdot 10^{-9}\text{m}\Omega\text{cm/Oe}}{-0.038 \cdot 10^{-9}\text{m}\Omega\text{cm/Oe}} \\ &= 0.315789474\end{aligned}$$

(We don't need to convert the units from Oe to T, right?)

4. In the figure, ρ_{ab} is the same as ρ_{xx}. We know

$$\rho_{xx} = \frac{m}{ne^2\tau} \implies \tau = \frac{m}{ne^2\rho_{xx}}$$

So,

$$\begin{aligned}\frac{\tau_{LT}}{\tau_{HT}} &= \frac{n_{HT} \cdot \rho_{xx,HT}}{n_{LT} \cdot \rho_{xx,LT}} \\ &= \frac{-0.012}{-0.038} \cdot \frac{-0.020}{-0.034}\end{aligned}$$

5.

6. Write this later.

7.

Question 2: Classical Model of Thermal Expansion
In classical statistical mechanics, we write the expectation of x as

$$\langle x\rangle_\beta = \frac{\int dx\ xe^{-\beta V(x)}}{\int dx\ e^{-\beta V(x)}}$$

Although one cannot generally do such integrals for arbitrary potential $V(x)$ as in Eq. 8.1, one can expand the exponentials as

$$e^{-\beta V(x)} = e^{-\frac{\beta\kappa}{2}(x-x_0)^2}\left[1+\frac{\beta\kappa_3}{6}(x-x_0)^3+\cdots\right]$$

and let limits of integration go to $\pm\infty$.
▷ Why is this expansion of the exponent and the extension of the limits of integration allowed?
▷ Use this expansion to derive $\langle x\rangle_\beta$ to lowest order in κ_3, and hence show that the coefficient of thermal expansion is

$$\alpha = \frac{1}{L}\frac{dL}{dT} \approx \frac{1}{x_0}\frac{d\langle x\rangle_\beta}{dT} = \frac{1}{x_0}\frac{k_B\kappa_3}{2\kappa^2}$$

with k_B Boltzmann's constant.
▷ In what temperature range is the above expansion valid?
▷ While this model of thermal expansion in a solid is valid if there are only two atoms, why is it invalid for the case of a many-atom chain?

Solution:
▷ We know we can do the expansion

$$V(x) = v(x_0) + \frac{\kappa}{2}(x-x_0)^2 + \frac{\kappa^3}{6}(x-x_0)^3+\cdots$$

when we're very close to x. If we further have that $-\beta V(x) \approx \beta\cdot\left[v(x_0)+\frac{\kappa}{2}(x-x_0)^2+\frac{\kappa^3}{6}(x-x_0)^3+\cdots\right]$ is small, then we can carry out the expansion of the exponential.

▷ We want to determine the conditions under which calculating

$$\langle x\rangle_\beta = \lim_{b\to\infty}\frac{\int_{-b}^{+b} dx\ xe^{-\beta V(x)}}{\int_{-b}^{+b} dx\ e^{-\beta V(x)}}$$

with the approximation

$$e^{-\beta V(x)} = e^{-\frac{\beta\kappa}{2}(x-x_0)^2}\left[1+\frac{\beta\kappa_3}{6}(x-x_0)^3+\cdots\right]$$

is valid.

Define $y = (x - x_0)$. Then, we have

$$\begin{aligned}\langle x \rangle_\beta &= \frac{\int dy\ (y + x_0) e^{-\frac{\beta\kappa}{2}y^2\left[1+\frac{\beta\kappa_3}{6}y^3+\cdots\right]}}{\int dy\ e^{-\frac{\beta\kappa}{2}y^2\left[1+\frac{\beta\kappa_3}{6}y^3+\cdots\right]}} \\ &= \frac{\int dy\ y \cdot e^{-\frac{\beta\kappa}{2}y^2}\left[1 + \frac{\beta\kappa_3}{6}y^3 + \cdots\right]}{\int dy\ e^{-\frac{\beta\kappa}{2}y^2}\left[1 + \frac{\beta\kappa_3}{6}y^3 + \cdots\right]} + x_0 \quad \text{Since } x_0 \text{ is constant}\end{aligned}$$

Now, we're trying to find the region of validity for the approximation where we drop the $\mathcal{O}(y^4)$ terms, so let's drop them and expand to get

$$\begin{aligned}\langle x \rangle_\beta &= \frac{\int dy\ y \cdot e^{-\frac{\beta\kappa}{2}y^2}\left[1 + \frac{\beta\kappa_3}{6}y^3\right]}{\int dy\ e^{-\frac{\beta\kappa}{2}y^2}\left[1 + \frac{\beta\kappa_3}{6}y^3\right]} + x_0 \quad \text{Since } x_0 \text{ is constant} \\ &= x_0 + \frac{\beta\kappa_3}{6}\frac{\int dy\ y^4 e^{-\frac{\beta\kappa}{2}y^2}}{\int dy\ e^{-\frac{\beta\kappa}{2}y^2}}\end{aligned}$$

Here, we've simplified the expression by using the fact that the integral of an odd function over an interval symmetric about 0 is zero.

