Handout 17

Lattice Waves (Phonons) in 1D Crystals: Monoatomic Basis and Diatomic Basis

In this lecture you will learn:

- Equilibrium bond lengths
- Atomic motion in lattices
- Lattice waves (phonons) in a 1D crystal with a monoatomic basis
- Lattice waves (phonons) in a 1D crystal with a diatomic basis
- Dispersion of lattice waves
- Acoustic and optical phonons

The Hydrogen Molecule: Equilibrium Bond Length

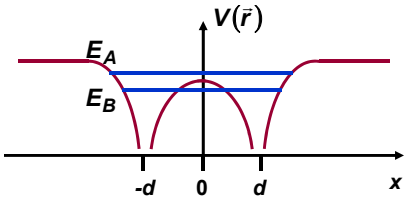
The equilibrium distance between the two hydrogen atoms in a hydrogen molecule is set by the balance among several different competing factors:

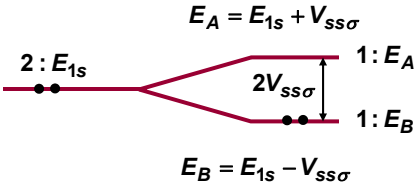
- The reduction in electronic energy due to co-valent bonding is $2V_{ss\sigma}$. If the atoms are too far apart, $V_{ss\sigma}$ becomes to small

$$\langle \phi_{1s}(\vec{r} - d\hat{x}) | \hat{H} | \phi_{1s}(\vec{r} + d\hat{x}) \rangle \approx -V_{ss\sigma}$$

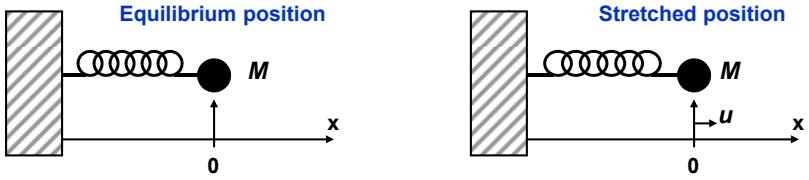
- If the atoms are too close, the positively charged nuclei (protons) will repel each other and this leads to an increase in the system energy

- Electron-electron repulsion also plays a role





A Mass Attached to a Spring: A Simple Harmonic Oscillator



Potential Energy:

$$PE = V(u) = \frac{1}{2} k\, u^2$$

spring constant = k
(units: Newton/meter)

PE varies quadratically with the displacement "*u* " of the mass from the equilibrium position

Kinetic Energy:

$$KE = \frac{M}{2}\left(\frac{du}{dt}\right)^2$$

Dynamical Equation (Newton's Second Law):

$$M\frac{d^2u}{dt^2} = -\frac{dV}{du} = -k\, u$$

Restoring force varies linearly with the displacement "*u* " of the mass from its equilibrium position

Solution:

$$u(t) = A\cos(\omega_o t) + B\sin(\omega_o t) \qquad \text{where:} \qquad \omega_o = \sqrt{\frac{k}{M}}$$

A 1D Crystal: Potential Energy

Consider a 1D lattice of *N* atoms:

Atoms can move only in the x-direction

• The potential energy of the entire crystal can be expressed in terms of the positions of the atoms. The potential energy will be minimum when all the atoms are at their equilibrium positions.

• Let the displacement of the atom at the lattice site given by $\vec{R}_n$ from its equilibrium position be $u(\vec{R}_n)$

• One can Taylor expand the potential energy of the entire crystal around its minimum equilibrium value:

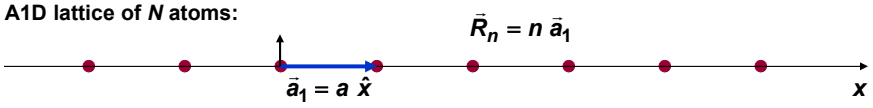
$$V\left[u(\vec{R}_1), u(\vec{R}_2), u(\vec{R}_3) \ldots\ldots\ldots u(\vec{R}_N)\right] = V_{EQ} + \sum_j \frac{\partial V}{\partial u(\vec{R}_j)}\bigg|_{EQ}^{0} u(\vec{R}_j)$$

$$+ \frac{1}{2}\sum_k \sum_j \frac{\partial^2 V}{\partial u(\vec{R}_j)\partial u(\vec{R}_k)}\bigg|_{EQ} u(\vec{R}_j)\,u(\vec{R}_k)$$

Potential energy varies quadratically with the displacements of the atoms from their equilibrium positions

A 1D Crystal: Potential and Kinetic Energies

A1D lattice of *N* atoms:



Potential Energy:

$$V = V_{EQ} + \frac{1}{2}\sum_k\sum_j \left.\frac{\partial^2 V}{\partial u(\vec{R}_j)\partial u(\vec{R}_k)}\right|_{EQ} u(\vec{R}_j,t)\,u(\vec{R}_k,t)$$

$$= V_{EQ} + \frac{1}{2}\sum_k\sum_j K(\vec{R}_j,\vec{R}_k)\,u(\vec{R}_j,t)\,u(\vec{R}_k,t) \qquad \left\{ K(\vec{R}_j,\vec{R}_k) = \left.\frac{\partial^2 V}{\partial u(\vec{R}_j)\partial u(\vec{R}_k)}\right|_{EQ}$$

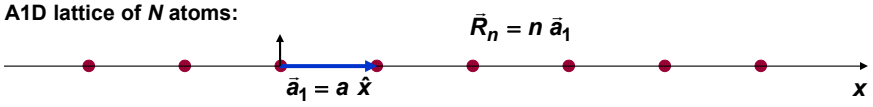
Kinetic Energy:

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

- The kinetic energy of all the atoms is the sum of their individual kinetic energies

A 1D Crystal: Dynamical Equation

A1D lattice of *N* atoms:



