
LECTURE 39: CONTINUUM LIMIT OF HARMONIC CHAIN
Friday, November 15, 2019

Allow me to restate the Hamiltonian, dropping the harmonic oscillator part, which isn't physical in real atomic structures:

$$\hat{H} = \sum_j \left(\frac{1}{2} m \dot{x}_j^2 + \frac{1}{2} m \omega_1^2 (x_{j+1} - x_j)^2 \right)$$

and

$$\Omega(k) = 2\omega_1 \left| \sin\left(\frac{kl}{2}\right) \right| = (\omega_1 l) k$$

where $m\omega_1^2$ is the strength of the atomic bond, roughly modeled as a spring.

When we go to the continuum limit, our discrete sum becomes an integral $\sim \int \frac{dx}{l}$. Now our discrete x_j should also be replaced by some continuous function $u(x)$, so $x_{j+1} - x_j \approx l \frac{\partial u(x)}{\partial x}$. If k corresponds to a length scale much larger than the size of the atoms, we no longer care about the mass of the atoms, but rather the mass density $\mu = \frac{m}{l}$. Of course, $\dot{x}_j \rightarrow \frac{\partial u(x)}{\partial t}$ and we will assign a new variable $m\omega_1^2 l^2 \rightarrow K$ such that $\omega_1 = \sqrt{\frac{K}{\mu}} - l$. K is an elastic constant.

$$H = \int dx \left\{ \frac{1}{2} \mu \left(\frac{\partial u}{\partial t} \right)^2 + \frac{1}{2} K \left(\frac{\partial u}{\partial x} \right)^2 \right\}$$

Solutions to this equation are

$$u_k(x, t) = A e^{i(kx - \omega t)}$$

where $\omega = vk$ with $v = \sqrt{\frac{K}{\mu}}$.

As l grows smaller, $\frac{\pi}{l}$ grows bigger—the Brillouin zone gets larger, and the dispersion relation grows as shown in Figure 0.0.1.

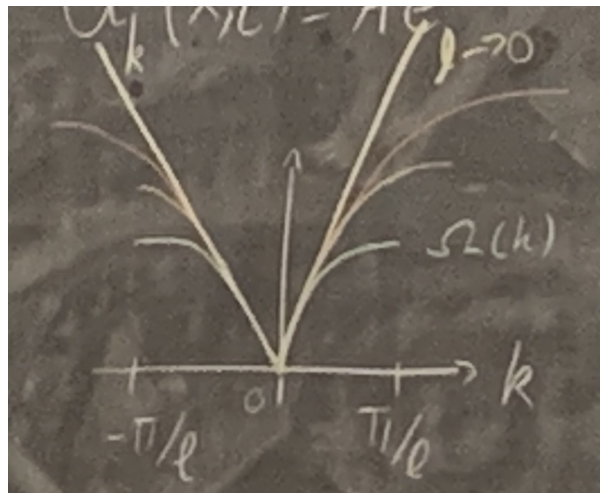


Figure 0.0.1: Dispersion relation as $l \rightarrow 0$

0.1 Blackbody Radiation

Think of a blackbody as a box of photons. Photons are allowed to leave (radiate) if they are excited.

Say we have a 1-D box which ranges from $[0, L]$ with boundary conditions where the field vanishes at the boundaries. We see that the set of wavenumbers which conform to these conditions are $k_j = \frac{\pi}{L} j$ and the

allowed frequencies are $\omega_j = ck_j$. Call the density of states $D(\omega)$ and we can define the number of states in an interval $(\omega, \omega + d\omega)$ as $D(\omega) d\omega$. The number of modes with frequency less than ω is $\mathcal{N}(\omega) = \frac{L\omega}{\pi c}$. Therefore,

$$D(\omega) = \frac{d\mathcal{N}}{d\omega} = \frac{L}{\pi c}$$

In 3-D,

$$\mathcal{N}(\omega) = \frac{4\pi}{3} \left(\frac{\omega L}{2\pi c} \right)^3$$

The values of allowed k form a discretely spaced set. If we then choose an ω , we can see how many k values lie in the dispersion band for a particular ω (again, see Figure 0.0.1).

