Density of states in 1 - dimension

Let's consider a chain of particles in 1D.
N+1 particles, separated by a distance a, in such a way that the chain has length L

→ The particles at $s=0$ and $s=N$ at the extremes of the chain/line are fixed.

→ Each normal mode of polarization p has the form of a standing wave

If the amplitude of the oscillation of the s^{th} particle is u_s

$$u_s = u\, e^{-i\omega_{k,p} t} \sin(ska)$$

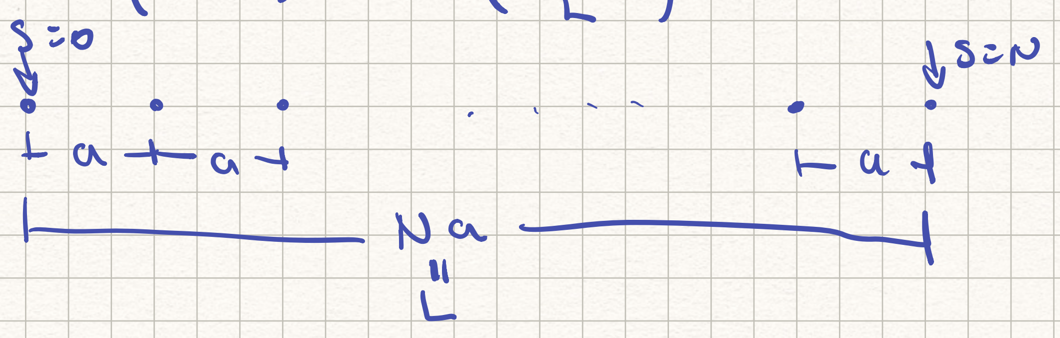
$\omega_{k,p}$ is related through k to the dispersion relation.

To force the amplitude at $s=0$ and $s=N$ to be zero we choose

$$k = \frac{n\pi}{L} \qquad n \in \mathbb{Z}$$

$$\sin(ska) = \sin\left(\frac{sn\pi}{L} a\right) \qquad \text{at } n=N \qquad \sin\left(s\pi \frac{Na}{L}\right)$$

$$= \sin(s\pi) = 0$$



If $n=N$, we have $u_s = 0$ for all particles

$$k = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \ldots, \frac{(N-1)\pi}{L}$$

A set of (N-1) values of k, which is equal to the number of particles that are allowed to move.

In a one-dimensional line of particles there is on mode for every interval $\Delta k = \frac{\pi}{L}$

The number of modes per unit range k is

$$\frac{1}{\Delta k} = \frac{L}{\pi} \quad \text{for} \quad k \leq \pi/a \qquad\qquad k = \frac{n\pi}{L} = \frac{\pi}{a}$$

$$0 \quad \text{for} \quad k > \pi/a$$

Other ways of counting are equally valid.

We can also consider a case where the line is not bounded, but we require the solutions to be periodic over the distance L.

$$u_s(sa) = u_s(sa + L)$$

This method is referred to as the method of periodic boundary conditions

Now we have a travelling wave

$$u_s = u\, e^{i(ska - \omega_{kp} t)}$$

For this wave to be periodic we need

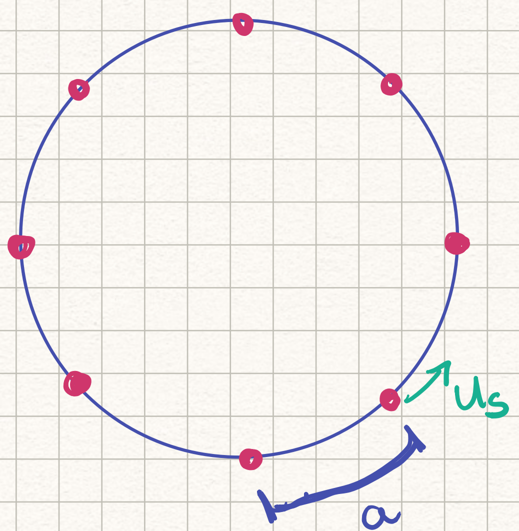
$$e^{iksa} = e^{ik(sa+L)} = e^{iksa} e^{ikL} \quad \Rightarrow \quad 1 = e^{ikL}$$

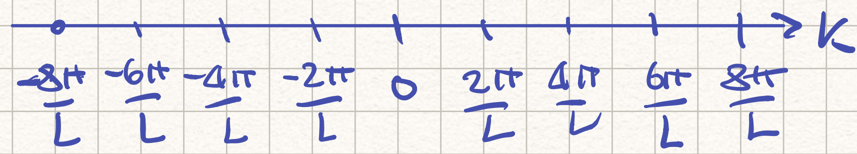
$$kL = \pm 2n\pi \quad \Rightarrow \quad k = \pm \frac{2n\pi}{L}$$

the valid k-values are $\pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \pm \frac{6\pi}{L}, \ldots$