Then, using the fact that

$$\int dy\ e^{-ay^2} = \sqrt{\frac{\pi}{a}}$$

and Feynman's trick we have

$$\begin{aligned}\int dy\ y^4 e^{-ay^2} &= \int dy\ \frac{\partial^2}{\partial a^2}\left(e^{-ay^2}\right) \\ &= \frac{d^2}{da^2}\int dy\ e^{-ay^2} \\ &= \frac{d^2}{da^2}\left(\sqrt{\frac{\pi}{a}}\right) \\ &= \frac{3}{4}\sqrt{\frac{\pi}{a^5}}\end{aligned}$$

Substituting this in, we get

$$\begin{aligned}\langle x \rangle_\beta &= x_0 + \frac{\beta\kappa_3}{6} \cdot \frac{\frac{3}{2}\sqrt{\frac{\pi}{(\beta\kappa/2)^5}}}{\sqrt{\frac{\pi}{(\beta\kappa/2)}}} \\ &= x_0 + \frac{\kappa_3 (k_B T)}{2\kappa^2}\end{aligned}$$

Thus,

$$\boxed{\frac{1}{x_0} \cdot \frac{d\langle x \rangle_\beta}{dT} = \frac{1}{x_0}\frac{k_B \kappa_3}{2\kappa^2}}$$

▷ In order for the result above to be valid, we need the cubic term to be much less important in contribution than the leading term.

And since we found $\langle x \rangle_\beta \sim k_B T$ we need the leading term $\kappa(x - x_0)^2 \sim k_B T \implies |x - x_0| \sim \sqrt{\frac{k_B T}{\kappa}}$. Then, we need

$$\begin{aligned} \kappa|x - x_0|^2 &>> \kappa_3 |x - x_0|^3 \\ \implies k_B T &>> \kappa_3 \left(\sqrt{\frac{k_B T}{\kappa}}\right)^{3/2} \\ \implies k_B T &<< \frac{\kappa^3}{\kappa_3^2} \end{aligned}$$

▷ For a many-atom chain, the quadratic term in the potential would introduce interaction (non-linear) terms, which would change the expression.

Question 3: Normal Modes of a One-Dimensional Monoatomic Chain

(a) Explain what is meant by "normal mode" and by "phonon".

(b) Skip derivation of dispersion relation $\omega(k)$ since it's done in the book and lectures.

(c) Show that the mode with wavevector k has the same pattern of mass displacements aas the node with wavevector $k + 2\pi/a$. Hence show that the dispersion relation is periodic in reciprocal space (k-space).
▷ How many *different* normal modes are there?

(d) Derive the phase and group velocities and sketch them as a function of k.
▷ What is the sound velocity?
▷ Show that the sound velocity iss also given by $v_s = 1/\sqrt{\beta\rho}$ where ρ is the chain density and β is the compressibility.

(e) Find the expression for $g(\omega)$, the density of states of modes per angular frequency.
▷ Sketch $g(\omega)$.

Solution:

(a) A normal mode is a collective oscillation of the atoms/particles in which all particles oscillate with the same frequency, usually denoted ω. A Phonon is a *quantum of vibration* i.e. an excitation of a normal mode up the QHO ladder. This is analogous to how a Photon is an excitation/quantum of an EM Wave.

(b) Skip this.

(c) Consider modes with wavevectors k and $k + 2\pi/a$.

The mass displacement of lattice point x_n is $\delta x_n = Ae^{i\omega t - ikna}$. Taking $k \to k + 2\pi/a$ we get

$$\begin{aligned}\delta x_n &= Ae^{i\omega t - i(k+2\pi/a)na} \\ &= Ae^{i\omega t - ikna} \cdot e^{-i2\pi n}\end{aligned}$$

and $e^{2\pi(-1)n} = 1$ so the mass displacements are the same.

▷ How many normal modes are there?
Recall that if we assume periodic boundary conditions then

$$k = \frac{2nm}{L}$$

but k is identified with $k + 2\pi/a$ so there are exactly $N = L/a$ different normal modes.

(d) The phase and group velocities are

$$v_{phase} = \frac{\omega(k)}{k} = 2\sqrt{\frac{\kappa}{m}}\frac{\left|\sin\left(\frac{ka}{2}\right)\right|}{k}$$

$$v_{group} = \frac{d\omega(k)}{dk} = \sqrt{\frac{\kappa}{m}} \cdot a\cos\left(\frac{|k|a}{2}\right) = \frac{a}{2}\omega_0\sqrt{1-\frac{\omega^2}{\omega_0^2}}$$

where $\omega_0 = 2\sqrt{\kappa/m}$