Phys. 528 Lecture 20

1D Harmonic System: fluctuations

Consider a one-dimensional crystal with lattice spacing a, and nearest-neighbor interactions:

$$\hat{H} = \sum_{n=1}^{L} \left[\frac{p_n^2}{2m} + \frac{C}{2}(x_n - x_{n-1})^2 \right]$$

$$C(0) = C_{nn} = 2C$$

$$C(1) = C_{n,n-1} = -C$$

$$C(-1) = C_{n-1,n} = -C$$

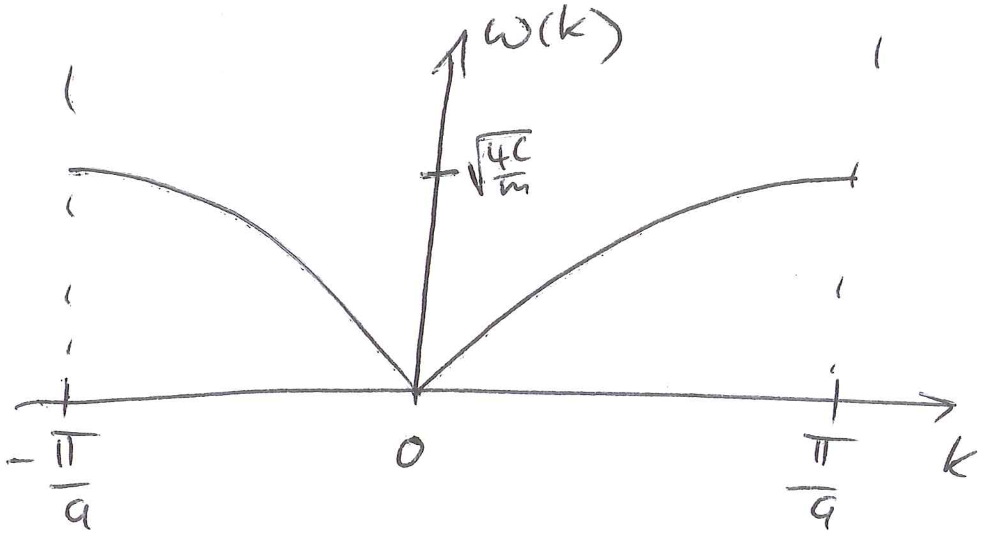
all others are zero

$$\tilde{C}(k) = C\left(2 - e^{ika} - e^{-ika}\right)$$

$$= 2C(1 - \cos ka)$$

$$\omega^2(k) = \frac{2C}{m}(1 - \cos ka) = \frac{4C}{m} \sin^2 \frac{ka}{2}$$

$$\omega(k) = \sqrt{\frac{4C}{m}} \left| \sin \frac{ka}{2} \right|$$



The group velocity is

$$V = \left|\frac{\partial \omega}{\partial k}\right| = \sqrt{\frac{Ca^2}{m}}\left|\cos\frac{ka}{2}\right|$$

In the long-wavelength limit $ka \ll 1$,

$$V_s = \lim_{ka\to 0}\left|\frac{\partial \omega}{\partial k}\right| = \sqrt{\frac{Ca^2}{m}} \quad \text{(speed of sound)}$$

Quantum fluctuations of the atoms

Recall, for the harmonic oscillator:

$$x^2 = \frac{\hbar}{2m\omega}(a+a^\dagger)^2 = \frac{\hbar}{2m\omega}\left[a^\dagger a + a a^\dagger + a^2 + (a^\dagger)^2\right]$$

$$a a^\dagger = a^\dagger a + 1$$

$$\langle x^2\rangle = \frac{\hbar}{2m\omega}\left(2a^\dagger a + 1 + \underbrace{\cancel{a^2}}_{0} + \underbrace{\cancel{(a^\dagger)^2}}_{0}\right)$$

$$\langle x^2 \rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{x}^2\}$$

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}\{e^{-\beta \hat{H}}\}} = \frac{e^{-\beta \hat{H}}}{Z}$$

