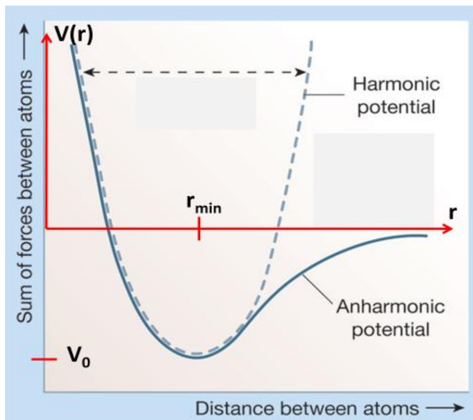
Lecture 12 Summary

Phys 404

We consider the energy stored in vibrational waves inside a solid at temperature τ. This problem is closely related to the Planck black body distribution law for photons in a box, considered in the last lecture.

A solid is made up of atoms that sit at equilibrium positions in a regular periodic array called a crystal. Consider the interatomic potential of atoms in a crystalline solid as shown in the figure below.



The atoms have an equilibrium separation from their neighbors at a distance r_{min}. Near the bottom of the potential well, the potential is described by $V(r) \cong V_0 + \frac{1}{2}k(r - r_{min})^2$ (dashed line in figure), where the "spring constant" k is the curvature of the potential. The quantum mechanical solutions for this potential are the harmonic oscillator eigenvalues, $E_s = s\hbar\omega$, where $\omega = \sqrt{k/m}$ is the resonant frequency of a mass m trapped in this potential, and $s = 0, 1, 2, 3, \ldots$ is the occupation number of the mode. The quanta of vibration in this single mode are called PHONONS, in analogy with the quanta of electromagnetic excitations of a single mode, called photons. We can now use all of the results of the photon mode statistical mechanics to describe what happens to the phonon occupation of this mode. In particular we have $< \varepsilon >=< s\hbar\omega >= \frac{\hbar\omega}{e^{\hbar\omega/\tau}-1}$, as before for the energy in this mode at temperature τ.

Now consider all of the modes of vibration of a cube of N atoms vibrating around their equilibrium positions. Take the cube to have sides L and to be in equilibrium with a reservoir at temperature τ. We can solve the wave equation for elastic vibrational modes in the cube: $\nabla^2\vec{u} = \frac{1}{v^2}\frac{\partial^2\vec{u}}{\partial t^2}$, where $\vec{u}(x, y, z)$ gives the displacement from equilibrium of the atom at position (x, y, z), and v is the speed of sound propagation. The result is essentially identical to the photon case, with the mode frequencies described by $\omega_n = \frac{n\pi c}{L}$, where $n = \sqrt{n_x^2 + n_y^2 + n_z^2}$, and $n_x = 1, 2, 3, \ldots$, $n_y = 1, 2, 3, \ldots$, $n_z = 1, 2, 3, \ldots$ However, here there is a difference. The number of elastic modes of the solid is not infinite (as in the electromagnetic case), but finite and equal to $3N$. The solid, made up of discrete atoms, cannot support waves whose wavelength is arbitrarily short. In fact it cannot support waves with wavelengths shorter than twice the interatomic separation. This limits the total number of modes to be just $3N$. The 3 comes from the fact that there are 3 polarizations of waves in the crystal; 2 transverse and one longitudinal. To include this constraint on the statistical physics, we have to count the modes from the lowest one and stop once we get to an upper bound, which we shall call n_{max}. To do this we once again convert from a sum on n_x, n_y, n_z to a continuous integral on n. We find that $3N = \sum_n^{n_{max}}$ becomes $3N = 3\frac{4\pi}{8}\int_0^{n_{max}} n^2\, dn$, which yields $n_{max} = (6N/\pi)^{1/3}$. The factor of 3 in front of the integral accounts for the three independent polarizations of the phonons (two transverse and one longitudinal).

The total energy of phonons in the solid is now given by $U = 3\frac{4\pi}{8}\int_0^{n_{max}} \frac{\hbar\omega_n}{e^{\hbar\omega_n/\tau}-1} n^2 dn$, which becomes after a change of variable, $U = \frac{3\pi}{2}\frac{V\tau^4}{(\pi\hbar v)^3}\int_0^{x_{max}} \frac{x^3 dx}{e^x-1}$, where $x_{max} = \frac{k_B\Theta_\mathrm{D}}{\tau}$, and $\Theta_\mathrm{D} = \frac{\hbar v}{k_B}(\frac{6\pi^2 \mathrm{N}}{\mathrm{V}})^{1/3}$ is called the Debye temperature, and is a characteristic of the material. Consider the low temperature limit $\tau \ll k_B\Theta_\mathrm{D}$. In this case, the upper limit of the integral can be extended to infinity with little error and we have the result $U = \frac{3}{5}\frac{Nk_B\pi^4}{{\Theta_\mathrm{D}}^3}T^4$ $(T \ll \Theta_\mathrm{D})$. This result is very similar to the Stefan-Boltzmann law for photons in a box. The heat capacity is a measure of how much energy must be added to the system to change its temperature by 1 degree, $C_V = \frac{\partial U}{\partial T}|_V = \frac{12Nk_B\pi^4}{5}\left(\frac{T}{\Theta_\mathrm{D}}\right)^3$. This famous result for the low temperature heat capacity due to phonons is widely reproduced in many materials. In the high temperature limit $(T \gg \Theta_\mathrm{D})$, the heat capacity tends to a constant value, $C_V = 3Nk_B$, which is known as the law of Dulong-Petit. The overall temperature dependence is shown in a figure on the class web site.