Physics 460 Lecture 16

Quantum Theory of Acoustic Waves

We have found that lattices support acoustic waves, which are waves in the displacement field $\vec{x}_n(t)$. In quantum mechanics, we know that the energy of a wave of frequency ω is quantized in units of $\hbar\omega$. Thus we expect the energy levels of the lattice to have the form:

$$E(\{n_{\vec{k}}\}) = \sum_{\vec{k}} \hbar\omega(\vec{k})\left(n_{\vec{k}} + \frac{1}{2}\right).$$

Each quantum of energy $\hbar\omega(\vec{k})$ in the mode with wavevector $\vec{k}$ is called a <u>phonon</u>.

In the text, phonons are posited following Planck's prescription for quantizing the energy levels of a field. However, it is instructive to derive phonons from a quantum mechanical treatment of the lattice Hamiltonian.

To simplify notation, let us continue to study a one-dimensional monatomic Bravais lattice composed of L atoms of mass M. The Hamiltonian was shown to be:

$$H = \sum_{n=1}^{L} \frac{p_n^2}{2M} + \frac{1}{2} \sum_{n,\ell} C(n-\ell) x_n x_\ell ,$$

where $C(-n) = C(n)$. Quantum mechanically, x_n and p_n are to be considered operators which obey the canonical commutation relation

$$[x_n, p_m] = i\hbar\,\delta_{nm}.$$

We impose periodic boundary conditions

$$x_{n+L} = x_n,$$

$$p_{n+L} = p_n.$$

H describes a system of L coupled harmonic oscillators.

Before diagonalizing H, let us review the quantum operator algebra for a <u>simple harmonic oscillator</u>:

$$H_1 = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \quad [x,p] = i\hbar$$

Define creation (a^+) and annihilation (a) operators:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\, x + \frac{ip}{\sqrt{2m\hbar\omega}}$$

$$a^+ = \sqrt{\frac{m\omega}{2\hbar}}\, x - \frac{ip}{\sqrt{2m\hbar\omega}}$$

Let $\hat{N} = a^+ a$:

$$\hat{N} = \frac{m\omega}{2\hbar} x^2 + \frac{p^2}{2m\hbar\omega} + \frac{i}{2\hbar}\overbrace{[x,p]}^{i\hbar}$$

$$= \frac{H}{\hbar\omega} - \frac{1}{2}.$$

Thus $H = \hbar\omega(\hat{N} + \frac{1}{2})$.

Let $|n\rangle$ be an eigenstate of $\hat{N}$ with eigenvalue n:

$$\hat{N}|n\rangle = n|n\rangle.$$

Then $\quad H|n\rangle = \hbar\omega(n+\frac{1}{2})|n\rangle.$

Notice that $\hat{N}$ is Hermitian

$$\hat{N}^{+} = (a^{+}a)^{+} = a^{+}a = \hat{N}.$$

Thus all eigenvalues of $\hat{N}$ are real. Furthermore $n \geq 0$, since

$$n = \langle n|\hat{N}|n\rangle = \langle n|a^{+}a|n\rangle = \langle\Phi|\Phi\rangle \geq 0,$$

where $|\Phi\rangle = a|n\rangle$.

To determine the eigenvalues of $\hat{N}$, let us first find the commutator

$$[a, a^{+}] = \frac{i}{2\hbar}\{[p,x]-[x,p]\} = 1.$$

(Obviously $[a,a] = [a^{+},a^{+}] = 0.$)

Now, $\hat{N} a = a^\dagger a a = (a a^\dagger - 1) a$

$$= a(\hat{N} - 1)$$

and $\hat{N} a^\dagger = a^\dagger (\hat{N} + 1)$.

