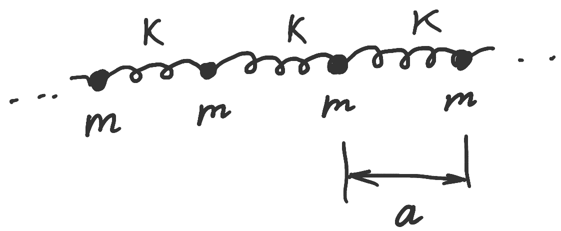
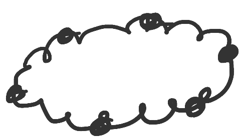
Phonons in solids II



$$H = \sum_i \left[\frac{p_i^2}{2m} + K(x_i - x_{i+1})^2 \right] \qquad (*)$$

How many momentum modes actually exist there? Since the boundary conditions are unimportant, make a ring out of the system



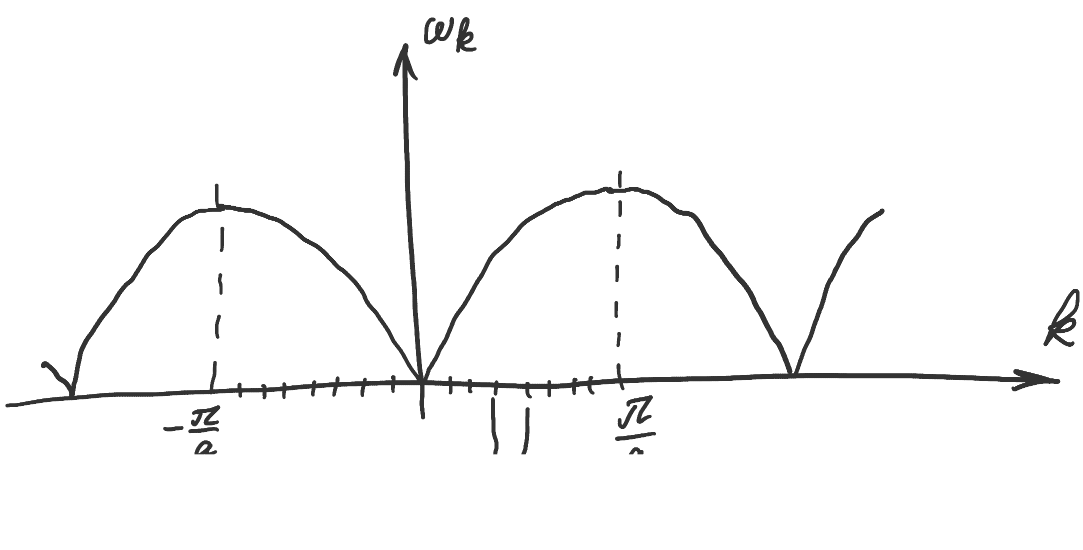
Periodic boundary condition:

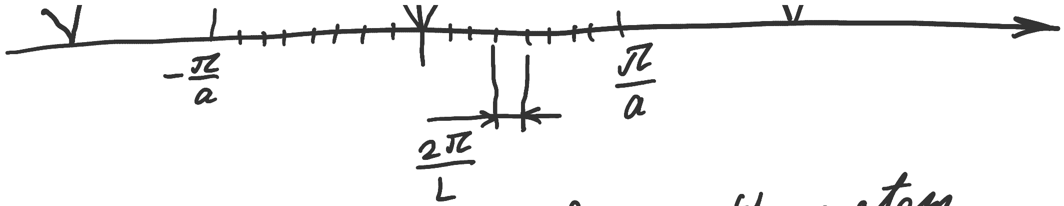
$$e^{ikL} = 1 \rightarrow$$

$$\rightarrow \quad kL = 2\pi n \rightarrow k_n = \frac{2\pi}{L} n$$

Note: since the distance between the atoms is a, $N = \frac{L}{a}$, and $k_n = \frac{2\pi}{a} \frac{n}{N}$

The spacing between the momenta of neighbouring modes is $\Delta k = \frac{2\pi}{L}$





There are $N = \frac{L}{a}$ modes in the system

Try to diagonalise (quantise) the Hamiltonian (*)

