Lecture 13 c Coupled oscillators

Consider a system of N atoms interacting via an N-body potential:

$$\hat{H} = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2M} + U(\{\vec{r}_i\})$$

At low temperatures, the configuration will be close to the minimum of the potential:

$$U_0 = \min\{U(\{\vec{r}_i\})\} = U(\{\vec{r}_i^{\,(0)}\})$$

Then we can Taylor expand

$$U(\{\vec{r}_i\}) \simeq U_0 + \frac{1}{2}\sum_{i,j} \vec{x}_i \cdot \left.\frac{\partial^2 U}{\partial \vec{r}_i \partial \vec{r}_j}\right|_{\{\vec{r}_k^{\,(0)}\}} \cdot \vec{x}_j$$

The 1st-order term is zero.

Here $\vec{x}_i = \vec{r}_i - \vec{r}_i^{\,(0)}$.

This gives us a Hamiltonian of many coupled oscillators

$N_{modes} = dN$, for $d = 1, 2, 3$ spatial dimensions. We can find the normal modes X_α:

$$\hat{H} = \sum_{\alpha=1}^{N_{modes}} \left(\frac{P_\alpha^2}{2m} + \frac{m\omega_\alpha^2}{2} X_\alpha^2 \right),$$

where the transformation

$$\{ \vec{X}_i \} \rightarrow \{ X_\alpha \}$$ is an

orthogonal transformation.

Quantizing the problem, we have

$$\hat{H} = \sum_{\alpha=1}^{N_{modes}} \hbar\omega_\alpha \left(a_\alpha^\dagger a_\alpha + \frac{1}{2} \right),$$

where $[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}$.

The mean-square displacement of an atom from its equilibrium position is

$$\langle \vec{x}_n^{\,2} \rangle = \frac{1}{N} \sum_{i=1}^{N} \langle \vec{x}_i^{\,2} \rangle = \frac{1}{N} \sum_{\alpha=1}^{N\text{modes}} \langle x_\alpha^2 \rangle .$$

The last equality holds because the transformation is orthogonal.

$$x_\alpha = \sqrt{\frac{\hbar}{2m\omega_\alpha}} \left(a_\alpha^\dagger + a_\alpha \right)$$

$$\langle x_\alpha^2 \rangle = \frac{\hbar}{2m\omega_\alpha} \langle (a_\alpha^\dagger)^2 + (a_\alpha)^2 + a_\alpha^\dagger a_\alpha + a_\alpha a_\alpha^\dagger \rangle$$

In an energy eigenstate

$$\langle n_\alpha | \underbrace{\cancel{(a_\alpha^\dagger)^2}}_{0} + \underbrace{\cancel{(a_\alpha)^2}}_{0} + a_\alpha^\dagger a_\alpha + a_\alpha a_\alpha^\dagger | n_\alpha \rangle$$

$$= 2n_\alpha + 1$$

In equilibrium at temperature T,

$$P(n_\alpha) = \frac{e^{-\beta E_{n_\alpha}}}{Z_\alpha} = \frac{e^{-\beta \hbar\omega_\alpha (n_\alpha + \frac{1}{2})}}{Z_\alpha}$$

$$Z_\alpha = \sum_{n_\alpha=0}^{\infty} e^{-\beta\hbar\omega_\alpha (n_\alpha + \frac{1}{2})}$$

(Here $\beta = \frac{1}{k_B T}$)

$$= \frac{e^{-\beta \frac{\hbar\omega_\alpha}{2}}}{1 - e^{-\beta\hbar\omega_\alpha}}$$

$$\langle E_\alpha \rangle = -\frac{\partial \ln Z_\alpha}{\partial \beta} = \hbar\omega_\alpha \left(\langle n_\alpha \rangle + \frac{1}{2} \right)$$

$$= \hbar\omega_\alpha \left(\frac{1}{e^{\beta\hbar\omega_\alpha} - 1} + \frac{1}{2} \right)$$

$$\boxed{\langle n \rangle = \frac{1}{e^{\beta\hbar\omega} - 1}}$$ Planck distribution

$$\langle x_\alpha^2 \rangle = \frac{\hbar}{2m\omega_\alpha}\left(\frac{1}{e^{\beta\hbar\omega_\alpha}-1} + \frac{1}{2}\right)$$

$$\langle \vec{X}_n^2 \rangle = \frac{1}{N}\sum_{\alpha=1}^{N\,\text{modes}} \frac{\hbar}{2m\omega_\alpha}\left(\frac{1}{e^{\beta\hbar\omega_\alpha}-1} + \frac{1}{2}\right)$$

Debye model

$$\omega_s(\vec{k}) = V|\vec{k}|, \quad s = 1, \dots, d$$

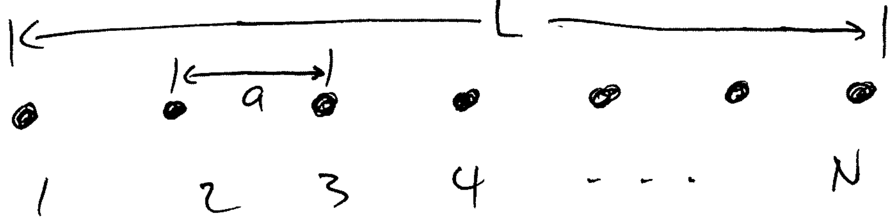
$$V = \sqrt{B/\rho} = \text{speed of sound in material}$$

i) 1 dimension

$$\langle X_n^2 \rangle = \frac{1}{N}\int \frac{dx\,dp}{h} \frac{\hbar^2}{2mV|p|}\left(\frac{1}{e^{\beta V|p|}-1} + \frac{1}{2}\right)$$

$$= \frac{L}{N}\frac{\hbar}{4\pi V}\int_{-\frac{\hbar\pi}{a}}^{\frac{\hbar\pi}{a}} dp\, \frac{1}{|p|}\left(\frac{1}{e^{\beta V|p|}-1} + \frac{1}{2}\right)$$

$\longrightarrow \infty$ even at $T = 0$!



Quantum fluctuations diverge!

Even though the mean positions of the atoms are arranged as shown above, the fluctuations about these mean positions are unbounded (for a very long system), indicating that such a system is a <u>fluid</u>, not a solid.

<u>Harmonic fluids</u> are ubiquitous in 1d interacting systems.

For the 2d case, one can show that

$$\langle \vec{x}_n^2 \rangle \Big|_{T=0} = \text{finite} \quad \text{but}$$

$$\langle \vec{x}_n^2 \rangle \Big|_{T>0} \to \infty .$$

A 2d crystal is not destroyed by quantum fluctuations, but is destroyed by thermal fluctuations at any finite temperature for a very large system. In 3d, everything is bounded for $T \geq 0$.

$\Rightarrow$ <u>Mermin-Wagner theorem</u>