7.5: Low-temperature Heat Capacity

If

$$G(\omega)d\omega = \text{ number of normal modes with frequencies from } \omega \text{ to } \omega + d\omega \tag{7.5.1}$$

then

$$E^{\text{crystal}} = \int_0^\infty G(\omega) e^{\text{SHO}}(\omega) d\omega \quad \text{and} \quad C_V^{\text{crystal}} = \int_0^\infty G(\omega) c_V^{\text{SHO}}(\omega) d\omega \tag{7.5.2}$$

and so forth.

Density of modes:

$$\begin{aligned} G(\omega)d\omega &= \sum_{\text{branches}} [\text{ vol. of shell in } k\text{-space }] (\text{density of modes in } k\text{-space}) \\ &= \sum_{\text{branches}} \left[4\pi (k_b(\omega))^2 dk_b\right] \left(\frac{V}{8\pi^3}\right) \end{aligned}$$

This formula holds for any isotropic dispersion relation $k_b(\omega)$. For small values of ω the dispersion relation for each branch is linear (with sound speed c_b) so

$$k_b = \frac{\omega}{c_b} \quad \text{and} \quad dk_b = \frac{d\omega}{c_b}, \tag{7.5.3}$$

whence

$$\begin{aligned} G(\omega)d\omega &= \sum\nolimits_{\text{branches}} \left[4\pi \left(\tfrac{\omega}{c_b}\right)^2 \tfrac{d\omega}{c_b}\right] \left(\tfrac{V}{8\pi^3}\right) \\ &= \frac{V}{2\pi^2} \left(\sum_{b=1}^{3} \frac{1}{c_b^3}\right) \omega^2 d\omega. \end{aligned} \tag{7.5.4}$$

If we define the "average sound speed" c_s through the so-called "harmonic cubed average",

$$\frac{1}{c_s^3} \equiv \frac{1}{3} \sum_{b=1}^{3} \frac{1}{c_b^3}, \tag{7.5.5}$$

then we have the small-ω density of modes

$$G(\omega)d\omega = \frac{3V}{2\pi^2} \frac{\omega^2}{c_s^3} d\omega. \tag{7.5.6}$$

At any temperature,

$$C_V^{\text{crystal}} = \int_0^\infty G(\omega) c_V^{\text{SHO}}(\omega) d\omega. \tag{7.5.7}$$

Recall from equation (5.78) that

$$c_V^{\text{SHO}}(\omega) = k_B \left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{e^{-\hbar\omega/k_B T}}{\left(1 - e^{-\hbar\omega/k_B T}\right)^2}, \tag{7.5.8}$$

and using the small-ω result (7.11), we have the low-temperature result

$$C_V^{\text{crystal}} = \frac{3V}{2\pi^2} \frac{1}{c_s^3} k_B \int_0^\infty \omega^2 d\omega \left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{e^{-\hbar\omega/k_B T}}{\left(1 - e^{-\hbar\omega/k_B T}\right)^2}. \tag{7.5.9}$$

For our first step, avoid despair — instead convert to the dimensionless variable

$$x = \frac{\hbar\omega}{k_B T} \tag{7.5.10}$$

and find

$$C_V^{\text{crystal}} = \frac{3V}{2\pi^2}\frac{1}{c_s^3}k_B\left(\frac{k_B T}{\hbar}\right)^3 \int_0^\infty \frac{x^4 e^{-x}}{\left(1-e^{-x}\right)^2}dx \tag{7.5.11}$$

The integral is rather hard to do, but we don't *need* to do it — the integral is just a number. We have achieved our aim, namely to show that at low temperatures, $C_V \sim T^3$.

However, if you want to chase down the right numbers, after some fiddling you'll find that

$$\int_0^\infty \frac{x^4 e^{-x}}{\left(1-e^{-x}\right)^2}dx = 4\Gamma(4)\zeta(4) = \frac{4}{15}\pi^4. \tag{7.5.12}$$

Thus, the low-temperature specific-heat of a solid due to a lattice vibration is

$$C_V^{\text{crystal}} = k_B V \frac{2\pi^2}{5}\left(\frac{k_B T}{\hbar c_s}\right)^3. \tag{7.5.13}$$

7.3 How far do the atoms vibrate?

> Consider a simplified classical Einstein model in which *N* atoms, each of mass *m*, move classically on a simple cubic lattice with nearest neighbor separation of a. Each atom is bound to its lattice site by a spring of spring constant *K*, and all the values of *K* are the same. At temperature *T*, what is the root mean square average distance of each atom from its equilibrium site? (Note: I am asking for an ensemble average, not a time average.)
