## Handout 20

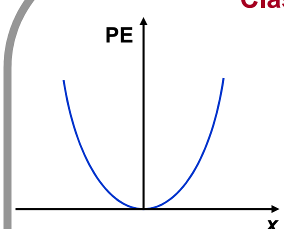
## Quantization of Lattice Waves: From Lattice Waves to Phonons

**In this lecture you will learn:**

- Simple harmonic oscillator in quantum mechanics
- Classical and quantum descriptions of lattice wave modes
- Phonons – what are they?



## Classical Simple Harmonic Oscillator




**Consider a particle of mass *m* in a parabolic potential**

$$\text{KE} = \frac{p_x^2(t)}{2m} \qquad \text{PE} = V(\hat{x}) = \frac{1}{2} m \omega_o^2 \, x^2(t)$$

**The total energy is:**

$$E_{Total} = \frac{p_x^2(t)}{2m} + \frac{1}{2} m \omega_o^2 \, x^2(t)$$

**In quantum mechanics, the dynamical variables and observables become operators:**

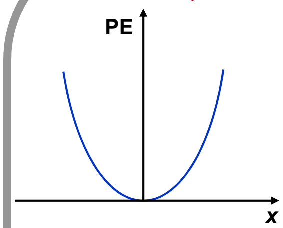
$$x(t) \Leftrightarrow \hat{x}$$

$$p_x(t) \Leftrightarrow \hat{p}_x$$

$$E_{Total} \Leftrightarrow \hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m \omega_o^2 \, \hat{x}^2$$

ECE 407 – Spring 2009 – Farhan Rana – Cornell University

## Quantum Simple Harmonic Oscillator Review - I




Consider a particle of mass *m* in a parabolic potential

$$\text{KE} = \frac{\hat{p}_x^2}{2m} \qquad \text{PE} = V(\hat{x}) = \frac{1}{2} m\omega_o^2\, \hat{x}^2$$

Hamiltonian operator is:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m\omega_o^2\, \hat{x}^2$$

The quantum mechanical commutation relations are:

$$[\ \hat{x}, \hat{p}_x\ ] = i\,\hbar$$

Define two new operators:

$$\hat{a} = \sqrt{\frac{m\omega_o}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\,\hbar\omega_o}}\hat{p}_x$$

$$\hat{a}^+ = \sqrt{\frac{m\omega_o}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2m\,\hbar\omega_o}}\hat{p}_x$$



## Quantum Simple Harmonic Oscillator Review - II

$$\hat{a} = \sqrt{\frac{m\omega_o}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\,\hbar\omega_o}}\hat{p}_x \qquad \hat{a}^+ = \sqrt{\frac{m\omega_o}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2m\,\hbar\omega_o}}\hat{p}_x$$

The quantum mechanical commutation relations are:

$$[\ \hat{x}, \hat{p}_x\ ] = i\,\hbar \qquad \Rightarrow \qquad \left[\hat{a}, \hat{a}^+\right] = 1$$

The Hamiltonian operator can be written as:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m\omega_o^2\, \hat{x}^2 = \hbar\,\omega_o\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$$

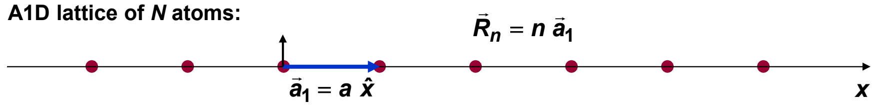
The Hamiltonian operator has eigenstates $|n\rangle$ that satisfy:

$$\hat{a}^+\hat{a}\,|n\rangle = n\,|n\rangle \qquad \{\ n = 0,1,2,3............$$

$$\hat{H}\,|n\rangle = \hbar\,\omega_o\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)|n\rangle = \hbar\,\omega_o\left(n + \frac{1}{2}\right)|n\rangle$$

## Lattice Waves in a 1D Crystal: Classical Description

A1D lattice of *N* atoms:




**Potential Energy:**

$$V = V_{EQ} + \frac{1}{2}\sum_k \sum_j K(\vec{R}_j , \vec{R}_k)\, u(\vec{R}_j,t)\, u(\vec{R}_k,t)$$

$$= \frac{1}{2}\sum_k \sum_j K(\vec{R}_j , \vec{R}_k)\, u(\vec{R}_j,t)\, u(\vec{R}_k,t)$$

$$\left\{ K(\vec{R}_j , \vec{R}_k) = \left.\frac{\partial^2 V}{\partial u(\vec{R}_j)\, \partial u(\vec{R}_k)}\right|_{EQ} \right.$$

