Physics 0551 Lecture #13

Boundary Conditions:

So far we have learned: What is a crystal?

How does it interact with waves?

How does it vibrate?

What are the important forces?

Now to address the thermodynamic properties this vibration process possesses:

Heat capacity and Thermal conductivity.

We have determined the types of lattice vibrations ω vs. k (or q), but we know nothing about their actual distribution. To answer this question we must determine two things:

(1) How are the lattice vibrations distributed?

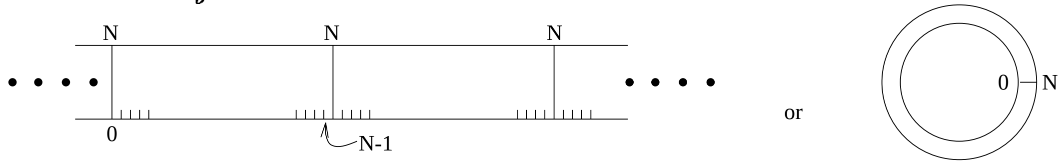
(2) What is their occupancy?

As of yet we have not considered boundary conditions. One possibility is to assume the ends of the crystal are held fixed

$$\vec{u}_0 = \vec{u}_N = 0$$

Another, (the one we will focus on)

Periodic boundary conditions

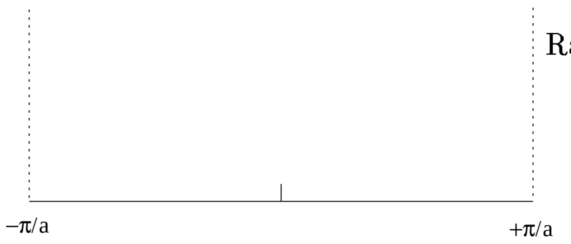


Thus $\vec{u}_0 = \vec{u}_N \qquad e^{ik\cdot 0a} = e^{ik\cdot Na} = 1$

$$kNa = 2\pi n \qquad \text{let } Na = L \qquad n = \text{integer}$$

$$k = 2\pi n/L \qquad \text{this gives a restricted set of } k\text{'s}$$

Question: How many k's are there in the first Brillouin zone of the one-dimensional chain?



Range of $k = \frac{2\pi}{a}$, each mode is $2\pi/L$ apart,

thus $\frac{L}{a}$ modes $= N$

There are N modes for *each* branch of the dispersion curve.

NEW CONCEPT: Density of states or (Density of modes)

$D(k)dk$ number of states with $|\vec{q}|$ vector between k and $k + dk$

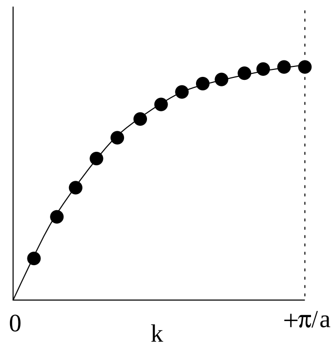
For 1D, states are $\frac{2\pi}{L}$ apart (in k), $\frac{dk}{2\pi/L} = \#$ of modes in dk

Thus $D(k)dk = \frac{L}{2\pi}dk$, $D(k) = \frac{L}{2\pi} =$ constant

Rather than $D(k)$, we will find it useful to consider quantity $D(\omega)$, density of states with respect to energy frequency.

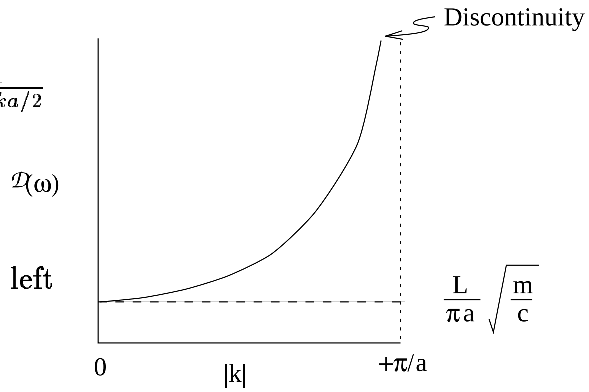
$$\begin{aligned} D(\omega) &= D(k)\frac{dk}{d\omega} = \frac{D(k)}{d\omega/dk} = D(k)/v_g \\ D(\omega) &= \frac{L}{2\pi}1/v_g \end{aligned}$$