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \sum_{n=0}^{\infty} \frac{\langle n | e^{-\beta \hat{H}} (2a^\dagger a + 1 + \cancelto{0}{a^2} + \cancelto{0}{(a^\dagger)^2}) | n \rangle}{Z}$$

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \frac{1}{Z} \sum_{n=0}^{\infty} e^{-\beta E_n} \langle n | 2a^\dagger a + 1 | n \rangle$$

$$\langle x^2 \rangle = \frac{\hbar}{m\omega} \sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) \frac{e^{-\beta \hbar\omega (n + \frac{1}{2})}}{Z}$$

$$= -\frac{1}{m\omega^2} \frac{\partial \ln Z}{\partial \beta}, \qquad Z = \frac{e^{-\beta \frac{\hbar\omega}{2}}}{1 - e^{-\beta\hbar\omega}}$$

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

Planck dist.

For the nth atom in the harmonic chain,

$$x_n = \frac{1}{\sqrt{L}} \sum_k \sqrt{\frac{\hbar}{2m\omega_k}} \left(a_k + a^\dagger_{-k}\right) e^{ikna}$$

The fluctuations in the distance between the nth atom and the $(n-\ell)$th atom are described by the operator

$$X_n - X_{n-\ell} = \frac{1}{\sqrt{L}} \sum_k \sqrt{\frac{\hbar}{2m\omega_k}} \left(a_k + a_{-k}^{+}\right) e^{ikna} \left(1 - e^{-ik\ell a}\right)$$

The mean-square fluctuations are

$$\langle (x_n - x_{n-\ell})^2 \rangle =$$

$$\frac{1}{L} \sum_k \sum_{k'} \frac{\hbar}{2m\sqrt{\omega_k \omega_{k'}}} e^{i(k+k')na} \left(1 - e^{-ik\ell a}\right)\left(1 - e^{-ik'\ell a}\right)$$

$$\times \left\langle \left(a_k + a_{-k}^{+}\right)\left(a_{k'} + a_{-k'}^{+}\right) \right\rangle$$

Again $\langle a_k a_{k'} \rangle = 0 = \langle a_{-k}^{+} a_{-k'}^{+} \rangle$.

$$\langle a_{-k}^{+} a_{k'} \rangle = \mathrm{Tr}\{ \hat{\rho}\, a_{-k}^{+} a_{k'} \}$$

$$= \frac{1}{Z} \sum_{\{n_k\}} \langle \{n_k\} | e^{-\beta \hat{H}} a_{-k}^{+} a_{k'} | \{n_k\} \rangle$$

$$\langle a^{+}_{-k} a_{k'} \rangle = \frac{1}{Z} \sum_{\{n_k\}} e^{-\beta E(\{n_k\})} \times \langle \{n_k\} | a^{+}_{-k} a_{k'} | \{n_k\} \rangle$$

$$a_{k'} : \quad n_{k'} \to n_{k'} - 1$$

$$a^{+}_{-k} : \quad n_{-k} \to n_{-k} + 1$$

matrix element is zero unless $k' = -k$.

$$\langle a^{+}_{-k} a_{k'} \rangle = \frac{1}{Z} \sum_{\{n_k\}} e^{-\beta E(\{n_k\})} n_{k'} \delta_{k',-k}$$

$$= \delta_{k',-k} \langle n_{k'} \rangle = \frac{\delta_{k',-k}}{e^{\beta \hbar \omega_{k'}} - 1}$$

Similarly,

$$\langle a_k a^{+}_{-k'} \rangle = \delta_{k,-k'} \left(1 + \frac{1}{e^{\beta \hbar \omega_k} - 1} \right)$$

Finally, $\langle (x_n - x_{n-\ell})^2 \rangle =$

$$\frac{1}{L} \sum_k \frac{\hbar}{2 m \omega_k} (1 - e^{-ik\ell a})(1 - e^{ik\ell a}) \left(\frac{2}{e^{\beta \hbar \omega_k} - 1} + 1 \right)$$

$$(1-e^{-ikla})(1-e^{ikla}) = 4\sin^2\left(\frac{kla}{2}\right)$$

Let's consider the fluctuations in the limit $T \to 0$ (ground state).

