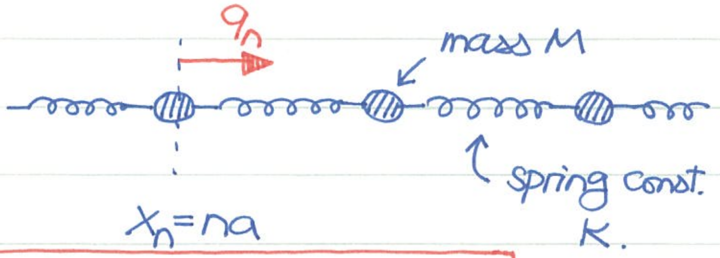
HH0065 Phonons and Debye Theory

Phonons are quantum version of sound waves, just like photons are quantized EM waves. To understand the "Maxwell eq." for phonons, it is helpful to start with 1D chain first.

⓪ One dimensional chain:



The Hamiltonian for a 1D chain with N particles connected by springs is

$$\boxed{H = \sum_{n=1}^{N} \frac{P_n^2}{2M} + \frac{1}{2}K(q_{n+1} - q_n)^2}$$

According to classical mechanics, equations of motion are

$$\frac{\partial H}{\partial P_n} = \dot{q}_n \quad \& \quad \frac{\partial H}{\partial q_n} = -\dot{P}_n \quad \longrightarrow \quad \frac{P_n}{M} = \dot{q}_n, \quad K(2q_n - q_{n+1} - q_{n-1}) = -\dot{P}_n$$

Combine both sets together to eliminate P_n,

$$\boxed{M\ddot{q}_n + K(2q_n - q_{n+1} - q_{n-1}) = 0}$$

becomes wave equation in the continuous limit.

(Can you find $\nabla^2 q$ here?)

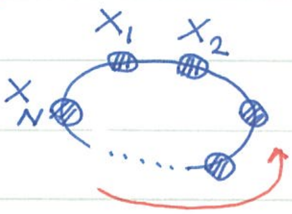
The above equation can be solved by Fourier transform,

$$\boxed{\begin{aligned} q_n &= \frac{1}{\sqrt{N}} \sum_k Q_k \, e^{ikx_n} \\ Q_k &= \frac{1}{\sqrt{N}} \sum_n q_n \, e^{-ikx_n} \end{aligned}}$$

$x_n = na \longrightarrow$ equilibrium positions.

$k = \frac{2m\pi}{Na} \longrightarrow$ quantized wave number from periodic B.C..

After Fourier transform, EOM coupling all q_n together is decoupled at different wave numbers:



$kL = 2m\pi \longrightarrow k = \frac{2m\pi}{L}$ and $L = Na$ ☺

$$\boxed{M\ddot{Q}_k + K(2 - 2\cos ka)\, Q_k = 0}$$

It's obvious that Q_k are normal modes!

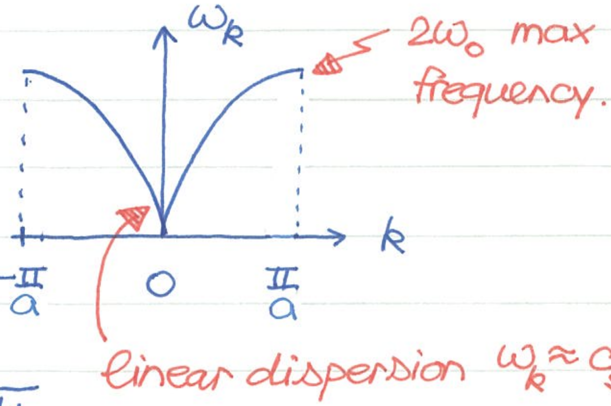
$Q_k(t) = Q_k e^{-i\omega_k t}$ to compute the frequency ω_k

The corresponding frequency is ω_k, satifying the characteritic equation

$$-M\omega_k^2 + K(2-2\cos ka) = 0$$

A bit algebra brings us to the final result.

$$\boxed{\omega_k = 2\omega_0 \,|\sin(ka/2)|}$$



where $\omega_0 = \sqrt{K/M}$. The speed of sound is the slope near $k=0$,

$$c_s = \lim_{k\to 0} \frac{d\omega_k}{dk} = \omega_0 a = a\sqrt{\frac{K}{M}}$$

One needs to be careful about mode counting here. We start with N-particle system and should get exactly N normal modes. For simplicity, assume N is even, the quantized wave numbers are

$$k = \frac{2m\pi}{Na} = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \cdots, \pm\frac{(N-1)\pi}{Na}, \frac{\pi}{a}.$$

important counting!

Great, we do get N quantized wave numbers ☺

Where are the phonons? Ok, we find N normal modes, but where are the phonons? Perform Fourier transform for both q_n and $P_n \longrightarrow Q_k$ and P_k. After some algebra, the Hamiltonian can be brought into the sum of normal modes

$$\boxed{H = \frac{1}{2M}\sum_k |P_k|^2 + M^2\omega_k^2 |Q_k|^2}$$

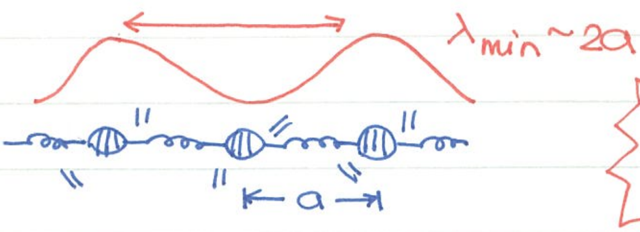
$P_k^* = P_{-k}$ and $Q_k^* = Q_{-k}$ have been used.