Write Newtons law for the atom sitting at the site $\vec{R}_n$:

$$M\frac{d^2u(\vec{R}_n,t)}{dt^2} = -\frac{\partial V}{\partial u(\vec{R}_n)} = -\sum_j K(\vec{R}_n,\vec{R}_j)\,u(\vec{R}_j,t)$$

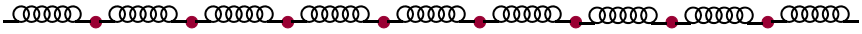
Remember that:

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

The restoring forces on the atoms vary linearly with the displacement of the atoms from their equilibrium positions

Dynamical Equation for Nearest-Neighbor Interactions

A1D lattice of *N* atoms:



$$M\frac{d^2u(\vec{R}_n,t)}{dt^2}=-\frac{\partial V}{\partial u(\vec{R}_n)}=-\sum_j K(\vec{R}_n,\vec{R}_j)\,u(\vec{R}_j,t)$$

Assume nearest-neighbor interactions:

$$K(\vec{R}_n,\vec{R}_j)=-\alpha\,\delta_{j,n+1}-\alpha\,\delta_{j,n-1}+2\alpha\,\delta_{j,n}$$

This gives:

$$M\frac{d^2u(\vec{R}_n,t)}{dt^2}=-\alpha\left[u(\vec{R}_n,t)-u(\vec{R}_{n-1},t)\right]-\alpha\left[u(\vec{R}_n,t)-u(\vec{R}_{n+1},t)\right]$$

The constants "α" provide restoring forces as if the atoms were connected together with springs of spring constant "α"

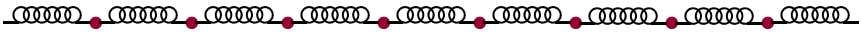
The constant α is called "force constant" (not spring constant) in solid state physics

We have *N* linear coupled differential equations for *N* unknowns

$$u(\vec{R}_n,t)\quad\{n=0,1,2.....(N-1)$$

Solution of the Dynamical Equation: Lattice Waves (Phonons)

A1D lattice of *N* atoms: $\vec{a}_1=a\,\hat{x}$ $\vec{R}_n=n\,\vec{a}_1$



$$M\frac{d^2u(\vec{R}_n,t)}{dt^2}=-\alpha\left[u(\vec{R}_n,t)-u(\vec{R}_{n-1},t)\right]-\alpha\left[u(\vec{R}_n,t)-u(\vec{R}_{n+1},t)\right]$$

Assume a solution of the form:

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

Represents a wave with wavevector $\vec{q}$, frequency ω, and amplitude $u(\vec{q})$

Or: $u(\vec{R}_n,t)=u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_n}\,e^{-i\,\omega\,t}$ → Slight abuse of notation

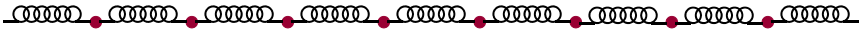
Note that:

$$u(\vec{R}_{n+1},t)=u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_{n+1}}\,e^{-i\,\omega\,t}=u(\vec{q})\,e^{i\,\vec{q}\,.\,(\vec{R}_n+\vec{a}_1)}\,e^{-i\,\omega\,t}$$
$$=e^{i\,\vec{q}\,.\,\vec{a}_1}u(\vec{q})\;e^{i\,\vec{q}\,.\,\vec{R}_n}\,e^{-i\,\omega\,t}$$

$$u(\vec{R}_{n-1},t)=u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_{n-1}}\,e^{-i\,\omega\,t}=u(\vec{q})\,e^{i\,\vec{q}\,.\,(\vec{R}_n-\vec{a}_1)}\,e^{-i\,\omega\,t}$$
$$=e^{-i\,\vec{q}\,.\,\vec{a}_1}u(\vec{q})\;e^{i\,\vec{q}\,.\,\vec{R}_n}\,e^{-i\,\omega\,t}$$

Solution of the Dynamical Equation: Lattice Waves (Phonons)

A1D lattice of N atoms: $\vec{a}_1 = a\,\hat{x}$ $\vec{R}_n = n\,\vec{a}_1$



$$M\frac{d^2u(\vec{R}_n,t)}{dt^2} = -\alpha\left[u(\vec{R}_n,t)-u(\vec{R}_{n-1},t)\right]-\alpha\left[u(\vec{R}_n,t)-u(\vec{R}_{n+1},t)\right]$$

Plug in the assumed solution: $u(\vec{R}_n,t) = u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_n}\,e^{-i\,\omega\,t}$ $\quad q = q_x\hat{x}$

To get:

$$-\omega^2\,M\,u(\vec{q}) = -\alpha\left[u(\vec{q})-e^{-i\,\vec{q}\,.\,\vec{a}_1}\,u(\vec{q})\right]-\alpha\left[u(\vec{q})-e^{+i\,\vec{q}\,.\,\vec{a}_1}\,u(\vec{q})\right]$$

Which simplifies to:

$$\omega^2 = \frac{2\alpha}{M}\left[1-\cos(\vec{q}\,.\,\vec{a}_1)\right]$$
$$= \frac{4\alpha}{M}\sin^2\left(\frac{\vec{q}\,.\,\vec{a}_1}{2}\right)$$

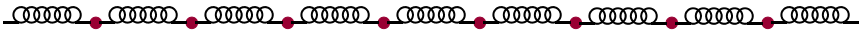
Or:

$$\omega = \pm\sqrt{\frac{4\alpha}{M}}\sin\left(\frac{\vec{q}\,.\,\vec{a}_1}{2}\right)$$