Let us apply the operator $\hat{N} a$ to the eigenstate $|n\rangle$ of $\hat{N}$:

$$\hat{N} a |n\rangle = a(\hat{N} - 1)|n\rangle = (n-1) a |n\rangle.$$

Thus $a|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $n-1$. If $\langle n|n\rangle = 1$, $a|n\rangle$ has normalization

$$(\langle n|a^\dagger)(a|n\rangle) = \langle n|a^\dagger a|n\rangle = \langle n|\hat{N}|n\rangle = n$$

so that

$$a|n\rangle = \sqrt{n}\,|n-1\rangle.$$

Similarly, $a^2|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue $n-2$, and

$$a^2|n\rangle = a\sqrt{n}\,|n-1\rangle = \sqrt{n(n-1)}\,|n-2\rangle.$$

Thus if n is an eigenvalue of $\hat{N}$, so are $n-1, n-2, n-3, \cdots$. But this sequence can't continue indefinitely, since eventually we would reach a negative eigenvalue, and we know all eigenvalues of $\hat{N}$ are positive. The only possibility is that n is an integer, for when we come to the eigenstate $|1\rangle$, we find:

$$a|1\rangle = |0\rangle$$

and $\quad a|0\rangle = 0$

Now consider

$$\hat{N} a^\dagger |n\rangle = a^\dagger (\hat{N}+1)|n\rangle = (n+1) a^\dagger |n\rangle .$$

Thus $n+1$ is also an eigenvalue

of $\hat{N}$, and it is easy to show

$$a^{+}|n\rangle = \sqrt{n+1}\ |n+1\rangle .$$

Therefore the eigenvalues of $\hat{N}$ are all integers from zero to infinity. One can construct all eigenstates $|n\rangle$ from $|0\rangle$ by successively applying a^{+}:

$$|n\rangle = \frac{(a^{+})^{n}}{\sqrt{n!}}\,|0\rangle .$$

- The eigenvalues of H are

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right) , \quad n = 0, 1, 2, \ldots$$

Let's return to the original problem of quantizing lattice waves:

$$H = \sum_{n=1}^{L} \frac{p_n^2}{2M} + \frac{1}{2}\sum_{n,\ell} C(n-\ell)\, x_n x_\ell .$$

To find the normal modes, let us perform a Fourier transform:

$$Q_k = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} x_n e^{-ikna} , \quad Q_k^+ = Q_{-k}$$

$$x_n = \frac{1}{\sqrt{L}} \sum_k Q_k e^{ikna} .$$

The allowed values of k are fixed by the boundary conditions $x_{n+L} = x_n$:

$$e^{ikLa} = 1,$$

whence $k = \frac{2\pi j}{La}$, $-\frac{L}{2} \le j \le \frac{L}{2}$.

Let's check the consistency of the definition of Q_k:

$$x_n = \frac{1}{\sqrt{L}} \sum_k Q_k e^{ikna}$$

$$= \frac{1}{L} \sum_k \sum_\ell x_\ell \, e^{ik(n-\ell)a}$$

$$= \sum_\ell x_\ell \; \frac{1}{L} \sum_k e^{ik(n-\ell)a}$$

now $\frac{1}{L} \sum_k e^{ik(n-\ell)a} = \frac{1}{L} \sum_{j=0}^{L-1} e^{i\frac{2\pi j(n-\ell)}{L}}$

$$= \frac{1}{L} \sum_{j=0}^{L-1} \left(e^{i\frac{2\pi(n-\ell)}{L}} \right)^j$$

$$= \frac{1}{L} \frac{1 - e^{i2\pi(n-\ell)}}{1 - e^{i\frac{2\pi(n-\ell)}{L}}} = \begin{cases} 0 & n \neq \ell \\ 1 & n = \ell \end{cases}$$

$$x_n = \sum_\ell x_\ell \, \delta_{n\ell} = x_n \quad \checkmark$$

(Here I used the conventional cell of the reciprocal lattice, rather than the first Brillouin zone, to simplify the algebra.)