Now $\hat{x}_i$ and $\hat{p}_i$ are quantum operators

$$\hat{x}_n = \frac{1}{\sqrt{N}} \sum_k \hat{x}_k e^{inak}, \quad \hat{p}_n = \frac{1}{\sqrt{N}} \sum_k \hat{p}_k e^{inka} \qquad (1)$$

$$\updownarrow$$

$$\hat{x}_k = \frac{1}{\sqrt{N}} \sum_n \hat{x}_n e^{-inak}$$

$$[\hat{p}_k, \hat{x}_{k'}] = \frac{1}{N} \left[\sum_n \hat{p}_n e^{-inak}, \sum_m \hat{x}_m e^{-imak'} \right] =$$

$$= \frac{1}{N} \sum_n [\hat{p}_n, \hat{x}_n] e^{ina(k+k')} =$$

Only $n=m$ contribute

$$= -i \delta_{k,-k'}$$

$$\boxed{[\hat{p}_k, \hat{x}_{k'}] = -i \delta_{k,-k'}}$$

One may say $\hat{p}_k = -i \frac{\partial}{\partial x_{-k}}$

Let's insert (1) into (*)

$$\sum \hat{p}_n^2 = \frac{1}{N} \sum_n \left(\sum_k \hat{p}_k e^{inka} \right) \left(\sum_{k'} \hat{p}_{k'} e^{ink'a} \right) =$$

$$\sum_n \hat{p}_n^2 = \frac{1}{N} \sum_n \left(\sum_k \hat{p}_k e^{inka} \right) \left(\sum_{k'} p_{k'} e^{\quad} \right) =$$

$$= \sum_k \hat{p}_k \hat{p}_{-k}$$

$$\sum_n e^{in(k+k')a} = N \delta_{k,-k'}$$

So, $\frac{1}{2m} \sum_n \hat{p}_n^2 = \sum_k \frac{\hat{p}_k \hat{p}_{-k}}{2m}$

$$\hat{x}_n - \hat{x}_{n+1} = \frac{1}{\sqrt{N}} \sum_k (1 - e^{ika}) e^{ikna}$$

$$\sum_n (\hat{x}_n - \hat{x}_{n+1})^2 = \sum_k \underbrace{(1 - e^{-ika})(1 - e^{ika})}_{2 - 2\cos(ka)} \hat{x}_k \hat{x}_{-k}$$

To sum up,

$$\boxed{\hat{H} = \sum_k \left[\frac{\hat{p}_k \hat{p}_{-k}}{2m} + \frac{K}{2} (2 - 2\cos(ka)) \hat{x}_k \hat{x}_{-k} \right]}$$

This is now easy to diagonalise because different ks are disentangled, except k and $-k$

Introduce $\omega_k = \sqrt{\frac{K}{m}(2 - 2\cos(ka))} = 2\sqrt{\frac{K}{m}} \left|\sin \frac{ka}{2}\right|$

Introduce $\hat{x}_k = \sqrt{\frac{\hbar}{m\omega_k}} \frac{b_k + b^+_{-k}}{\sqrt{2}}$

$$\hat{p}_k = \sqrt{\hbar m \omega_k} \frac{b_k - b^+_{-k}}{i\sqrt{2}}$$

$$\hat{H} = \sum_k \left(\hat{b}_k^+ \hat{b}_k + \frac{1}{2} \right) \hbar \omega_k$$

The system is equivalent to a set of harmonic oscillators. Their excitation quanta = phonons = quanta of vibrations of the crystalline lattice

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Similarly, for an arbitrary Hamiltonian one may diagonalise it and arrive at a set of oscillators

$$\hat{H} = \sum_{\vec{k}\alpha} \left(\hat{b}_{\vec{k}\alpha}^+ \hat{b}_{\vec{k}\alpha} + \frac{1}{2} \right) \hbar \omega_{\vec{k}\alpha}$$

How many modes are there?

For each branch there are 3 polarisations

We may again choose, e.g., the periodic boundary conditions. Then

$$\vec{k} = \frac{2\pi}{L} (n_x, n_y, n_z) \quad \text{(in a cube)}$$

The number of momentum modes is $\left(\frac{2\pi}{a}\right)^3 / \left(\frac{2\pi}{L}\right)^3 = N$

(with polarisations it's $3N$, for multiatomic lattices $3\nu N$)

The number of momentum modes in the element $d\vec{k}$ of momentum space is given by