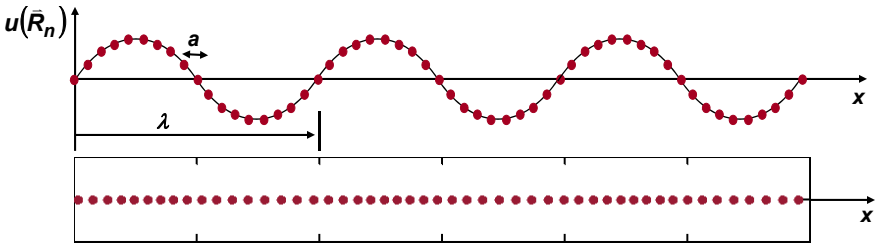
Since ω is always positive, the negative sign is chosen when the sine term is negative

Solution of the Dynamical Equation: Lattice Waves (Phonons)

A1D lattice of N atoms: $\vec{a}_1 = a\,\hat{x}$ $\vec{R}_n = n\,\vec{a}_1$



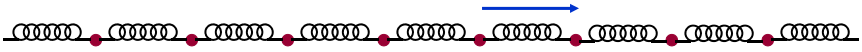
Solution is: $u(\vec{R}_n,t) = u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_n}\,e^{-i\,\omega\,t}$ and $\omega = \sqrt{\frac{4\alpha}{M}}\sin\left(\frac{\vec{q}\,.\,\vec{a}_1}{2}\right)$



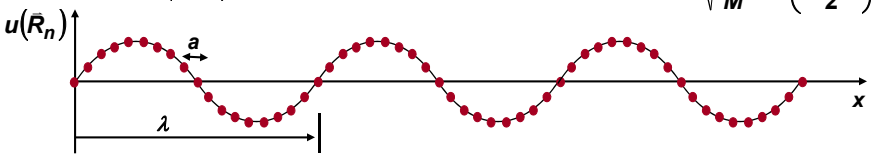
- The lattice waves are like the compressional sound waves in the air

Solution of the Dynamical Equation: Lattice Waves (Phonons)

A1D lattice of *N* atoms: $\vec{a}_1 = a\,\hat{x}$ $\vec{R}_n = n\,\vec{a}_1$



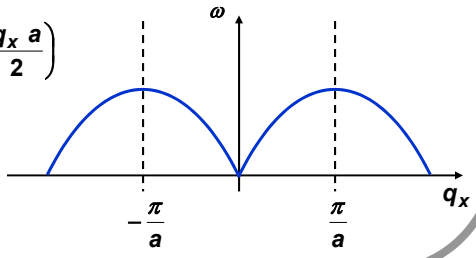
Solution is: $u(\vec{R}_n, t) = u(\vec{q})\, e^{i\,\vec{q}\,.\,\vec{R}_n}\, e^{-i\,\omega\,t}$ and $\omega = \sqrt{\frac{4\alpha}{M}} \sin\left(\frac{\vec{q}\,.\,\vec{a}_1}{2}\right)$



The relation:

$$\omega = \pm\sqrt{\frac{4\alpha}{M}} \sin\left(\frac{\vec{q}\,.\,\vec{a}_1}{2}\right) = \pm\sqrt{\frac{4\alpha}{M}} \sin\left(\frac{q_x\, a}{2}\right)$$

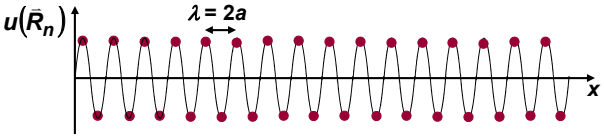
represents the dispersion of the lattice waves or phonons



Lattice Waves and the First BZ

Solution is: $u(\vec{R}_n, t) = u(\vec{q})\, e^{i\,\vec{q}\,.\,\vec{R}_n}\, e^{-i\,\omega\,t}$ and $\omega = \sqrt{\frac{4\alpha}{M}} \sin\left(\frac{\vec{q}\,.\,\vec{a}_1}{2}\right)$

Question: What is the shortest wavelength (or the largest wavevector) the lattice waves can have?



⇒For the shortest wavelength:

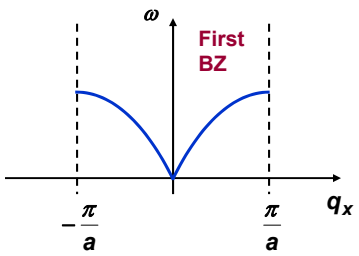
$$\lambda = 2a$$

⇒The largest wavevector is then:

$$|q_x| = \frac{2\pi}{\lambda} = \frac{\pi}{a}$$

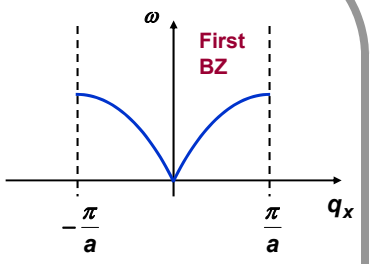
⇒The wavevector values can be restricted to the First BZ

• No new solutions are found for values of the wavevector outside the first BZ



Phase and Group Velocities

$$\omega = \pm\sqrt{\frac{4\alpha}{M}}\sin\left(\frac{q_x a}{2}\right)$$



Phase velocity and group velocity of lattice waves are defined as:

$$\vec{v}_p(\vec{q}) = \frac{\omega(\vec{q})}{|\vec{q}|}\hat{q} \xrightarrow{1D} \frac{\omega}{q_x}\hat{x}$$

$$\vec{v}_g(\vec{q}) = \nabla_{\vec{q}}\,\omega(\vec{q}) \xrightarrow{1D} \frac{d\omega}{dq_x}\hat{x}$$

Case I: For $q_x \approx 0$ (i.e. $q_x a << \pi$):

$$\omega \approx \sqrt{\frac{\alpha}{M}}\,q_x a \longrightarrow \text{Linear dispersion} \quad \Rightarrow \quad v_p = \sqrt{\frac{\alpha}{M}}\,a = v_g$$

