

1. Show that the exact distribution of frequencies for a one-dimensional crystal,

$$g(\nu) = \frac{2N}{\pi} \frac{1}{(\nu_{\max}^2 - \nu^2)^{1/2}}$$

agrees with that of the Debye approximation for a one-dimensional crystal as $\nu \rightarrow 0$.

In the exact distributions, as $\nu \rightarrow 0$, $g(\nu) = \frac{2N}{\pi\nu_{\max}}$

For long wavelengths, $\nu = \frac{\omega}{k} = \lambda\nu = \frac{a\omega_{\max}}{2} = \frac{a}{2}2\pi\nu_{\max}$

$$\Rightarrow \nu_{\max} = \frac{\nu}{\pi a}$$

Thus, $g(\nu) = \frac{2Na}{\nu}$

In the Debye expression in one dimension,

$$n_x^2 \left(\frac{\pi}{L} \right)^2 = k^2 \quad \text{Noting } \frac{2\pi\nu}{k} = \nu, \quad \frac{2\pi\nu}{\nu} = k, \quad \text{so}$$

$$n_x^2 \left(\frac{\pi}{L} \right)^2 = \left(\frac{2\pi\nu}{\nu} \right)^2$$

$$n_x^2 = \left(\frac{2\pi\nu}{\nu} \right)^2 \left(\frac{L}{\pi} \right)^2 = \left(\frac{2L\nu}{\nu} \right)^2$$

$$n_x = \left(\frac{2L\nu}{\nu} \right)$$

The density of state becomes:

$$g(\nu) = \frac{\partial n_x}{\partial \nu} = \frac{2L}{\nu} = \frac{2Na}{\nu}$$

2. Derive the following exact expression for the energy of the 1-dimensional crystal:

$$E = \frac{Na}{\pi} \int_0^{\pi/a} \frac{\hbar\omega(k) dk}{\exp(\hbar\omega(k)/kT) - 1}$$

The total partition function is $Q = e^{-U(0)/kT} \prod_{j=1}^N q(\hbar\omega_j/kT)$.

where $\theta_j = \hbar\omega_j/k$ and $q = \frac{e^{-\hbar\omega/2kT}}{1 - e^{-\hbar\omega/kT}}$

Excluding the U(0) term,

$$\ln Q = \sum_j \left[-\hbar\omega_j/kT - \ln \left[1 - \exp(-\hbar\omega_j/kT) \right] \right]$$

The crystal energy is

$$kT^2 \frac{\partial \ln Q}{\partial T} = kT^2 \left[\frac{\hbar\omega}{2kT^2} - \sum_j \frac{-\hbar\omega_j e^{-\hbar\omega_j/kT} / kT^2}{1 - \exp(-\hbar\omega_j/kT)} \right] = \sum_j \frac{\hbar\omega_j}{2} + \sum_j \frac{\hbar\omega_j e^{-\hbar\omega_j/kT}}{1 - \exp(-\hbar\omega_j/kT)}$$

$$\text{Thus, } E = \sum_j \frac{\hbar\omega_j}{2} + \sum_j \frac{\hbar\omega_j}{\exp(\hbar\omega_j/kT) - 1}$$

$$\text{Use } k = \frac{2\pi j}{Na}$$

The number of states with $k < k'$: $\Phi(k) = \frac{Nka}{2\pi}$

Thus, in terms of an integral over

$$0 \rightarrow +k: E = \frac{Na}{\pi} \int_0^{\pi/a} \frac{\hbar\omega(k)}{\exp(\hbar\omega(k)/k_B T) - 1} dk$$

3. Derive an exact expression for the heat capacity of the 1D crystal and take the low temperature limit. Is it consistent with Debye?

$$\begin{aligned} C_V &= \frac{\partial E}{\partial T} \\ &= k_B \int_0^{\nu_{\max}} \frac{(h\nu/kT)^2 e^{h\nu/kT} g(\nu)}{(e^{h\nu/kT} - 1)^2} d\nu \end{aligned}$$