Recall that $[q_n, P_m] = i\hbar\,\delta_{nm}$. Because Fourier transform is unitary, the commutators remain canonical,

$$[Q_k, P_{k'}] = i\hbar\,\delta_{k,k'}$$

The Hamiltonian can be viewed as N oscillators with frequencies ω_k.

Note that the Hamiltonian for phonons is basically the same as that for photons. But, there is a fundamental difference,



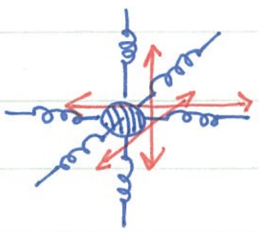
It leads to $k_{max} \sim \frac{2\pi}{\lambda_{min}} \sim \frac{\pi}{a}$.

The existence of k_{max} indicates the underlying lattice.

no λ_{min} for EM waves

There is no underlying lattice to generate EM waves and thus no λ_{min} (k_{max}) for photons.

⊘ Mode counting: The difference between phonons and photons arises from the underlying lattice. We already find the effect due to finite lattice constant $\underline{a}$. Another important feature is the total number of atoms $\underline{\underline{N}}$.



Generalize to 3D. There are three "polarizations". The total degrees of freedom is $3N$ (not N)!

Counting modes...

$$\sum_n (\cdots) = 3 \cdot \frac{1}{8} \int 4\pi n^2 dn \, (\cdots)$$

Want to find n_{max} to account for $3N$.

$$3N = 3 \cdot \frac{1}{8} \int_0^{n_{max}} 4\pi n^2 dn \longrightarrow \boxed{n_D \equiv n_{max} = \left(\frac{6N}{\pi}\right)^{\frac{1}{3}}}$$

Stands for Debye

The thermal energy for phonons is

$$U = \sum_n \langle s_n \rangle \hbar\omega_n = \sum_n \frac{\hbar\omega_n}{e^{\hbar\omega_n/\tau} - 1}$$

$$= 3 \cdot \frac{1}{8} \int_0^{n_D} 4\pi n^2 \cdot \frac{\hbar\omega_n}{e^{\hbar\omega_n/\tau} - 1} dn, \quad \omega_n = \frac{n\pi c_s}{L}$$

$$= \left(\frac{3\pi^2\hbar c_s}{2L}\right) \times \left(\frac{\tau L}{\pi\hbar c_s}\right)^4 \times \int_0^{x_D} dx \frac{x^3}{e^x - 1}, \quad x_D = \left(\frac{\pi\hbar c_s}{\tau L}\right) n_D$$

In the literature, it is more common to write the dimensionless parameter as $x_D = \theta_D/\tau$ $\boxed{\theta_D = \hbar c_s (6\pi^2 n)^{\frac{1}{3}}}$ Debye temperature.

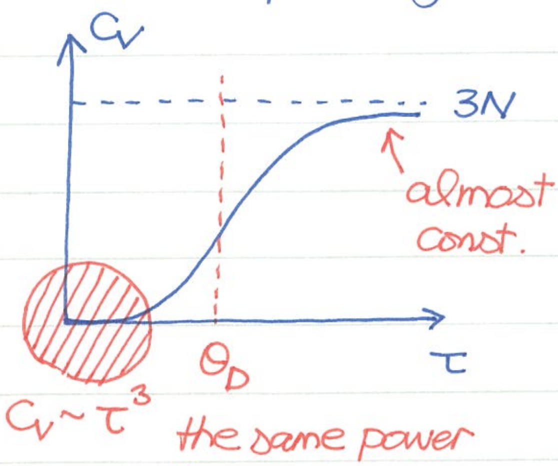
① Low temperature limit ($x_D \gg 1$).

$$\int_0^{x_D} dx \frac{x^3}{e^x - 1} \approx \frac{\pi^4}{15} \longrightarrow U \sim \tau^4, \quad C_V = \left(\frac{\partial U}{\partial \tau}\right)_{N,V} \sim \tau^3$$

② High temperature limit ($x_D \ll 1$)

$$\int_0^{x_D} dx \frac{x^3}{e^x - 1} \approx \int_0^{x_D} dx\, x^2 = \frac{1}{3} x_D^3 \longrightarrow U \approx 3N\tau$$

The corresponding specific heat is $C_V \approx 3N$



The temperature trend of C_V can be understood this way:

$\boxed{\tau \gg \theta_D,}$ all modes are activated.

Equipartition of energy:

1 S.H.O $\rightarrow$ 1τ thus $U = 3N\tau$

$\boxed{\tau \ll \theta_D,}$ not all modes are activated. $U \ll 3N\tau$. The temp. dependence $U \sim \tau^4$ is the same as photons.

2012.1113

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