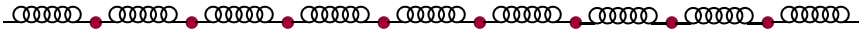
Case II: For $q_x a = \pi$:

$$\omega = \sqrt{\frac{4\alpha}{M}} \quad \Rightarrow \quad v_p = \sqrt{\frac{4\alpha}{M}}\,\frac{a}{\pi}$$

$$\Rightarrow \quad v_g = 0$$

Periodic Boundary Conditions

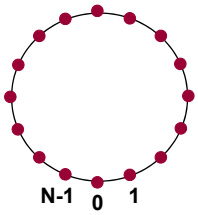
A1D lattice of N atoms: $\vec{a}_1 = a\,\hat{x}$ $\qquad \vec{R}_n = n\,\vec{a}_1$



In the solution:

$$u(\vec{R}_n, t) = u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_n}\,e^{-i\,\omega\,t}$$

allowed values of the wavevector depend on the boundary conditions



Periodic Boundary Condition:

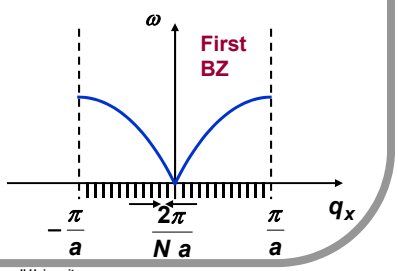
The N-th atom is the same as the 0-th atom
This implies:

$$u(\vec{R}_N, t) = u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_N}\,e^{-i\,\omega\,t} = u(\vec{R}_0, t) = u(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{R}_0}\,e^{-i\,\omega\,t}$$

$$\Rightarrow e^{i\,\vec{q}\,.\,(\vec{R}_N - \vec{R}_0)} = 1$$

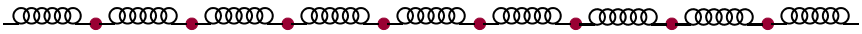
$$\Rightarrow e^{i\,q_x N a} = 1$$

$$\Rightarrow q_x = \frac{m}{N}\frac{2\pi}{a} \qquad \begin{cases} m = \text{integer} \\ -\frac{N}{2} < m \le \frac{N}{2} \end{cases}$$



Counting and Conserving Degrees of Freedom

A1D lattice of *N* atoms: $\vec{a}_1 = a\,\hat{x}$ $\vec{R}_n = n\,\vec{a}_1$

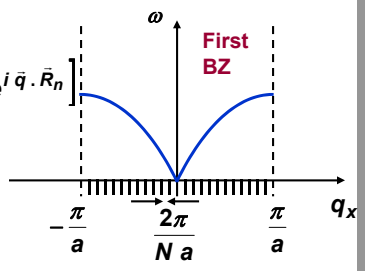


- We started with *N* degrees of freedom which were related to the motion in 1D of *N* different atoms
- The dynamical variables were the amplitudes of the displacements of *N* different atoms

$$u(\vec{R}_n, t) \quad \{ n = 0,1,2.....(N-1)$$

We then ended up with lattice waves:

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



- There are *N* different lattice wave modes corresponding to the *N* different possible wavevector values in the first BZ
- The dynamical variables are the amplitudes of the *N* different lattice wave modes

$$u(\vec{q}, t) \quad \left\{ q_x = \frac{m}{N}\frac{2\pi}{a} \quad \text{and} \quad -\frac{N}{2} < m \le \frac{N}{2} \right.$$

The number of degrees of freedom are the same before and after – as they should be!

Counting and Conserving Degrees of Freedom

The atomic displacements,

$$u(\vec{R}_n, t) \quad \{ n = 0,1,2.....(N-1)$$

taken together provide a complete description of the motion of all the atoms in the crystal

In general, one can expand the atomic displacements in terms of all the lattice wave modes (resembles a Fourier series expansion):

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

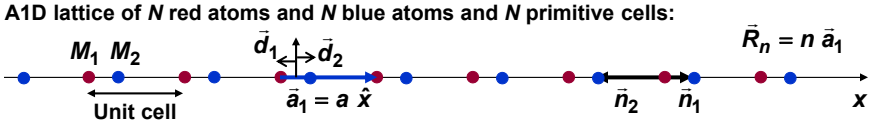
$$= \sum_{\vec{q}\,\text{in FBZ}} \frac{u(\vec{q})}{2}\, e^{i\,\vec{q}\,.\,\vec{R}_n}\; e^{-i\,\omega(\vec{q})\,t} + \frac{u^*(\vec{q})}{2}\, e^{-i\,\vec{q}\,.\,\vec{R}_n}\; e^{i\,\omega(\vec{q})\,t}$$

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

Therefore, the lattice wave amplitudes also provide a complete description of the motion of all the atoms in the crystal

Lattice Waves (Phonons) in a 1D crystal: Diatomic Basis

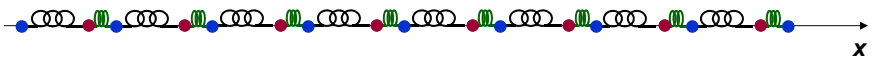
A1D lattice of *N* red atoms and *N* blue atoms and *N* primitive cells:



The basis vectors are: $\vec{d}_1$ $\vec{d}_2$

The nearest neighbor vectors are: $\vec{n}_1$ $\vec{n}_2$

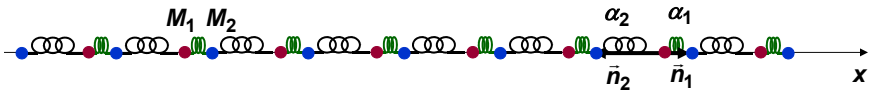
The spring model for nearest neighbor interactions:



Let the displacement of the red atom in the *n*-th cell be: $u_1\left(\vec{R}_n + \vec{d}_1, t\right)$

Let the displacement of the blue atom in the *n*-th cell be: $u_2\left(\vec{R}_n + \vec{d}_2, t\right)$