For the 1-D monoatomic lattice: $\omega = \sqrt{\frac{4c}{m}}\ \sin\frac{ka}{2}$ $\quad \frac{d\omega}{dk} = \frac{a}{2}\sqrt{\frac{4c}{n}}\ \cos\frac{ka}{2}$



$$D(\omega) = 2\frac{L}{2\pi a}\sqrt{\frac{m}{c}}\ \frac{1}{\cos\ ka/2}$$

Factor of two for the left and right



Now extend this to 3 dimensions (and assume an orthogonal basis)

A plane wave propagating in the $\hat{k}$ directions

$$\lambda = 2\pi/|k| \qquad \vec{k} = k_1\hat{a}_1^* + k_2\hat{a}_2^* + k_3\hat{a}_3^*$$
$$u = u_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)} \qquad \vec{r} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

For a discrete lattice $\quad \vec{k}$ is not necessarily a reciprocal lattice vector

$$u_{n_1,n_2,n_3} = u_0 e^{i(k_1a_1n_1+k_2a_2n_2+k_3a_3n_3)}$$

Consider a volume $Na_1 \times Na_2 \times Na_3$ $\quad N^3$ cells

Apply periodic boundary conditions

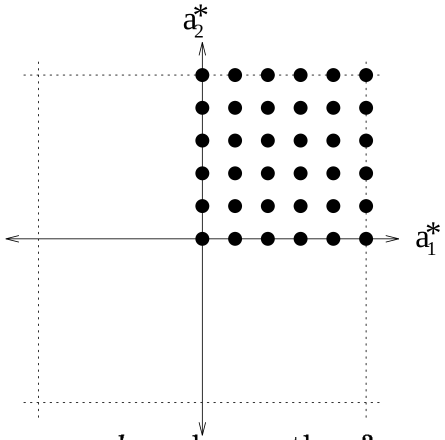
$$\begin{aligned} a_1 \rightarrow &\quad e^{ik_1n_1a_1} = e^{ik_1(N+n_1)a_1} \\ a_2 \rightarrow &\quad e^{ik_2n_2a_2} = e^{ik_2(N+n_2)a_2} \\ a_3 \rightarrow &\quad e^{ik_3n_3a_3} = e^{ik_3(N+n_3)a_3} \end{aligned}$$

This gives $e^{ik_1Na_1} = e^{ik_2Na_2} = e^{ik_3Na_3} = 1$

$k_1Na_1 = m2\pi \qquad k_2Na_2 = n2\pi \qquad k_2Na_3 = \ell 2\pi$ with $m, n, \ell =$ integer

If $a_1 = a_2 = a_3 = a$ then $k_1 = 2\pi n/L$, $k_2 = 2\pi n/L$, and $k_3 = 2\pi \ell/L$

Now examine the k_1, k_2 plane



spacing $2\pi/L$ $\qquad Na = L$

If L is large, k's form
a closely spaced lattice
within lst B.Z.

How many k-modes are there?

$$\frac{\text{Volume}}{\text{1st BZ}} = \left(\frac{2\pi}{a}\right)^3 \frac{\text{Volume}}{\text{one mode}} = \left(\frac{2\pi}{L}\right)^3$$

Modes = $(2\pi/a)^3/(2\pi/L)^3 = \left(\frac{L}{a}\right)^3 = \#$ of lattice points in

N^3 quantization volume

For one atom/lattice point and three branches (2TA,1LA) there are $\underline{3N^3 \text{ modes.}}$
(Along high symmetry directions)
Density of states in k-space

$$D(k)d^3k = \left(\frac{L}{2\pi}\right)^3 d^3k = \frac{V}{(2\pi)^3} d^3k$$

This is just the number of allowed states/per branch in an element d^3k of k-space. It is a constant since k's are uniformly spaced. How about spherical in coordinates:
All the modes between $|k|$ and $|dk| + |k|$

Spherical shells of $4\pi|k|^2 d|k|$

$D(|k|)d|k| = \frac{4\pi k^2 d|k|}{(2\pi/L)^3} = \frac{V}{2\pi^2} \; k^2 d|k|$

Again we want the number of modes with ω between ω and ω+dω
$D(\omega)d\omega = \frac{D(|k|)}{d\omega dk} d\omega = \frac{D(|k|)}{v_g} d\omega$

For k small

$$\begin{aligned} (\text{ non-dispersive})\ v_g &= v_s \qquad D(\omega) = \frac{Vk^2}{2\pi^2 v_s} = \frac{V\omega^2}{2\pi^2 v_s^3}\ (\text{ for each branch}) \\ \frac{\omega}{k} &= v_s \end{aligned}$$