For the monatomic crystal:

$$g(\nu) = \frac{2N}{\pi} \frac{1}{\left[v_m^2 - \nu^2 \right]^{1/2}}$$

At low temperatures, where only low frequency modes are populated:

$$g(\nu) \approx \frac{2N}{\pi v_m}$$

Thus,

$$\begin{aligned} C_V &= k \frac{2N}{\pi v_m} \int_0^{v_m} \frac{(h\nu/kT)^2 e^{h\nu/kT}}{(e^{h\nu/kT} - 1)^2} d\nu \\ &\rightarrow k \frac{2N}{\pi v_m} \left(\frac{h}{k}\right)^2 \frac{1}{T^2} \int_0^\infty \frac{\nu^2 e^{h\nu/kT}}{(e^{h\nu/kT} - 1)^2} d\nu \end{aligned}$$

$$\text{Let } x = h\nu/kT, \quad \frac{xkT}{h} = \nu; \quad dx = \frac{h}{kT} d\nu$$

$$\rightarrow k \frac{2N}{\pi v_m} \left(\frac{h}{k}\right) \frac{1}{T^2} \left(\frac{kT}{h}\right)^3 \int_0^\infty \frac{x^2 e^x}{(e^x - 1)^2} dx$$

For low temperatures, include only the low frequency modes:

$$\int_0^\infty \frac{x^2 e^x}{(e^x - 1)^2} dx = \frac{\pi^2}{3}$$

$$\begin{aligned} C_V &= k \frac{2N}{\pi v_m} \left(\frac{h}{k}\right) \frac{1}{T^2} \left(\frac{kT}{h}\right)^3 \left(\frac{\pi^2}{3}\right) \\ &\propto T \end{aligned}$$

Agrees with Debye in 1D.

4. Derive an expression relating the Debye frequency, ν_D and the maximum frequency in the exact treatment of the 1D crystal.

The 1D density of states in the Debye model is (see Problem #1):

$$\begin{aligned} g(\nu) &= \frac{2Na}{v} \quad \nu \leq \nu_D \\ &= 0 \quad \nu \geq \nu_D \end{aligned}$$

where the cutoff is determined by

$$\int_0^{\nu_D} g(\nu) d\nu = N, \quad \text{thus } \frac{2Na}{v} \int_0^{\nu_D} d\nu = N, \quad \text{so } \nu_D = \frac{v}{2a}.$$

Compare this with v_{\max} in the low frequency limit in the "exact" treatment of the 1D crystal. From Problem #1, we have

$$v_{\max} = \frac{v}{\pi a}$$

The ratio is therefore
$$\frac{v_D}{v_{\max}} = \frac{\frac{v}{2a}}{\frac{v}{\pi a}} = \frac{\pi}{2} = 1.57$$

5. The Debye theory treats the crystal as a continuum body, and hence the dispersion relation for the phonons is $\omega = ck$, where c is the speed of sound in the body. In a ferromagnetic solid at low temperatures, there exist quantized waves of magnetization called spin waves, and the dispersion relation for these type of waves is $\omega \propto k^2$. Find the low temperature heat capacity due to spin waves. Assume that spin waves are quantized with energies

$$\varepsilon_k = \left(n_k + \frac{1}{2} \right) \hbar \omega \quad \text{where } \omega_k = Ak^2.$$

The partition function for the spin waves may be written:

$$q = \sum_{n_k=0}^{\infty} e^{-\varepsilon_k / kT} \\ = \frac{e^{-\hbar \omega_k / 2kT}}{1 - e^{-\hbar \omega_k / kT}}$$

Take N spin waves. The total partition function becomes

$$Q = \prod_{i=1}^N q_i$$

Thus,

$$\ln Q = \ln \prod_{i=1}^N q_i = \sum_{i=1}^N \ln q_i = \sum_{i=1}^N \left[-\frac{\hbar \omega_i}{2kT} - \ln \left(1 - e^{-\hbar \omega_i / kT} \right) \right]$$