Lattice Waves (Phonons) in a 1D crystal: Diatomic Basis



Write the dynamical equations for both the atoms assuming nearest neighbor interactions

$$M_1 \frac{d^2 u_1\left(\vec{R}_n + \vec{d}_1, t\right)}{dt^2} = -\alpha_2\left[u_1\left(\vec{R}_n + \vec{d}_1, t\right) - u_2\left(\vec{R}_{n-1} + \vec{d}_2, t\right)\right] - \alpha_1\left[u_1\left(\vec{R}_n + \vec{d}_1, t\right) - u_2\left(\vec{R}_n + \vec{d}_2, t\right)\right]$$

$$M_2 \frac{d^2 u_2\left(\vec{R}_n + \vec{d}_2, t\right)}{dt^2} = -\alpha_1\left[u_2\left(\vec{R}_n + \vec{d}_2, t\right) - u_1\left(\vec{R}_n + \vec{d}_1, t\right)\right] - \alpha_2\left[u_2\left(\vec{R}_n + \vec{d}_2, t\right) - u_1\left(\vec{R}_{n+1} + \vec{d}_1, t\right)\right]$$

The constants α_1 and α_2 are called "force constants" (not spring constants) in solid state physics

Assume a solution of the form:

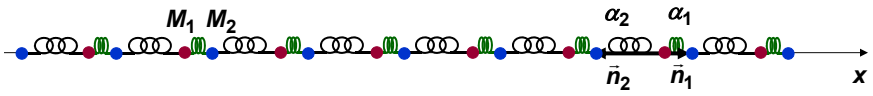
$$u_1\left(\vec{R}_n + \vec{d}_1, t\right) = u_1(\vec{q})\, e^{i\,\vec{q}\,.\,\left(\vec{R}_n + \vec{d}_1\right)}\, e^{-i\,\omega\,t}$$

$$u_2\left(\vec{R}_n + \vec{d}_2, t\right) = u_2(\vec{q})\, e^{i\,\vec{q}\,.\,\left(\vec{R}_n + \vec{d}_2\right)}\, e^{-i\,\omega\,t}$$

Notice the phases

This is again a wave-like solution with a wavevector $\vec{q}$ and frequency ω and different amplitudes for the two atoms

Lattice Waves (Phonons) in a 1D crystal: Diatomic Basis



Plug the solutions in the dynamical equations to get:

$$-\omega^2 M_1 u_1(\vec{q}) = -\alpha_2\left[u_1(\vec{q}) - e^{i\,\vec{q}\,.\,\vec{n}_2} u_2(\vec{q})\right] - \alpha_1\left[u_1(\vec{q}) - e^{i\,\vec{q}\,.\,\vec{n}_1} u_2(\vec{q})\right]$$

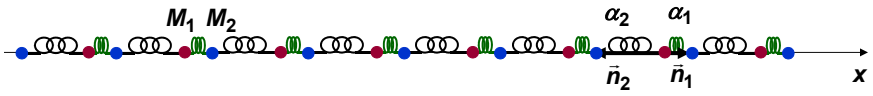
$$-\omega^2 M_2 u_2(\vec{q}) = -\alpha_1\left[u_2(\vec{q}) - e^{-i\,\vec{q}\,.\,\vec{n}_1} u_1(\vec{q})\right] - \alpha_2\left[u_2(\vec{q}) - e^{-i\,\vec{q}\,.\,\vec{n}_2} u_1(\vec{q})\right]$$

Write the equations in a matrix form:

$$\begin{bmatrix} \alpha_1+\alpha_2 & -\left(\alpha_1 e^{i\,\vec{q}\,.\,\vec{n}_1} + \alpha_2 e^{i\,\vec{q}\,.\,\vec{n}_2}\right) \\ -\left(\alpha_1 e^{-i\,\vec{q}\,.\,\vec{n}_1} + \alpha_2 e^{-i\,\vec{q}\,.\,\vec{n}_2}\right) & \alpha_1+\alpha_2 \end{bmatrix} \begin{bmatrix} u_1(\vec{q}) \\ u_2(\vec{q}) \end{bmatrix} = \omega^2 \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} \begin{bmatrix} u_1(\vec{q}) \\ u_2(\vec{q}) \end{bmatrix}$$

This is a 2x2 matrix eigenvalue equation that needs to be solved for each value of the wavevector to get the dispersion of the lattice waves

The Dynamical Matrix



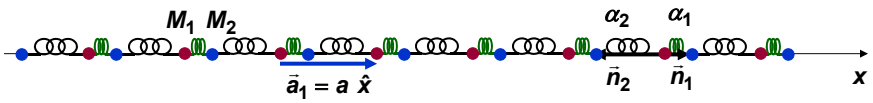
$$\begin{bmatrix} \alpha_1+\alpha_2 & -\left(\alpha_1 e^{i\,\vec{q}\,.\,\vec{n}_1} + \alpha_2 e^{i\,\vec{q}\,.\,\vec{n}_2}\right) \\ -\left(\alpha_1 e^{-i\,\vec{q}\,.\,\vec{n}_1} + \alpha_2 e^{-i\,\vec{q}\,.\,\vec{n}_2}\right) & \alpha_1+\alpha_2 \end{bmatrix} \begin{bmatrix} u_1(\vec{q}) \\ u_2(\vec{q}) \end{bmatrix} = \omega^2 \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} \begin{bmatrix} u_1(\vec{q}) \\ u_2(\vec{q}) \end{bmatrix}$$

Or:
$$\overline{\overline{D}}(\vec{q}) \begin{bmatrix} u_1(\vec{q}) \\ u_2(\vec{q}) \end{bmatrix} = \omega^2\, \overline{\overline{M}} \begin{bmatrix} u_1(\vec{q}) \\ u_2(\vec{q}) \end{bmatrix}$$