What is the momentum variable conjugate to Q_k? Consider the classical Lagrangian

$$\mathcal{L} = \sum_{n=1}^{L} \frac{m}{2} \dot{x}_n^2 - \frac{1}{2} \sum_{n,\ell} C_{n\ell} x_n x_\ell$$

Now

$$\sum_{n=1}^{L} \dot{x}_n^2 = \frac{1}{L} \sum_k \sum_{k'} \sum_n \dot{Q}_k \dot{Q}_{k'} e^{i(k+k')na}$$

$$= \sum_k \dot{Q}_k \dot{Q}_{-k}$$

Furthermore,

$$\sum_{n,\ell} C_{n\ell} x_n x_\ell = \frac{1}{L} \sum_k \sum_{k'} Q_k Q_{k'} \sum_{n,\ell} C_{n\ell} e^{i(kn+k'\ell)a}$$

Now

$$\frac{1}{L}\sum_{n\ell} C_{n\ell}\, e^{i(kn+k'\ell)a} = \frac{1}{L}\sum_{n\ell} C(n-\ell)\, e^{i(kn+k'\ell)a}$$

let $n-\ell = j$

$$= \underbrace{\sum_j C(j)\, e^{ikja}}_{\tilde{C}(k)} \; \underbrace{\frac{1}{L}\sum_{\ell} e^{i(k+k')\ell a}}_{\delta_{k,-k'}}$$

Thus

$$\mathcal{L} = \sum_k \left\{ \frac{m}{2}\dot{Q}_k \dot{Q}_{-k} - \frac{\tilde{C}(k)}{2} Q_k Q_{-k} \right\}$$

$$P_k = \frac{\partial \mathcal{L}}{\partial \dot{Q}_k} = m\dot{Q}_{-k}$$

The Hamiltonian becomes

$$H = \sum_k \left\{ \frac{P_k P_{-k}}{2m} + \frac{\tilde{C}(k)}{2} Q_k Q_{-k} \right\}.$$

In terms of the original coordinates,

$$P_k = m\dot{Q}_{-k} = \frac{1}{\sqrt{L}} \sum_n m \dot{x}_n e^{ikna}$$

$$= \frac{1}{\sqrt{L}} \sum_{n=1}^{L} p_n e^{ikna}$$

$$P_k^\dagger = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} p_n e^{-ikna} = P_{-k}$$

Let's check the commutator:

$$[Q_k, P_{k'}] = \frac{1}{L} \sum_{n\ell} [x_n, p_\ell] e^{-i(kn-k'\ell)a}$$

$$= i\hbar \delta_{kk'} \quad \checkmark$$

Crystal momentum

- The total momentum of the system is

$$P_{tot} = \sum_{n=1}^{L} P_n = \sqrt{L}\, P_0 .$$

Thus the total momentum involves only the $k=0$ mode. Modes with $k \neq 0$ correspond to internal coordinates, and do not contribute to the total momentum of the system.

Many interaction processes in crystals proceed as if the total wave vector $\sum \vec{k}$ were conserved for the interacting particles. For this reason, $\hbar\vec{k}$ is referred to as <u>crystal momentum</u> or <u>quasimomentum</u>.

As we shall see in forthcoming lectures, the conservation law for crystal momentum is

$$\Delta \sum_{\nu} \vec{k}_{\nu} = \vec{G}, \quad \text{where}$$

$\vec{G}$ is a reciprocal lattice vector. However, this conservation law is distinct from the conservation of the center-of-mass momentum.

- <u>Diagonalizing H</u>

The Hamiltonian is not quite in the form of a collection of independent harmonic oscillators due to the mixture of terms involving k and $-k$. Let $\omega_k = \sqrt{\tilde{C}(k)/m}$. Consider the operators:

$$a_k = \sqrt{\frac{m\omega_k}{2\hbar}}\, Q_k + \frac{i\, P_{-k}}{\sqrt{2m\hbar\omega_k}}$$

$$a_k^+ = \sqrt{\frac{m\omega_k}{2\hbar}}\, Q_{-k} - \frac{i\, P_k}{\sqrt{2m\hbar\omega_k}}$$

$$[a_k, a_{k'}^+] = \frac{i}{2\hbar}\left\{[P_{-k}, Q_{-k'}] - [Q_k, P_{k'}]\right\}$$