We want to convert the integral to a summation. For this we need to derive the frequency distribution function. Assuming the ends of the chain enforce the boundary condition, we have in 3D:

$$k^2 = \left(\frac{\pi}{L} \right)^2 \left(n_x^2 + n_y^2 + n_z^2 \right)$$

Substituting in the dispersion relation, $\omega_k = Ak^2$,

$$\frac{\omega_k}{A} = \left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

$$\text{Rearranging, } R \equiv (n_x^2 + n_y^2 + n_z^2) = \left(\frac{L}{\pi}\right)^2 \frac{\omega_k}{A}$$

The number of states having frequency $< \omega$ is the volume enclosed in the octant of a sphere with radius R is

$$\Phi(\omega) = \frac{1}{8} \cdot \frac{4}{3} \cdot \pi R^3 = \frac{V}{6\pi^2} \left(\frac{\omega}{A}\right)^{3/2}$$

$$\text{The frequency distribution is } g(\omega) = \frac{\partial}{\partial \omega} \Phi(\omega) = \frac{V}{4\pi^2 A^{3/2}} \omega^{1/2}$$

We can substitute this into our expression for $\ln Q$:

$$\begin{aligned} \ln Q &= \int_0^{\omega_{\max}} \left[-\frac{\hbar \omega_i}{2kT} - \ln(1 - e^{-\hbar \omega_i / kT}) \right] g(\omega) d\omega \\ &= \frac{V}{4\pi^2 A^{3/2}} \int_0^{\omega_{\max}} \left[-\frac{\hbar \omega_i}{2kT} - \ln(1 - e^{-\hbar \omega_i / kT}) \right] \omega^{1/2} d\omega \\ &= -\frac{V}{4\pi^2 A^{3/2}} \left[\frac{\hbar}{2kT} \int_0^{\omega_{\max}} \omega^{3/2} d\omega + \int_0^{\omega_{\max}} \ln(1 - e^{-\hbar \omega_i / kT}) \omega^{1/2} d\omega \right] \end{aligned}$$

Calculate the energy, $E = kT^2 \frac{\partial \ln Q}{\partial T}$

$$\begin{aligned} kT^2 \frac{\partial \ln Q}{\partial T} &= -\frac{VkT^2}{4\pi^2 A^{3/2}} \left[\frac{-\hbar}{2kT^2} \int_0^{\omega_{\max}} \omega^{3/2} d\omega - \int_0^{\omega_{\max}} \frac{\omega^{1/2} e^{-\hbar \omega / kT}}{(1 - e^{-\hbar \omega / kT})} \left[\frac{\hbar \omega}{kT^2} \right] d\omega \right] \\ &= \frac{V\hbar}{4\pi^2 A^{3/2}} \left[\frac{1}{2} \int_0^{\omega_{\max}} \omega^{3/2} d\omega + \int_0^{\omega_{\max}} \frac{\omega^{3/2} e^{-\hbar \omega / kT}}{(1 - e^{-\hbar \omega / kT})} d\omega \right] \\ &= \frac{V\hbar}{4\pi^2 A^{3/2}} \left[\frac{1}{2} \int_0^{\omega_{\max}} \omega^{3/2} d\omega + \int_0^{\omega_{\max}} \frac{\omega^{3/2}}{(e^{\hbar \omega / kT} - 1)} d\omega \right] \end{aligned}$$

Lastly, we want to get the heat capacity, so take derivative w.r.t T again. The first term vanishes since it is T independent z.p.e.

$$C_v = \frac{V\hbar}{4\pi^2 A^{3/2}} \int_0^{\omega_{\max}} \frac{\omega^{3/2} e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT} - 1)^2} \left(\frac{\hbar\omega}{kT^2} \right) d\omega$$

$$= \frac{V\hbar^2}{4\pi^2 A^{3/2} kT^2} \int_0^{\omega_{\max}} \frac{\omega^{5/2} e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT} - 1)^2} d\omega$$

We can easily approximate C_v in the low temperature regime.