Or:
$$\overline{\overline{M}}^{-1}\, \overline{\overline{D}}(\vec{q}) \begin{bmatrix} u_1(\vec{q}) \\ u_2(\vec{q}) \end{bmatrix} = \omega^2 \begin{bmatrix} u_1(\vec{q}) \\ u_2(\vec{q}) \end{bmatrix}$$

- **The matrix $\overline{\overline{D}}(\vec{q})$ is called the dynamical matrix of the medium**
- **For any medium, in any dimension, the dispersion relations for the lattice waves (phonons) are obtained by solving a similar matrix eigenvalue equation**

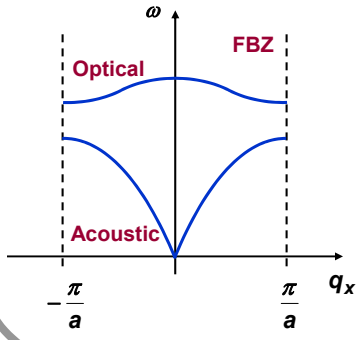
Optical and Acoustic Phonons



The frequency eigenvalues are:

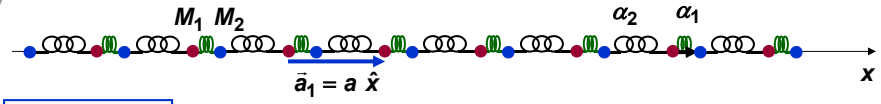
$$\omega^2(\vec{q}) = \frac{(\alpha_1+\alpha_2)}{2M_r} \pm \frac{1}{2}\sqrt{\frac{(\alpha_1+\alpha_2)^2}{M_r^2} - 16\frac{\alpha_1\alpha_2}{M_1M_2}\sin^2\left(\frac{\vec{q}\,.\,\vec{a}_1}{2}\right)}$$

$$\frac{1}{M_r} = \frac{1}{M_1} + \frac{1}{M_2}$$



- The two frequency eigenvalues for each wavevector value in the FBZ give two phonon bands
- The higher frequency band is called the optical phonon band
- The lower frequency band is called the acoustic phonon band

Optical and Acoustic Phonons: Special Cases



Case I: $\vec{q} \approx 0$

Acoustic band:

$$\omega(\vec{q}\approx 0) \approx \sqrt{\frac{\alpha_1\alpha_2}{(\alpha_1+\alpha_2)(M_1+M_2)}}\,q_x a \qquad \begin{bmatrix} u_1(\vec{q}\approx 0) \\ u_2(\vec{q}\approx 0) \end{bmatrix} \approx A\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$u_1(\vec{R}_n + \vec{d}_1, t) = A\, e^{i\,\vec{q}\,.\,(\vec{R}_n+\vec{d}_1)}\, e^{-i\,\omega\,t}$$

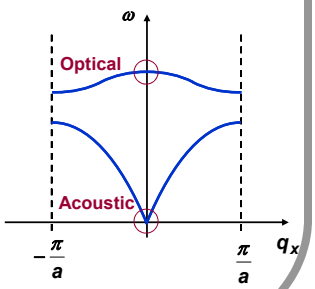
$$u_2(\vec{R}_n + \vec{d}_2, t) = A\, e^{i\,\vec{q}\,.\,(\vec{R}_n+\vec{d}_2)}\, e^{-i\,\omega\,t}$$

Optical band:

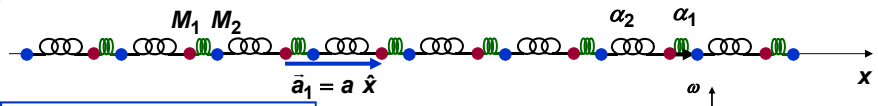
$$\omega(\vec{q}\approx 0) \approx \sqrt{\frac{(\alpha_1+\alpha_2)}{M_r}} \qquad \begin{bmatrix} u_1(\vec{q}\approx 0) \\ u_2(\vec{q}\approx 0) \end{bmatrix} \approx A\begin{bmatrix} 1 \\ -M_1/M_2 \end{bmatrix}$$

$$u_1(\vec{R}_n + \vec{d}_1, t) = A\, e^{i\,\vec{q}\,.\,(\vec{R}_n+\vec{d}_1)}\, e^{-i\,\omega\,t}$$

$$u_2(\vec{R}_n + \vec{d}_2, t) = -A\frac{M_1}{M_2}\, e^{i\,\vec{q}\,.\,(\vec{R}_n+\vec{d}_2)}\, e^{-i\,\omega\,t}$$



Optical and Acoustic Phonons: Special Cases

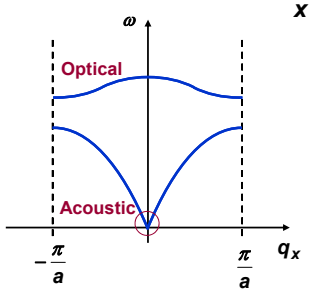


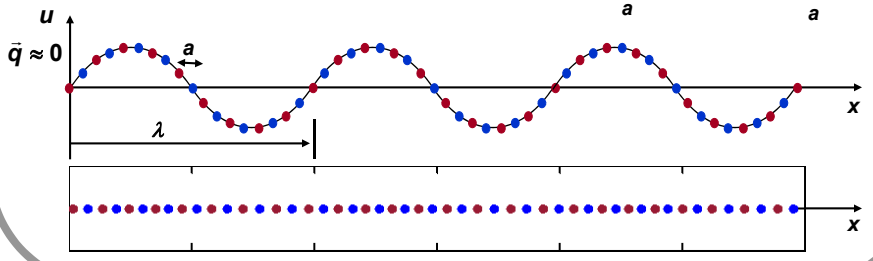
Case I: $\vec{q} \approx 0$ Acoustic Mode

Acoustic band (basis atoms move in-phase):