$$= \delta_{kk'}$$

$$a_k^+ a_k = \frac{m\omega_k}{2\hbar} Q_{-k} Q_k + \frac{P_k P_{-k}}{2m\hbar\omega_k}$$

$$+ \frac{i}{2\hbar}\left[Q_{-k} P_{-k} - P_k Q_k\right]$$

$$a_k^{+} a_k + a_{-k}^{+} a_{-k} =$$

$$\frac{m\omega_k}{\hbar} Q_k Q_{-k} + \frac{P_k P_{-k}}{m\hbar\omega_k} + \frac{i}{2\hbar}[Q_k, P_k]$$

$$+ \frac{i}{2\hbar}[Q_{-k}, P_{-k}]$$

$$\hbar\omega_k \left(a_k^{+} a_k + a_{-k}^{+} a_{-k} \right) =$$

$$\frac{P_k P_{-k}}{m} + m\omega_k^2 Q_k Q_{-k} - 1$$

$$\Rightarrow \quad H = \sum_k \hbar\omega_k \left(a_k^{+} a_k + \frac{1}{2} \right)$$

(since $\sum_k$ includes k and $-k$)

From the commutation relation $[a_k, a^\dagger_{k'}] = \delta_{kk'}$, we know that the eigenvalues of $a^\dagger_k a_k$ are non-negative integers (c.f. harmonic oscillator).

- Thus we have <u>derived</u> the Planck's ansatz that the energy of a wave of frequency ω is quantized in units of $\hbar\omega$ — for the particular case of acoustic waves in one dimension. The generalization to higher dimensions is straightforward. The generalization to E+M waves requires relativistic quantum mechanics, and is quite a bit more complicated.

The inverse transformation is:

$$Q_k = \sqrt{\frac{\hbar}{2m\omega_k}}\left(a_k + a_{-k}^{+}\right)$$

$$P_k = i\sqrt{\frac{m\hbar\omega_k}{2}}\left(a_k^{+} - a_{-k}\right)$$

The displacement of the nth atom/ion from its equilibrium position is described by the operator

$$x_n = \frac{1}{\sqrt{L}}\sum_k Q_k e^{ikna}$$

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

where the sum is over the 1st Brillouin zone.

Each quantum of energy $\hbar\omega_k$ in the mode of wave-vector k is called a <u>phonon</u> (for quantized acoustic wave). A phonon in a crystal behaves like a particle of energy $\hbar\omega_k$ and momentum $\hbar k$ (although, strictly speaking, it carries no momentum). As for the harmonic oscillator, the energy eigenstates can be expressed in terms of the ground state $|0\rangle$ of the crystal and the creation operators a_k^{+} for phonons:

The state with energy

$$E(\{n_k\}) = \sum_k \hbar\omega_k \left(n_k + \tfrac{1}{2}\right)$$

is given by

$$|\{n_k\}\rangle = \left(\prod_k \frac{(a_k^{\dagger})^{n_k}}{\sqrt{n_k!}}\right)|0\rangle .$$

- phonons are bosons

Consider a state with two phonons with wave vectors k_1 and k_2:

$$|k_1\, k_2\rangle = a_{k_1}^{\dagger} a_{k_2}^{\dagger} |0\rangle = |\Psi\rangle.$$

What happens to $|\Psi\rangle$ if we interchange the two phonons?

$$\Pi_{12} : k_1 \rightleftarrows k_2$$

$$\Pi_{12}|\Psi\rangle = |k_2 k_1\rangle$$
$$= a^+_{k_2} a^+_{k_1} |0\rangle$$

But $[a^+_k, a^+_{k'}] = 0$,

so $\Pi_{12}|\Psi\rangle = a^+_{k_1} a^+_{k_2} |0\rangle$
$$= |k_1 k_2\rangle$$
$$= |\Psi\rangle.$$

The phonon wave function $|\Psi\rangle$ is thus <u>symmetric</u> under interchange of two phonons $\Longrightarrow$ phonons obey <u>Bose-Einstein statistics</u>.

- Expressing H in terms of creation and annihilation operators is called "2nd quantization."