$$\langle 0|(x_n - x_{n-l})^2|0\rangle = \frac{1}{L}\sum_k \frac{2\hbar}{m\omega_k}\sin^2\left(\frac{kla}{2}\right)$$

$$= \frac{1}{L}\sum_k \frac{\hbar}{\sqrt{mC}} \frac{\sin^2\left(\frac{kla}{2}\right)}{|\sin(ka/2)|}$$

using $\omega_k = \sqrt{\frac{4C}{m}}|\sin(ka/2)|$.

For large L, $\frac{1}{L}\sum_k \to \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk$

$$\langle 0|(x_n - x_{n-l})^2|0\rangle \underset{L\to\infty}{=} \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk\, \frac{\hbar}{\sqrt{mC}} \frac{\sin^2(kla/2)}{|\sin(ka/2)|}$$

$$= \frac{2\hbar}{\pi\sqrt{mC}}\int_0^{\pi/2} dx\, \frac{\sin^2(lx)}{\sin x}$$

$$\boxed{\langle 0|(x_n - x_{n-l})^2|0\rangle = \begin{cases} \dfrac{2\hbar}{\pi\sqrt{mC}}, & l = 1 \\ \dfrac{\hbar}{\pi\sqrt{mC}}\ln l, & l \to \infty \end{cases}}$$

The nearest-neighbor bond length is well ~~defined~~ provided

$$\langle 0 | (x_n - x_{n-1})^2 | 0 \rangle \ll a^2$$

$$\frac{2}{\pi} \frac{\hbar}{m v_s} \ll a \,, \quad \text{where} \quad v_s = \sqrt{\frac{C a^2}{m}}$$

is the speed of sound.

Q: What is the mean-square displacement of the nth atom from its equilibrium position?

$$x_n^2 = \frac{1}{L} \sum_k \sum_{k'} \frac{\hbar \, e^{i(k+k')na}}{2m\sqrt{\omega_k \omega_{k'}}} (a_k + a_{-k}^\dagger)(a_{k'} + a_{-k'}^\dagger)$$

Using the same method as above, we find

$$\langle x_n^2 \rangle = \frac{1}{L} \sum_k \frac{\hbar}{2m\omega_k} \left(\frac{2}{e^{\beta\hbar\omega_k} - 1} + 1 \right)$$

$$\sum_k \longrightarrow \int_0^{\omega_D} d\omega \, g(\omega)$$

$$\langle x_n^2 \rangle = \frac{1}{L} \int_0^{\omega_D} d\omega\, g(\omega) \frac{\hbar}{m\omega} \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right)$$

cf. HW 8.2

Leaving it in terms of k, we get

$$\langle 0 | x_n^2 | 0 \rangle \underset{L \to \infty}{=} \frac{a}{2\pi} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \, \frac{\hbar}{2m\,\omega(k)}$$

$$= \frac{a}{2\pi} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \, \frac{\hbar}{4\sqrt{cm}\, |\sin(\frac{ka}{2})|}$$

$$= \frac{\hbar}{2\sqrt{cm}} \int_0^{\pi/2} \frac{dx}{\sin x} = \infty \; !$$

Here, we have omitted the term in the $\sum_k$ with $k=0$, which describes the motion of the center of mass; we are interested in the displacement of the nth atom relative to the c.m.

Thus, the nth atom is totally delocalized! This implies that crystalline order is destroyed by quantum fluctuations in one dimension. Indeed, <u>Mermin and Wagner</u> proved that long-range order is always destroyed by quantum fluctuations in one dimension (and by thermal fluctuations in two dimensions).

What we thought was the Hamiltonian of a 1D crystal really describes a <u>fluid</u>. The "harmonic fluid" is ubiquitous in 1D systems of both bosons and fermions.