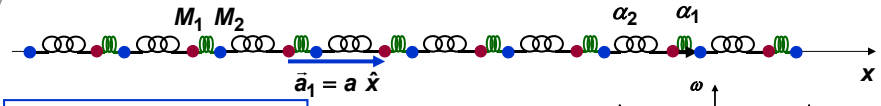
$$u_1\left(\vec{R}_n + \vec{d}_1, t\right) = A\, e^{i\,\vec{q}\cdot\left(\vec{R}_n + \vec{d}_1\right)}\, e^{-i\,\omega\,t}$$

$$u_2\left(\vec{R}_n + \vec{d}_2, t\right) = A\, e^{i\,\vec{q}\cdot\left(\vec{R}_n + \vec{d}_2\right)}\, e^{-i\,\omega\,t}$$





Optical and Acoustic Phonons: Special Cases

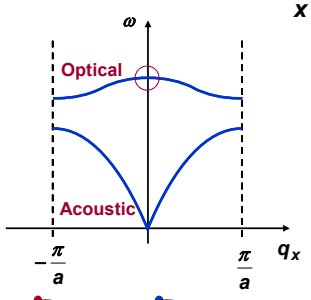


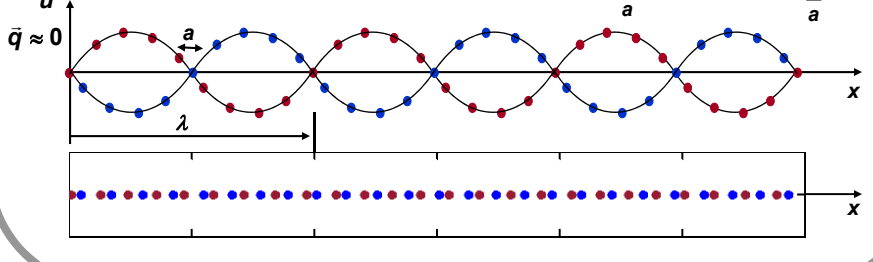
Case I: $\vec{q} \approx 0$ Optical Mode

Optical band (basis atoms move 180° out-of-phase):

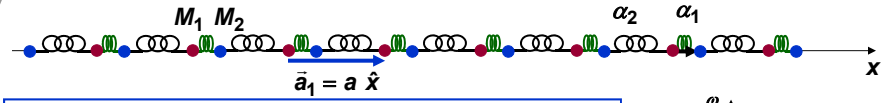
$$u_1\left(\vec{R}_n + \vec{d}_1, t\right) = A\, e^{i\,\vec{q}\cdot\left(\vec{R}_n + \vec{d}_1\right)}\, e^{-i\,\omega\,t}$$

$$u_2\left(\vec{R}_n + \vec{d}_2, t\right) = -A\,\frac{M_1}{M_2}\, e^{i\,\vec{q}\cdot\left(\vec{R}_n + \vec{d}_2\right)}\, e^{-i\,\omega\,t}$$



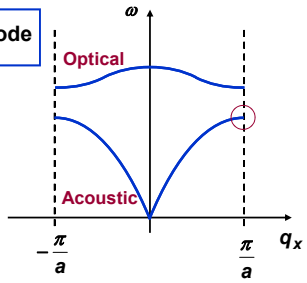


Optical and Acoustic Phonons: Special Cases



Case II: $\vec{q} = \frac{\pi}{a}\hat{x}$, $M_1 = M_2 = M$, $\alpha_1 > \alpha_2$ Acoustic Mode

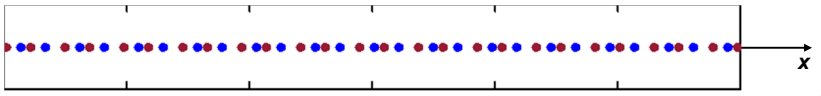
$$\omega\left(\frac{\pi}{a}\hat{x}\right) = \sqrt{\frac{2\alpha_2}{M}} \qquad \begin{bmatrix} u_1\left(\frac{\pi}{a}\hat{x}\right) \\ u_2\left(\frac{\pi}{a}\hat{x}\right) \end{bmatrix} = A\begin{bmatrix} 1 \\ e^{-i\,\vec{q}\,.\,\vec{n}_1} \end{bmatrix}$$



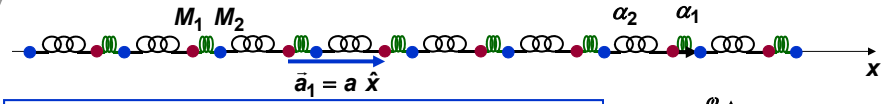
$$u_1\left(\vec{R}_n + \vec{d}_1, t\right) = A\, e^{i\,\vec{q}\,.\,\left(\vec{R}_n + \vec{d}_1\right)} e^{-i\,\omega\,t}$$

$$u_2\left(\vec{R}_n + \vec{d}_2, t\right) = A\, e^{-i\,\vec{q}\,.\,\vec{n}_1} e^{i\,\vec{q}\,.\,\left(\vec{R}_n + \vec{d}_2\right)} e^{-i\,\omega\,t}$$

$$= A\, e^{i\,\vec{q}\,.\,\left(\vec{R}_n + \vec{d}_1\right)} e^{-i\,\omega\,t}$$

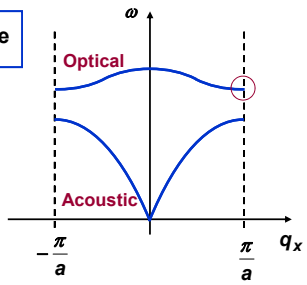


Optical and Acoustic Phonons: Special Cases



Case II: $\vec{q} = \frac{\pi}{a}\hat{x}$, $M_1 = M_2 = M$, $\alpha_1 > \alpha_2$ Optical Mode