$\boxed{N=8}$

$k=0$: uniform mode





There are 8 modes of oscillation

The amplitude of oscillation

$1, e^{\pm \pi s/4}$

$L = 8a$

$$u_s = u\, e^{i(ska - \omega_{kp} t)}$$

$$k = \pm \frac{2\pi}{L} = \frac{\pm 2\pi}{8a} = \pm \frac{\pi}{4a}$$

$$e^{is\frac{\pi}{4a}a} = e^{is\pi/4}$$

$$e^{is\frac{6\pi}{8a}a} =$$

$$e^{is\frac{8\pi}{8a}a} = e^{is\pi}$$

$k=0$ $\qquad u_s = 1\, u e^{-i\omega t}$

$k = \pm\frac{2\pi}{L}$ $\qquad u_s = e^{\pm is\pi/4}\, u e^{-i\omega t}$

$k = \pm\frac{4\pi}{L}$ $\qquad u_s = e^{\pm s\pi/2}\, u e^{-i\omega t}$

$k = \pm\frac{6\pi}{L}$ $\qquad u_s = e^{\pm 3s\pi/4}\, u e^{-i\omega t}$

$k = -\frac{8\pi}{L}$ $\qquad u_s = e^{-i\pi s}\, u e^{-i\omega t}$

we have one solution (for k) per mobile atom but now we have ± values of k

$$\Delta k = \frac{2\pi}{L}$$

$$\left.\begin{array}{ll} -\frac{\pi}{a} < k < \frac{\pi}{a} : & \frac{L}{2\pi} \\ \text{otherwise} : & 0 \end{array}\right\} \text{density of } k \text{ values}$$

we need to obtain $D(\omega)$, the number of modes per unit frequency range for a given polarization.

In 1D:

$$D_1(k)\,d\omega = \frac{L}{\pi}\frac{dk}{d\omega}\,d\omega \qquad \frac{dk}{d\omega} = \frac{1}{d\omega/dk} = \frac{1}{\frac{d\omega}{dk}}$$

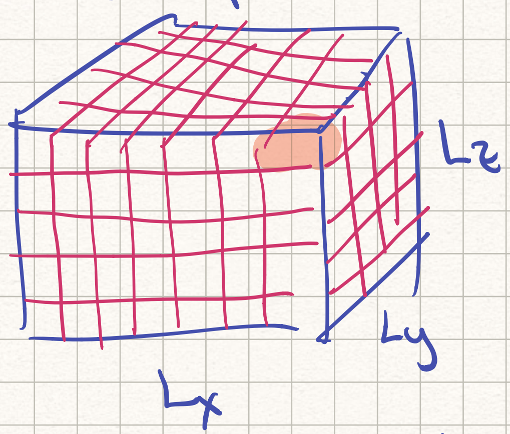
$$= \frac{L}{\pi}\frac{1}{v_g}\,d\omega \qquad v_g = \frac{d\omega}{dk}$$

Related to the dispersion relation

Note that we have a singularity in $D_1(\omega)$ whenever the dispersion relation $\omega(k)$ is horizontal $\Rightarrow v_g = 0$

Density of states in three dimensions

Periodic bound. cond. method $\quad N^3$ cells within a cube of side $L_x \cdot L_y \cdot L_z$



$N a_x = L_x \qquad N a_y = L_y$

$N a_z = L_z$

$a_x \cdot a_y \cdot a_z$

$\vec{k} = (k_x, k_y, k_z) \qquad \vec{L} = (L_x, L_y, L_z)$

$\vec{r} = (x, y, z)$

$$e^{i\vec{k}\cdot\vec{r}} = e^{i\vec{k}\cdot(\vec{r}+\vec{L})}$$

$$\vec{k}\cdot\vec{r} = (k_x x + k_y y + k_z z) \qquad \vec{r}+\vec{L} = (x+L_x, y+L_y, z+L_z)$$

$$e^{ik_x x}\, e^{ik_y y}\, e^{ik_z z} = e^{ik_x(x+L_x)}\, e^{ik_y(y+L_y)}\, e^{ik_z(z+L_z)}$$

So that

$$k_x = 0;\ \pm\frac{2\pi}{L_x};\ \pm\frac{4\pi}{L_x}\ \ldots;\ -\frac{N\pi}{L_x} \qquad N = \text{even number}$$

$$k_y = 0;\ \pm\frac{2\pi}{L_y};\ \pm\frac{4\pi}{L_y}\ \ldots;\ -\frac{N\pi}{L_y}$$

$$k_z = 0;\ \pm\frac{2\pi}{L_z};\ \pm\frac{4\pi}{L_z}\ \ldots;\ -\frac{N\pi}{L_z}$$

There's 1 $\vec{k}$-vector per unit volume $\frac{(2\pi)^3}{L_x L_y L_z}$

$$\frac{(2\pi)^3}{L_x L_y L_z} = \frac{2\pi}{L_x} \cdot \frac{2\pi}{L_y} \cdot \frac{2\pi}{L_z}$$

The density of $\vec{k}$-vectors is $\frac{L_x L_y L_z}{(2\pi)^3} = \frac{V}{(2\pi)^3}$

$V = L_x L_y L_z$: volume

The total number of modes that have wavevector less than k is given by $\frac{V}{(2\pi)^3}$ multiplied by the volume of a sphere with radius k.

$$N = \frac{V}{(2\pi)^3} \frac{4\pi k^3}{3} = \frac{1}{3} \frac{V k^3}{2\pi^2}$$

Therefore, the density of states for each polarization is

$$D_3(\omega)\, d\omega = \frac{\partial N}{\partial \omega} d\omega = \frac{\partial N}{\partial k} \frac{\partial k}{\partial \omega} d\omega$$

$$= \frac{V k^2}{2\pi^2} \frac{\partial k}{\partial \omega} d\omega$$

$\omega(k)$