Choose the zero of energy so the constant term $V_{EQ}$ goes away

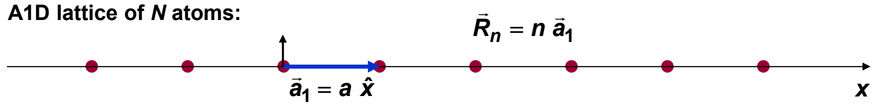
**Kinetic Energy:**

$$\text{KE} = \sum_j \frac{M}{2}\left(\frac{du(\vec{R}_j,t)}{dt}\right)^2$$



## Lattice Waves in a 1D Crystal: Classical Description

A1D lattice of *N* atoms:




**Potential Energy:**

$$V = \frac{1}{2}\sum_k \sum_j K(\vec{R}_j , \vec{R}_k)\, u(\vec{R}_j,t)\, u(\vec{R}_k,t)$$

$$K(\vec{R}_k , \vec{R}_j) = -\alpha\,\delta_{j,k+1} - \alpha\,\delta_{j,k-1} + 2\alpha\,\delta_{j,k}$$ ⟶ Nearest-neighbor interaction

$K(\vec{R}_j , \vec{R}_k)$ is always a function of only the difference $\vec{R}_j - \vec{R}_k$

$$\Rightarrow\; V = \frac{1}{2}\sum_k \sum_j K(\vec{R}_j - \vec{R}_k)\, u(\vec{R}_j,t)\, u(\vec{R}_k,t)$$

## Lattice Waves in a 1D Crystal: Classical Description

The energy for the entire crystal becomes:

Atomic displacements coupled in the PE term

$$E = \text{KE} + \text{PE}$$

$$= \sum_j \frac{M}{2}\left(\frac{d\,u(\vec{R}_j,t)}{dt}\right)^2 + \frac{1}{2}\sum_k \sum_j K(\vec{R}_j - \vec{R}_k)\,u(\vec{R}_j,t)\,u(\vec{R}_k,t)$$

The atomic displacement can be expanded in terms of all the lattice wave modes:

$$u(\vec{R}_n,t) = \sum_{\vec{q}\text{ in FBZ}} \text{Re}\left[u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_n}\,e^{-i\,\omega(\vec{q})\,t}\right]$$

$$= \sum_{\vec{q}\text{ in FBZ}} \frac{u(\vec{q})}{2}\,e^{i\,\vec{q}\,.\,\vec{R}_n}\,e^{-i\,\omega(\vec{q})\,t} + \frac{u^*(\vec{q})}{2}\,e^{-i\,\vec{q}\,.\,\vec{R}_n}\,e^{i\,\omega(\vec{q})\,t}$$

$$= \sum_{\vec{q}\text{ in FBZ}} \frac{u(\vec{q},t)}{2}\,e^{i\,\vec{q}\,.\,\vec{R}_n} + \frac{u^*(\vec{q},t)}{2}\,e^{-i\,\vec{q}\,.\,\vec{R}_n}$$

$$= \sum_{\vec{q}\text{ in FBZ}} \frac{u(\vec{q},t)}{2}\,e^{i\,\vec{q}\,.\,\vec{R}_n} + \frac{u^*(-\vec{q},t)}{2}\,e^{i\,\vec{q}\,.\,\vec{R}_n}$$

$$= \sum_{\vec{q}\text{ in FBZ}} U(\vec{q},t)\,e^{i\,\vec{q}\,.\,\vec{R}_n} \qquad \left\{\; U(-\vec{q},t) = U^*(\vec{q},t)\right.$$



## Lattice Waves in a 1D Crystal: Classical Description

Take the expansion in terms of the lattice wave modes:

$$u(\vec{R}_n,t) = \sum_{\vec{q}\text{ in FBZ}} U(\vec{q},t)\,e^{i\,\vec{q}\,.\,\vec{R}_n} \qquad \left\{\; U(-\vec{q},t) = U^*(\vec{q},t)\right.$$

