Solutions for Homework Set 4

Jock McOrist

1. Kittel Problem 5.3

Solution

(a) We are given that

$$\langle R^2 \rangle = \frac{\hbar}{2\rho V} \sum \omega^{-1},$$

where the sum is over all independent phonon modes. We may replace this summation by an integral over the density of states in the Debye approximation, and account for the 3-fold degeneracy in the modes (we are in an isotropic medium, so polarisation is independent of velocity). Also the density of states is given by

$$\mathcal{D}(\omega) = \frac{V\omega^2}{2\pi^2 v^3}.$$

Hence,

$$\langle R^2 \rangle = \frac{3\hbar}{2\rho V} \int_0^{\omega_D} \mathcal{D}(\omega) \omega^{-1} \mathrm{d}\omega,$$

= $\frac{3\hbar\omega_D^2}{8\pi^2 v^3 \rho}.$ (1)

(b) In one dimension we have

$$\langle R^2 \rangle \propto \sum \omega^{-1},$$

so we show that the sum over modes diverges. One approach is to note that the allowed wavevectors take the form $K = 2\pi n/L$, with n an integer. In the Debye approximation we have $\omega = Kv$, and so $\omega \propto n$. Hence,

$$\langle R^2 \rangle \propto \sum \omega^{-1} \propto \sum_n n^{-1} = \infty$$

as a harmonic series diverges. Therefore, $\langle R^2\rangle$ and $\sum \omega^{-1}$ both diverge. However, more explicitly

$$\langle R^2 \rangle \propto \sum \omega^{-1} = \int_0^{\omega_D} \mathcal{D}(\omega) \omega^{-1},$$

$$= \int_0^{\omega_D} \frac{L}{\pi v \omega} d\omega$$

$$= \infty,$$
 (2)

as $\ln 0 = \infty$.

The mean square strain is given by $\langle (\partial R/\partial x)^2 \rangle = \sum K^2 u_0/2$ where $u_0 = \hbar/2\rho V \sum \omega^{-1}$.

For a line of N atoms of mass M including only longitudinal modes we convert the sum to an integral giving:

$$\left\langle \left(\frac{\partial R}{\partial x}\right)^2 \right\rangle = \int_0^{\omega_D} \mathcal{D}(\omega) k^2 \frac{\hbar}{2\rho V \omega}$$
$$= \frac{\hbar}{2\rho V \omega} \int_0^{\omega_D} \frac{L}{\pi v} \frac{\omega}{v^2} d\omega$$
$$= \frac{L\hbar \omega_D^2}{4MNv^3}, \tag{3}$$

where $\rho L = MN$ is the mass of the lattice, and so the mean square strain is

$$\frac{L\hbar\omega_D^2}{4MNv^3}.$$
(4)

Note that in this problem there is an ambiguity of a factor of 2. This originates from a typo in Kittel – Equation (4.29) has an extra factor of a 1/2. Try and work it out for yourself!

Solution

(a) The layers are de-coupled so the problem becomes a 2D one, with modes propagating only in the plane of layers. Hence, the 2D density of states within a plane is given by

$$\mathcal{D}(\omega) = \frac{L^2}{2\pi} \frac{\omega}{v^2}.$$

Then, the energy of the system is given by in the Debye approximation:

$$U = \int_{0}^{\infty} \mathcal{D}(\omega) \langle n(\omega) \rangle \hbar \omega d\omega,$$

$$= \int_{0}^{\omega_{D}} \frac{A\omega}{2\pi v^{2}} \frac{\hbar \omega}{e^{\hbar \omega/k_{b}T} - 1} d\omega$$

$$= \frac{Ak_{b}^{3}T^{3}}{2\pi \hbar^{2} v^{2}} \int_{0}^{x_{D}} \frac{x^{2}}{e^{x} - 1},$$
 (5)

where in the last line we define $x = \hbar \omega / (k_b T)$. In the low temperature limit the integral extends to infinity, and is now independent of temperature. To find the heap capacity, one can then differentiate the resulting expression with respect to T, or alternatively differentiate the second line in (5) above for a general temperature. In any case one finds that,

$$C_V \propto T^2.$$
 (6)

(b) As the coupling between layers becomes stronger we expect that the heat capacity should go from the 2D result to the 3D result. That is, we expect $C \propto T^n$, where n goes from $n = 2 \rightarrow 3$. In 2D, at low temperatures $x_D \rightarrow \infty$, giving

$$C_v \propto \frac{3Ak_b^2}{\pi v^2 \hbar^2} \zeta(3) T^2, \tag{7}$$

where $\zeta(z)$ is the Riemann zeta function. Similarly we know that at low temperatures $C_v \propto T^3$ for 3D, and hence, with weak coupling between layers $C_V \propto T^2$, as T^2 dominates T^3 at low temperatures.

3. Kittel Problem 5.4

Solution

The energy of an arbitrary system is given by

$$U = \int_0^\infty \varepsilon n(\varepsilon) \mathcal{D}(\varepsilon) \mathrm{d}\varepsilon, \tag{8}$$

which for a free electron gas coincides exactly with the kinetic energy (i.e. no potential energy). Also, $\mathcal{D}(\varepsilon)$ is the density of states for the free electron gas in 3D. Explicitly this is given by,

$$\mathcal{D}(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2}.$$
(9)

Hence, as we are at T = 0 the Fermi-Dirac distribution is given by the usual step-function giving:

$$U_{0} = \int_{0}^{\varepsilon_{f}} \frac{V}{2\pi^{2}} \left(\frac{2m}{\hbar^{2}}\right)^{3/2} \varepsilon^{3/2} d\varepsilon,$$

$$= \frac{V}{2\pi^{2}} \left(\frac{2m}{\hbar^{2}}\right)^{3/2} \frac{2v e_{f}^{5/2}}{5},$$

$$= \frac{3}{5} N \varepsilon_{f},$$
 (10)

where in the last line we use

$$N = \frac{V}{3\pi^2} \left(\frac{2m\varepsilon}{\hbar^2}\right)^{3/2}$$

4. Kittel Problem 6.3

Solution

We use the definition of N in terms of $\mathcal{D}(\varepsilon)$ and the Fermi-Dirac distribution function to determine μ the chemical potential. In 2D the density of states is a constant given by

$$\mathcal{D}(\varepsilon) = \frac{m}{\pi\hbar^2}.$$

The number density of electrons n = N/V in our system at a temperature T is then,

$$n = \int_{0}^{\infty} \mathcal{D}(\varepsilon)n(\varepsilon),$$

$$= \frac{m}{\pi\hbar^{2}} \int_{0}^{\infty} \frac{\mathrm{d}\varepsilon}{e^{(\varepsilon-\mu)/k_{b}T} + 1},$$

$$= \frac{mk_{b}T}{\pi\hbar^{2}} \int_{0}^{\infty} \frac{e^{-x}}{e^{-\mu/T} + e^{-x}} \mathrm{d}x,$$

$$= \frac{mk_{b}T}{\pi\hbar^{2}} \log(1 + e^{\mu/T}).$$
(11)

Therefore, rearranging for μ :

$$\mu = k_B T \log(e^{\pi \hbar^2 n/mk_b T} - 1).$$
(12)