For photons in 3-D space, we actually need to multiply this value by two, since we can have two different polarized states:

$$\mathcal{N}(\omega) = \frac{4\pi}{3} \left(\frac{\omega L}{2\pi c} \right)^3 \times 2$$

Given this \mathcal{N} ,

$$D(\omega) = \frac{\omega^2}{\pi^2} \frac{1}{c^3} V$$

where V is the volume of the box.

Recall from this morning we discussed the expectation value of the Hamiltonian for a particular temperature and value of ω :

$$\hat{\mathbf{H}} = \int dk \hat{\mathbf{H}}(k)$$

so

$$\langle \hat{\mathbf{H}} \rangle(\omega) - \frac{1}{2} \hbar \omega = \frac{\omega^2}{\pi^2} \frac{1}{c^3} V \frac{\hbar \omega}{e^{\frac{\hbar \omega}{kT}} - 1}$$

because many of the modes in the 3-D box are degenerate (just in different directions). The spectral energy density is the famous blackbody spectrum (see Figure 0.1.1)

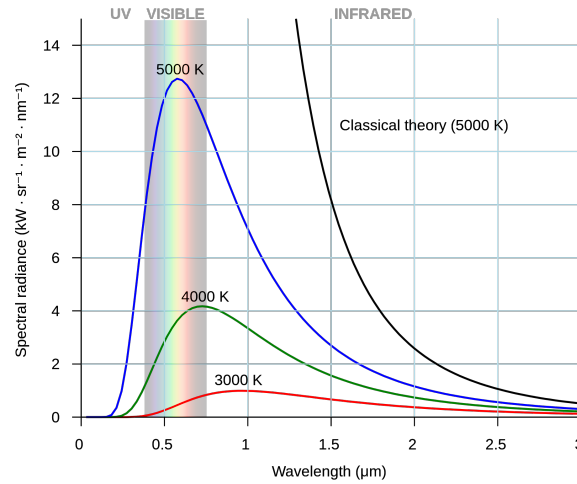


Figure 0.1.1: The Blackbody Energy Density Spectrum

We can see that the spectrum increases with $\omega^2 T$ at low ω , but at some point ($\omega = \frac{kT}{\hbar}$) we leave this Classical behavior and the spectrum changes like $e^{-\frac{\hbar \omega}{kT}}$.

0.2 Heat Capacity

We can describe a characteristic called heat capacity which corresponds to the way the heat contained in an object changes with temperature:

$$C_v = \frac{\partial U(T)}{\partial T}$$

For a harmonic solid (something with quadratic terms in the Hamiltonian, no higher-order terms), the total energy constant is proportional to the total number of atoms present and the average amount of energy per atom:

$$U = 3N \langle \hat{\mathbf{H}} \rangle$$

Note that phonon modes have three polarizations (degenerate eigenstates in 3-D). Let's examine the Einstein model, where the density of states is described by

$$D(\omega) = 3N\delta(\omega - \omega_E)$$

This is equivalent to bringing back the local harmonic oscillators which we threw away in the continuum limit, and it removes the interaction between nearby atoms. It's not a great model. For this model,

$$C_v \sim e^{-\frac{\hbar\omega_E}{k_B T}}, \quad T \rightarrow 0$$

This explains nicely why heat capacity vanishes at low T and approaches $3k_B$ as $T \rightarrow \infty$, the Classical limit. The Classical (high temp) and quantum (low temp) regions are separated by characteristic temperature $\frac{\hbar\omega_E}{k_B}$.

There is another model by Debye which takes into account the low frequency modes:

$$D(\omega) = \frac{\omega^2}{\pi^2} \frac{1}{c^3} V \div 2 \times 3$$

Note that c here is the speed of sound, not light.

We divide by 2 to eliminate the degeneracy of photon polarizations which was present in the blackbody derivation, but multiply by 3 to reintroduce the degeneracy of the phonon states.

While both models behave the same way in their extremes, the Debye model varies like T^3 at low temperatures while Einstein's model varies like $e^{-\frac{\hbar\omega_E}{k_B T}}$.