And plug it into the expression for the energy:

$$E = \sum_j \frac{M}{2}\left(\frac{d\,u(\vec{R}_j,t)}{dt}\right)^2 + \frac{1}{2}\sum_k \sum_j K(\vec{R}_j - \vec{R}_k)\,u(\vec{R}_j,t)\,u(\vec{R}_k,t)$$

The KE term becomes:

$$\sum_j \frac{M}{2}\left(\frac{d\,u(\vec{R}_j,t)}{dt}\right)^2 = \sum_{\vec{q}\text{ in FBZ}} \frac{NM}{2}\,\frac{dU(\vec{q},t)}{dt}\,\frac{dU^*(\vec{q},t)}{dt}$$

The PE term becomes:

$$\frac{1}{2}\sum_k \sum_j K(\vec{R}_j - \vec{R}_k)\,u(\vec{R}_j,t)\,u(\vec{R}_k,t) = \sum_{\vec{q}\text{ in FBZ}} \frac{NM\,\omega^2(\vec{q})}{2}\,U(\vec{q},t)\,U^*(\vec{q},t)$$

where: $\omega^2(\vec{q}) = \frac{1}{M}\sum_j K(\vec{R}_j)\,e^{i\,\vec{q}\,.\,\vec{R}_j} = \frac{4\alpha}{M}\sin^2\left(\frac{\vec{q}\,.\,\vec{a}_1}{2}\right)$

## From Classical to Quantum Description

So we have finally:

$$E = \sum_j \frac{M}{2}\left(\frac{d\,u(\vec{R}_j,t)}{dt}\right)^2 + \frac{1}{2}\sum_k \sum_j K(\vec{R}_j - \vec{R}_k)\,u(\vec{R}_j,t)\,u(\vec{R}_k,t)$$

$$= \sum_{\vec{q}\text{ in FBZ}} \left[\frac{NM}{2}\frac{dU(\vec{q},t)}{dt}\frac{dU^*(\vec{q},t)}{dt} + \frac{NM}{2}\omega^2(\vec{q})U(\vec{q},t)\,U^*(\vec{q},t)\right]$$

Lattice wave amplitudes uncoupled in the PE term

**Going from classical to quantum description:**

The atomic displacements and the atomic momenta become operators:

$$u(\vec{R}_n,t) \;\Rightarrow\; \hat{u}(\vec{R}_n)$$

$$M\frac{du(\vec{R}_n,t)}{dt} \;\Rightarrow\; \hat{p}(\vec{R}_n)$$

Commutation relations are:

$$\left[\hat{u}(\vec{R}_n),\,\hat{p}(\vec{R}_n)\right] = i\,\hbar$$



## From Classical to Quantum Description

The amplitudes of lattice waves are now also operators:

| | | |
|---|---|---|
| Classical: | $u(\vec{R}_n,t) = \sum_{\vec{q}\text{ in FBZ}} U(\vec{q},t)\,e^{i\,\vec{q}\cdot\vec{R}_n}$ | $\{\; U(-\vec{q},t) = U^*(\vec{q},t)$ |
| Quantum: | $\hat{u}(\vec{R}_n) = \sum_{\vec{q}\text{ in FBZ}} \hat{U}(\vec{q})\,e^{i\,\vec{q}\cdot\vec{R}_n}$ | $\{\; \hat{U}(-\vec{q}) = \hat{U}^+(\vec{q},t)$ |
| Classical: | $p(\vec{R}_n,t) = \sum_{\vec{q}\text{ in FBZ}} P(\vec{q},t)\,e^{i\,\vec{q}\cdot\vec{R}_n}$ | $\{\; P(-\vec{q},t) = P^*(\vec{q},t)$ |
| Quantum: | $\hat{p}(\vec{R}_n) = \sum_{\vec{q}\text{ in FBZ}} \hat{P}(\vec{q})\,e^{i\,\vec{q}\cdot\vec{R}_n}$ | $\{\; \hat{P}(-\vec{q}) = \hat{P}^+(\vec{q})$ |

The commutation relations for the lattice wave amplitudes are:

$$\left[\hat{u}(\vec{R}_j),\,\hat{p}(\vec{R}_j)\right] = i\,\hbar \quad \text{can hold only if} \quad \left[\hat{U}(\vec{q}),\,\hat{P}^+(\vec{q}')\right] = \frac{i\hbar}{N}\delta_{\vec{q},\vec{q}'}$$

