Physics 560A Lecture 5, Part 2

Zero-point fluctuations in 1D

Consider a one-dimensional monatomic crystal with lattice spacing a. The Hamiltonian is

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

a) Calculate the zero-point fluctuations of the nearest-neighbor bond length, $\langle 0|(x_n - x_{n-1})^2|0\rangle$. Hint: the displacement operator for the nth atom may be expressed as

$$x_n = L^{-1/2} \sum_k \sqrt{\frac{\hbar}{2m\omega_k}} (a_k e^{ikna} + a_k^\dagger e^{-ikna}).$$

Also, in the limit $L \to \infty$ (which you may utilize) the sum over k may be replaced by an integral, $L^{-1} \sum_k \to (a/2\pi) \int dk$.

b) Calculate the mean squared deviation of the nth atom from its equilibrium position, $\langle 0|x_n^2|0\rangle$. (In evaluating the sum over normal modes, the mode with $k = 0$ should be omitted. This corresponds to displacements of the center of mass, and we are only interested in the displacement of the atom relative to a frame in which the center of mass of the crystal is fixed.)

What does this result suggest about the possible existence of crystalline order in one dimension?

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S.H.O. $x^2 = \frac{\hbar}{2m\omega}(a+a^+)(a+a^+)$

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

$\langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega}\langle 0|aa^+|0\rangle$

$= \frac{\hbar}{2m\omega}\langle 0|1 + a^+a|0\rangle = \frac{\hbar}{2m\omega}$

3a) $X_n - X_{n-\ell} = \frac{1}{\sqrt{L}}\sum_k Q_k \left(e^{ikna} - e^{ik(n-\ell)a}\right)$.

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

$\langle 0|(X_n - X_{n-\ell})^2|0\rangle =$

$\frac{1}{L}\sum_{kk'} \frac{\hbar}{2m\sqrt{\omega_k\omega_{k'}}} e^{i(k+k')na}\left(1-e^{-ik\ell a}\right)\left(1-e^{-ik'\ell a}\right)\underbrace{\langle 0|a_k a_{-k'}^+|0\rangle}_{\delta_{k,-k'}}$

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

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

$$= \frac{1}{L} \sum_k \frac{2\hbar}{m\omega_k} \sin^2 \frac{k\ell a}{2}$$

$$= \frac{1}{L} \sum_k \frac{\hbar}{\sqrt{mC}} \frac{\sin^2 k\ell a}{\left|\sin \frac{ka}{2}\right|} ,$$

using $\omega_k = \sqrt{\frac{4C}{m}} \left|\sin \frac{ka}{2}\right|$.

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

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

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

This integral can be evaluated. One finds:

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

The nearest-neighbor bond length is well defined provided

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

$$\Rightarrow \quad a \gg \frac{\hbar}{mv} \,,$$

where $v = \sqrt{\frac{Ca^2}{\mu}}$ is the speed of sound.

3b) $\langle 0|x_n^2|0\rangle = \frac{1}{L}\sum_{kk'} \frac{\hbar}{2m\sqrt{\omega_k\omega_{k'}}} e^{inq(k-k')}$

$\times \underbrace{\langle 0|a_k a_{k'}^+|0\rangle}_{\delta_{kk'}}$

$= \frac{1}{L}\sum_k \frac{\hbar}{2m\omega_k}$

$\xrightarrow[L\to\infty]{} \frac{q}{2\pi}\int_{-\frac{\pi}{q}}^{\pi/q} dk \frac{\hbar}{2m\omega(k)}$ (omitting the term $k=0$, which describes the center of mass of the crystal).

$= \frac{q}{2\pi}\int_{-\frac{\pi}{q}}^{\frac{\pi}{q}} dk \frac{\hbar}{4\sqrt{Cm}\left|\sin\frac{kq}{2}\right|}$

$= \frac{\hbar}{2\sqrt{Cm}}\int_0^{\frac{\pi}{2}} \frac{dx}{\sin x}$

$\longrightarrow \infty$!

Thus the nth atom is totally delocalized! This suggests that crystalline order is destroyed by quantum fluctuations in one dimension. Indeed, Mermin & Wagner proved that quantum fluctuations always destroy long range order in one dimension.

What we thought was the Hamiltonian of a 1D crystal really describes a fluid. This "harmonic fluid" is ubiquitous in 1D systems.