$d\vec{k}$ of momentum space is given by

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

That matches the Bohr-Sommerfeld quantisation rule

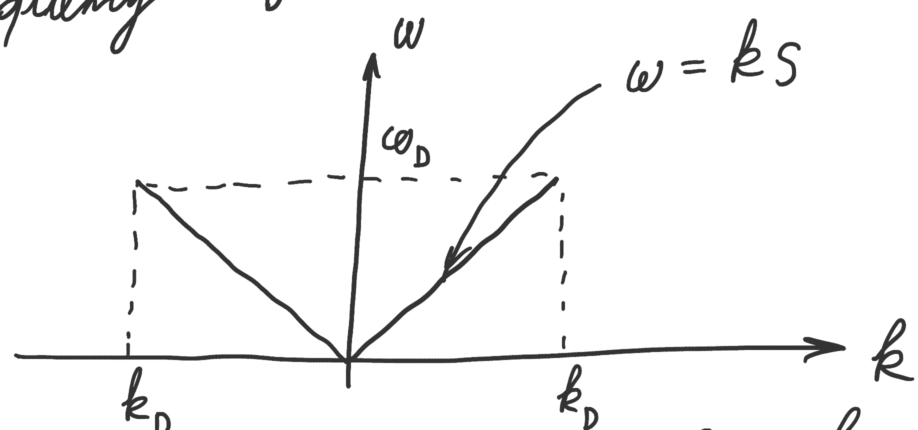
Compute, e.g., the internal energy

$$E = \sum_{\alpha} V \int \frac{d\vec{k}}{(2\pi)^3} \frac{\hbar \omega_{\vec{k}\alpha}}{e^{\frac{\hbar\omega_{\vec{k}\alpha}}{T}} - 1}$$

In general, this integral is arbitrarily ugly. That is why one often uses the simplified

<u>Debye model</u>

The phonon dispersion is linear up to some frequency ω_D



Require that the number of modes is still the same (within a branch!)

$$\frac{4\pi}{3} k_D^3 \cdot \frac{1}{\cdots} = N \rightarrow k_D = \left(6\pi^2 \frac{N}{V}\right)^{\frac{1}{3}} \equiv \left(6\pi^2 n\right)^{\frac{1}{3}}$$

the same (wa...

$$\frac{4\pi}{3} k_D^3 V \frac{1}{(2\pi)^3} = N \rightarrow k_D = \left(6\pi^2 \frac{N}{V}\right)^{\frac{1}{3}} \equiv \left(6\pi^2 n\right)^{\frac{1}{3}}$$

$$\boxed{\omega_D = \left(6\pi^2 n\right)^{\frac{1}{3}} s}$$

Now it's easier to compute the internal energy

$$E = 3V \int_0^{k_D} \frac{4\pi k^2 dk}{(2\pi)^3} \frac{\hbar s k}{e^{\frac{\hbar s k}{T}} - 1} = 3V \int_0^{\omega_D} \underbrace{\frac{\omega^2}{2\pi^2 s^3}}_{\substack{\text{DoS (per volume)} \\ \text{(per branch)}}} \frac{\hbar\omega}{e^{\hbar\omega/T} - 1} d\omega =$$

$$= \frac{3VT^4}{2\pi^2 s^3 \hbar^3} \int_0^{x_D} \frac{x^3 dx}{e^x - 1} \quad \text{, where } x_D = \frac{\hbar\omega_D}{T}$$

<u>The case of low temperatures, $T \ll \hbar\omega_D$</u>

$x_D \rightarrow \infty$

$$\int_0^\infty dx \frac{x^3}{e^x - 1} = \frac{\pi^4}{15}$$

Then $E = \dfrac{\pi^2 V T^4}{5 s^3 \hbar^3}$

$$\boxed{C_V = \frac{4\pi^2 V}{5 s^3 \hbar^3} T^3 = \frac{12}{5}\pi^4 N \left(\frac{T}{\hbar\omega_D}\right)^3}$$

$C_V \propto T^3$

High temperatures, $T \gg \hbar\omega_D$

Then $x_D \ll 1$

$$\frac{x^3}{e^x - 1} \approx \frac{x^3}{x} = x^2$$

$$E = \frac{3VT^4}{2\pi^2 s^3 \hbar^3} \int_0^{x_D} x^2 \, dx = \frac{VT^4}{2\pi^2 s^3 \hbar^3} x_D^3 = \frac{V\omega_D^3}{2\pi^2 s^3} T = 3NT$$

$$\boxed{C_V = 3N}$$