Let $x = \frac{\hbar\omega}{kT}$ and $u = \frac{\hbar\omega_{\max}}{kT}$

$$C_v = \frac{V\hbar^2}{4\pi^2 A^{3/2} kT^2} \frac{kT}{\hbar} \left(\frac{kT}{\hbar} \right)^{5/2} \int_0^u \frac{x^{5/2} e^x}{(e^x - 1)^2} d\omega$$

$$= \frac{V\hbar^2}{4\pi^2 A^{3/2} kT^2} \left(\frac{kT}{\hbar} \right)^{7/2} \int_0^u \frac{x^{5/2} e^x}{(e^x - 1)^2} d\omega$$

$$= \frac{V\hbar^2 k k^{3/2} T^{3/2}}{4\pi^2 A^{3/2} \hbar^{3/2}} \int_0^u \frac{x^{5/2} e^x}{(e^x - 1)^2} d\omega = \frac{V\hbar^2 k}{4\pi^2} \left(\frac{kT}{A\hbar} \right)^{3/2} \int_0^u \frac{x^{5/2} e^x}{(e^x - 1)^2} d\omega$$

Note the $T^{3/2}$ dependence of the heat capacity.

6. Consider a planar square lattice of identical atoms which vibrate perpendicular to the plane of the lattice. If we let x_{lm} be the displacement of the atom in the l th column and m th row, show that the equation of motion is:

$$m \frac{\partial^2 x_{lm}^2}{\partial t^2} = f \left[(z_{l+1,m} + z_{l-1,m} - 2z_{lm}) + (z_{l,m+1} + z_{l,m-1} - 2z_{lm}) \right]$$

where m is the mass of an atom, and f is the force constant. Assume a solution of the form

$$x_{lm} = \exp \left[i(lk_y a + mk_x a + \omega t) \right]$$

The potential function in 1D is

$$U(z) = \sum_1^N u(a + z_{i+1} - z_i) = \sum_1^N u(a + \delta)$$

To generalize to vibrations perpendicular to the plane, we need to indices, l and m to locate each atom. The potential function becomes

$$U(x) = \sum_{l,m}^N \left[u(a + z_{l+1,m} - z_{l,m}) + u(a + z_{l,m+1} - z_{l,m}) \right]$$

Now expand the potential about $z=a$ using a Taylor series.

$$U(z) \approx U(0) + \sum_{l,m}^{N_l N_m} \left[\frac{1}{2} u''(a) (z_{l+1,m} - z_{l,m})^2 + \frac{1}{2} u''(a) (z_{l,m+1} - z_{l,m})^2 \right]$$

Now differentiate to get the wave equation.

$$m \frac{\partial^2 z_{lm}}{\partial t^2} = \frac{\partial U}{\partial z} = f \left[(z_{l+1,m} + z_{l-1,m} - 2z_{lm}) + (z_{l,m+1} + z_{l,m-1} - 2z_{lm}) \right]$$

a. Derive the dispersion function $\omega(k)$.

Try a solution of the form $x_{lm}(t) = e^{i\omega t} y_l y_m$

We get

$$-m\omega^2 y_l y_m = f \left[(y_{l+1} y_m - y_{l-1} y_m - 2y_l y_m) + (y_l y_{m+1} - y_l y_{m-1} - 2y_l y_m) \right]$$

Now we need to make a guess at the solution for the difference equation.