The Hamiltonian operator in terms of the lattice wave amplitude operators is:

$$\hat{H} = \sum_{\vec{q}\text{ in FBZ}} \left[\frac{N}{2M}\hat{P}(\vec{q})\,P^+(\vec{q}) + \frac{NM}{2}\omega^2(\vec{q})\hat{U}(\vec{q},t)\,\hat{U}^+(\vec{q},t)\right]$$

## From Classical to Quantum Description

**Define two new operators:**

$$\hat{a}(\vec{q}) = \sqrt{\frac{NM\omega(\vec{q})}{2\hbar}}\,\hat{U}(\vec{q}) + i\sqrt{\frac{N}{2M\,\hbar\omega(\vec{q})}}\hat{P}(\vec{q})$$

$$\hat{a}^{+}(\vec{q}) = \sqrt{\frac{NM\omega(\vec{q})}{2\hbar}}\,\hat{U}^{+}(\vec{q}) - i\sqrt{\frac{N}{2M\,\hbar\omega(\vec{q})}}\hat{P}^{+}(\vec{q})$$

**The commutation relations are:**

$$\left[\hat{U}(\vec{q})\,,\,\hat{P}^{+}(\vec{q}')\right] = \frac{i\hbar}{N}\delta_{\vec{q}\,,\,\vec{q}'} \qquad \Rightarrow \qquad \left[\,\hat{a}(\vec{q})\,,\hat{a}^{+}(\vec{q}')\,\right] = \delta_{\vec{q}\,,\,\vec{q}'}$$

**Note the inverse expressions:**

$$\hat{U}(\vec{q}) = \sqrt{\frac{\hbar}{2NM\omega(\vec{q})}}\left[\,\hat{a}(\vec{q}) + \hat{a}^{+}(-\vec{q})\,\right]$$

$$\hat{P}(\vec{q}) = -i\sqrt{\frac{M\,\hbar\omega(\vec{q})}{2N}}\left[\,\hat{a}(\vec{q}) - \hat{a}^{+}(-\vec{q})\,\right]$$



## From Classical to Quantum Description

**Use the expressions:**

$$\hat{U}(\vec{q}) = \sqrt{\frac{\hbar}{2NM\omega(\vec{q})}}\left[\,\hat{a}(\vec{q}) + \hat{a}^{+}(-\vec{q})\,\right]$$

$$\hat{P}(\vec{q}) = -i\sqrt{\frac{M\,\hbar\omega(\vec{q})}{2N}}\left[\,\hat{a}(\vec{q}) - \hat{a}^{+}(-\vec{q})\,\right]$$

**in the Hamiltonian operator:**

$$\hat{H} = \sum_{\vec{q}\text{ in FBZ}}\left[\frac{N}{2M}\hat{P}(\vec{q})\,P^{+}(\vec{q}) + \frac{NM}{2}\omega^{2}(\vec{q})\hat{U}(\vec{q},t)\,\hat{U}^{+}(\vec{q},t)\right]$$

**to get:**

$$\hat{H} = \sum_{\vec{q}\text{ in FBZ}}\hbar\,\omega(\vec{q})\left(\hat{a}^{+}(\vec{q})\,\hat{a}(\vec{q}) + \frac{1}{2}\right)$$

## From Classical to Quantum Description

The final answer:

$$\hat{H} = \sum_{\vec{q} \text{ in FBZ}} \hbar\, \omega(\vec{q}) \left( \hat{a}^{+}(\vec{q})\, \hat{a}(\vec{q}) + \frac{1}{2} \right)$$

and the commutation relations

$$\left[ \hat{a}(\vec{q}) , \hat{a}^{+}(\vec{q}) \right] = 1$$

tell us that:

1) The Hamiltonians of different lattice wave modes are uncoupled
2) The Hamiltonian of each lattice mode resembles that of a simple harmonic oscillator

Finally, the atomic displacements can be expanded in terms of the phonon creation and destruction operators

$$\hat{u}\left(\vec{R}_j\right) = \sum_{\vec{q} \text{ in FBZ}} \hat{U}(\vec{q})\, e^{i\, \vec{q} \,.\, \vec{R}_j}$$

$$= \sum_{\vec{q} \text{ in FBZ}} \sqrt{\frac{\hbar}{2NM\omega(\vec{q})}} \left[ \hat{a}(\vec{q}) + \hat{a}^{+}(-\vec{q}) \right] e^{i\, \vec{q} \,.\, \vec{R}_j}$$