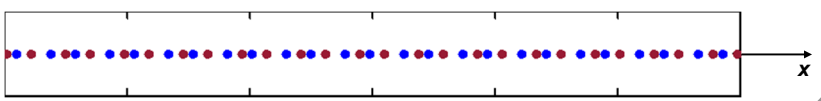
$$\omega\left(\frac{\pi}{a}\hat{x}\right) = \sqrt{\frac{2\alpha_1}{M}} \qquad \begin{bmatrix} u_1\left(\frac{\pi}{a}\hat{x}\right) \\ u_2\left(\frac{\pi}{a}\hat{x}\right) \end{bmatrix} = A\begin{bmatrix} 1 \\ -e^{-i\,\vec{q}\,.\,\vec{n}_1} \end{bmatrix}$$



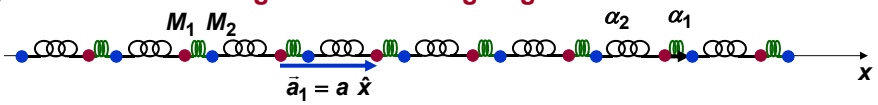
$$u_1\left(\vec{R}_n + \vec{d}_1, t\right) = A\, e^{i\,\vec{q}\,.\,\left(\vec{R}_n + \vec{d}_1\right)} e^{-i\,\omega\,t}$$

$$u_2\left(\vec{R}_n + \vec{d}_2, t\right) = -A\, e^{-i\,\vec{q}\,.\,\vec{n}_1} e^{i\,\vec{q}\,.\,\left(\vec{R}_n + \vec{d}_2\right)} e^{-i\,\omega\,t}$$

$$= -A\, e^{i\,\vec{q}\,.\,\left(\vec{R}_n + \vec{d}_1\right)} e^{-i\,\omega\,t}$$



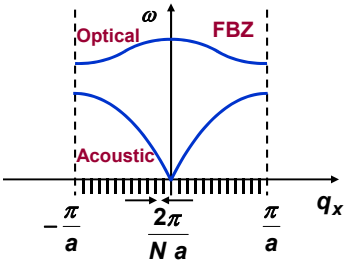
Counting and Conserving Degrees of Freedom



- We started with $2N$ degrees of freedom which were related to the motion in 1D of $2N$ different atoms
- The dynamical variables were the amplitudes of the displacements of $2N$ different atoms

$$u_1\left(\vec{R}_n + \vec{d}_1, t\right) \quad u_2\left(\vec{R}_n + \vec{d}_2, t\right) \quad \{ n = 0,1,2.....(N-1)$$

We then ended up with lattice waves:



- There are N different modes per phonon band corresponding to the N different possible wavevector values in the first BZ
- There are 2 phonon bands and therefore a total of $2N$ different phonon modes
- The dynamical variables are the amplitudes of the $2N$ different phonon modes

The number of degrees of freedom are the same before and after – as they should be!

Counting and Conserving Degrees of Freedom

The atomic displacements,

$$u_1\left(\vec{R}_n + \vec{d}_1, t\right) \quad u_2\left(\vec{R}_n + \vec{d}_2, t\right) \quad \{ n = 0,1,2.....(N-1)$$

taken together provide a complete description of the motion of all the $2N$ atoms in the crystal

In general, one can expand the atomic displacements in terms of all the lattice wave modes – all wavevectors and all bands:

$$\begin{bmatrix} u_1\left(\vec{R}_n + \vec{d}_1, t\right) \\ u_2\left(\vec{R}_n + \vec{d}_2, t\right) \end{bmatrix} = \sum_{\eta=A,O} \sum_{\vec{q}\ \text{in FBZ}} \text{Re}\left[\begin{bmatrix} u_{1\eta}(\vec{q})\, e^{i\,\vec{q}\,.\,\vec{d}_1} \\ u_{2\mu}(\vec{q})\, e^{i\,\vec{q}\,.\,\vec{d}_2} \end{bmatrix} e^{i\,\vec{q}\,.\,\vec{R}_n}\, e^{-i\,\omega_\eta(\vec{q})\,t} \right]$$

$$= \sum_{\eta=A,O} \sum_{\vec{q}\ \text{in FBZ}} \frac{1}{2} \begin{bmatrix} u_{1\eta}(\vec{q})\, e^{i\,\vec{q}\,.\,\vec{d}_1} \\ u_{2\eta}(\vec{q})\, e^{i\,\vec{q}\,.\,\vec{d}_2} \end{bmatrix} e^{i\,\vec{q}\,.\,\vec{R}_n}\, e^{-i\,\omega_\eta(\vec{q})\,t} + \frac{1}{2} \begin{bmatrix} u^*_{1\eta}(\vec{q})\, e^{-i\,\vec{q}\,.\,\vec{d}_1} \\ u^*_{2\eta}(\vec{q})\, e^{-i\,\vec{q}\,.\,\vec{d}_2} \end{bmatrix} e^{-i\,\vec{q}\,.\,\vec{R}_n}\, e^{i\,\omega_\eta(\vec{q})\,t}$$

$$= \sum_{\eta=A,O} \sum_{\vec{q}\ \text{in FBZ}} \frac{1}{2} \begin{bmatrix} u_{1\eta}(\vec{q},t)\, e^{i\,\vec{q}\,.\,\vec{d}_1} \\ u_{2\eta}(\vec{q},t)\, e^{i\,\vec{q}\,.\,\vec{d}_2} \end{bmatrix} e^{i\,\vec{q}\,.\,\vec{R}_n} + \frac{1}{2} \begin{bmatrix} u^*_{1\eta}(\vec{q},t)\, e^{-i\,\vec{q}\,.\,\vec{d}_1} \\ u^*_{2\eta}(\vec{q},t)\, e^{-i\,\vec{q}\,.\,\vec{d}_2} \end{bmatrix} e^{-i\,\vec{q}\,.\,\vec{R}_n}$$

Therefore, the lattice wave amplitudes also provide a complete description of the motion of all the atoms in the crystal