Try $y_l y_m = e^{i\varphi_l l} e^{i\varphi_m m}$

$$-m\omega^2 e^{i\varphi_l l} e^{i\varphi_m m} = f e^{i\varphi_l l} e^{i\varphi_m m} \left[(e^{i\varphi_m} + e^{-i\varphi_m} - 2) + (e^{i\varphi_l} + e^{-i\varphi_l} - 2) \right]$$

$$m\omega^2 = f \left[\sin^2 \left(\frac{\varphi_m}{2} \right) + \sin^2 \left(\frac{\varphi_l}{2} \right) \right]$$

$$\omega = \omega_{\max} \left[\sin^2 \left(\frac{\varphi_m}{2} \right) + \sin^2 \left(\frac{\varphi_l}{2} \right) \right]^{1/2}$$

To summarize, our solution is $x_m(t) = \exp[i(l\varphi_l + m\varphi_m + \omega t)]$

It repeats itself every $\Delta l = 2\pi/\varphi_l$ and every $\Delta m = 2\pi/\varphi_m$. This is a wave in both dimension with wavelengths

$$\lambda_l = \frac{2\pi a}{\phi_l} \quad \text{and} \quad \lambda_m = \frac{2\pi a}{\phi_m}.$$

Thus, we solve for ϕ_l and ϕ_m .

This results in the dispersion relation we are looking for.

$$\omega = \omega_{\max} \left[\sin^2 \left(\frac{k_m a}{2} \right) + \sin^2 \left(\frac{k_l a}{2} \right) \right]^{1/2}$$

b. Simplify the expression $\omega(k)$ in the long wavelength limit to obtain

$$\omega = ka \left(\frac{f}{m} \right)^{1/2} \quad \text{where} \quad k = (k_x^2 + k_y^2)^{1/2}$$

We use the approximation $\sin(x) = x$ for small x . Thus,

$$\begin{aligned} \omega &= \omega_{\max} \left[\sin^2 \left(\frac{k_m a}{2} \right) + \sin^2 \left(\frac{k_l a}{2} \right) \right]^{1/2} \\ &\approx \frac{a\omega_{\max}}{2} \left[k_m^2 + k_l^2 \right]^{1/2} \end{aligned}$$

c. Derive an energy expression for this 2D lattice.

$$\text{In 2D, } k^2 = \left(\frac{\pi}{L} \right)^2 (n_x^2 + n_y^2) \quad , \quad \text{or} \quad k^2 = \left(\frac{\pi}{L} \right)^2 (n_x^2 + n_y^2)$$

$$\text{Letting } R^2 = n_x^2 + n_y^2,$$

The area in the positive quadrant is

$$\Phi = \frac{1}{4} \pi R^2 = \frac{1}{4} \pi \left(\frac{L}{\pi} \right)^2 k^2 = \frac{Ak^2}{4\pi}$$

Now insert the dispersion relation, in the long wavelength limit:

$$\left(\frac{2\omega}{a\omega_{\max}} \right)^2 \approx k^2$$

$$\Phi = \frac{1}{4}\pi R^2 = \frac{1}{4}\pi\left(\frac{L}{\pi}\right)^2 k^2 = \frac{A}{4\pi}\left(\frac{2\omega}{a\omega_{\max}}\right)^2$$

The frequency distribution function is:

$$g(\omega) = \frac{\partial\Phi}{\partial\omega} = \frac{A}{2\pi}\left(\frac{2\omega}{a\omega_{\max}}\right)\frac{2}{a\omega_{\max}} = \frac{2A\omega}{\pi a^2\omega_{\max}^2}$$

The energy expression, derived previously, is

$$E = \sum_j \frac{\hbar\omega_j}{2} + \sum_j \frac{\hbar\omega_j}{\exp(\hbar\omega_j/kT) - 1}$$

Converting to an integral over $0 \rightarrow \omega_{\max}$

$$E = \int_0^{\omega_{\max}} \frac{\hbar\omega g(\omega)d\omega}{\exp(\hbar\omega/kT) - 1} = \frac{2A\hbar}{\pi a^2\omega_{\max}^2} \int_0^{\omega_{\max}} \frac{\omega^2 d\omega}{\exp(\hbar\omega/kT) - 1}$$