## What are Phonons?

Consider the Hamiltonian of just a single lattice wave mode:

$$\hat{H} = \hbar\, \omega(\vec{q}) \left( \hat{a}^{+}(\vec{q})\, \hat{a}(\vec{q}) + \frac{1}{2} \right)$$

In analogy to the simple harmonic oscillator, its eigenstates, and the corresponding eigenenergies, must be of the form:

$$\left| n_{\vec{q}} \right\rangle \qquad \left\{ \text{where} \quad n_{\vec{q}} = 0,1,2,3............ \right.$$

$$\hat{H} \left| n_{\vec{q}} \right\rangle = \hbar\, \omega(\vec{q}) \left( \hat{a}^{+}(\vec{q})\, \hat{a}(\vec{q}) + \frac{1}{2} \right) \left| n_{\vec{q}} \right\rangle = \hbar\, \omega(\vec{q}) \left( n_{\vec{q}} + \frac{1}{2} \right) \left| n_{\vec{q}} \right\rangle$$

This eigenstate corresponds to $n_{\vec{q}}$ phonons in the lattice wave mode

• A phonon corresponds to the minimum amount by which the energy of a lattice wave mode can be increased or decreased – it is the quantum of lattice wave energy

• A lattice wave mode with $n_{\vec{q}}$ phonons means the total energy of the lattice wave above the ground state energy of $\hbar\, \omega(\vec{q})/2$ is $n_{\vec{q}}\, \hbar\, \omega(\vec{q})$

• The ground state energy is not zero but equals $\hbar\, \omega(\vec{q})/2$ and corresponds to quantum fluctuations of atoms around their equilibrium positions (but no phonons)

## What are Phonons?

In general the quantum state of all the lattice wave modes can be written as follows:

$$|\psi\rangle = |n_{\vec{q}_1}\rangle |n_{\vec{q}_2}\rangle |n_{\vec{q}_3}\rangle |n_{\vec{q}_4}\rangle \ldots\ldots\ldots |n_{\vec{q}_N}\rangle = \prod_{\vec{q}\ \text{in FZB}} |n_{\vec{q}}\rangle$$

where the wavevectors run over all the *N* lattice wave modes in the FBZ, and the total energy for this quantum state is:

$$\hat{H}|\psi\rangle = \sum_{\vec{q}\ \text{in FBZ}} \hbar\,\omega(\vec{q}) \left( \hat{a}^{+}(\vec{q})\,\hat{a}(\vec{q}) + \frac{1}{2} \right) |\psi\rangle$$

$$= \sum_{\vec{q}\ \text{in FBZ}} \hbar\,\omega(\vec{q}) \left( n_{\vec{q}} + \frac{1}{2} \right) |\psi\rangle$$

"Phonons are to lattice waves as photons are to electromagnetic waves"



## Hamiltonian for Multiple Phonon Bands

If the crystal has multiple phonon bands (TA, LA, TO, etc) then it can be shown that the Hamiltonian can be written as follows:

$$\hat{H} = \sum_{\eta} \sum_{\vec{q}\ \text{in FBZ}} \hbar\,\omega_{\eta}(\vec{q}) \left( \hat{a}^{+}_{\eta}(\vec{q})\,\hat{a}_{\eta}(\vec{q}) + \frac{1}{2} \right)$$

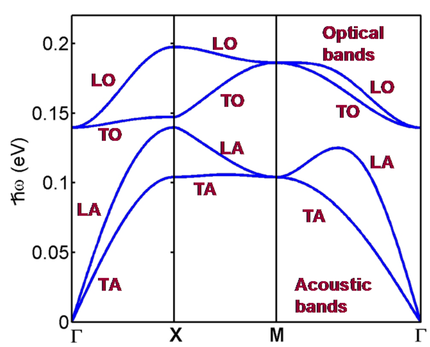
where the summation over "$\eta$" represents the summation over different phonon bands.

$\eta = 1 \Rightarrow$ TA

$\eta = 2 \Rightarrow$ LA

$\eta = 3 \Rightarrow$ TO

$\eta = 4 \Rightarrow$ LO



Phonons bands of a 2D diatomic crystal