SEOUL NATIONAL UNIVERSITY – SCHOOL OF PHYSICS

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SPRING SEMESTER 2004

Solid State Physics II

Chapter 2 Lattice Dynamics in One Dimension

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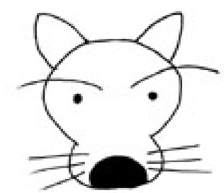

Lattice Dynamics in One Dimension

We may consider crystalline solids as a periodic array of atoms or molecules at fixed positions, i.e., lattice points. However, since, at finite temperature, the atoms in a solid are in constant motion induced by the thermal energy, we need to device a picture or model for the description of such thermal motion of atoms.

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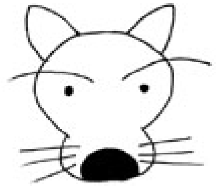
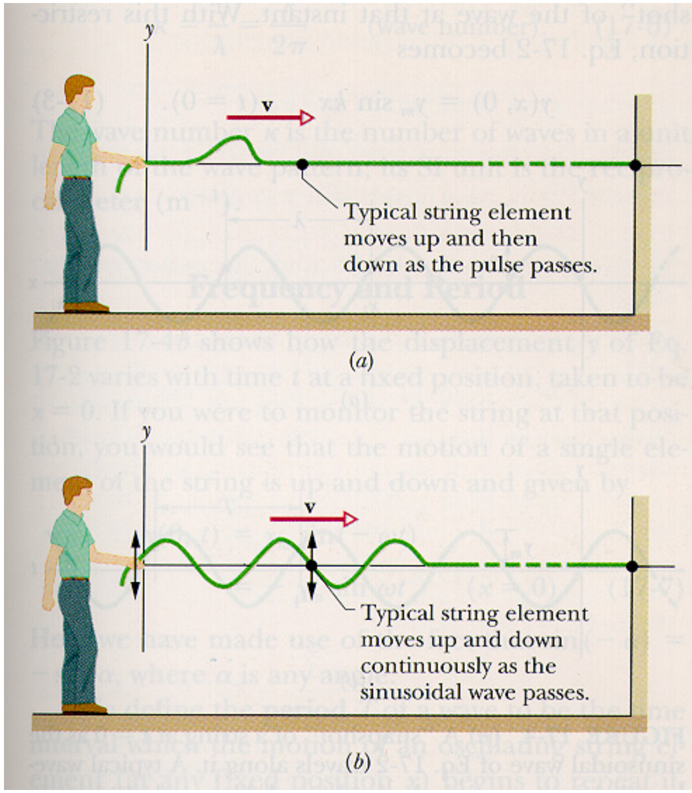
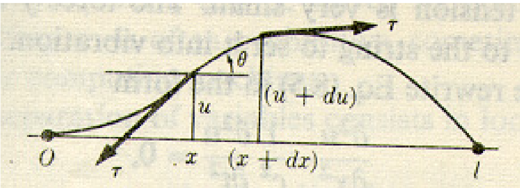
The basic ideas behind this picture are:

- Harmonic motions of atoms about their equilibrium positions
- Normal modes of lattice waves



Dynamics of a string — continuous medium





$$\tau_u = \tau \sin\theta \approx \tau \frac{\partial u}{\partial x}$$

$$dF = \tau_u\big|_{x+dx} - \tau_u\big|_x \approx \frac{\partial}{\partial x}\left(\tau \frac{\partial u}{\partial x}\right) dx$$

$$\sigma dx \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(\tau \frac{\partial u}{\partial x}\right) dx$$

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{{v_s}^2}\frac{\partial^2 u}{\partial t^2} = 0$$

$$v_s = \left(\frac{\tau}{\sigma}\right)^{1/2}$$

What do we measure in the motion of continuum string?
How do we observe in the vibrational motion?

In particle dynamics, we are interested in the dynamic variables $\{\mathbf{x}_i, \mathbf{p}_i\}$ of each individual particles. When the number of particle $N \to \infty$, it becomes no longer possible to observe them all. Then, what do we do?

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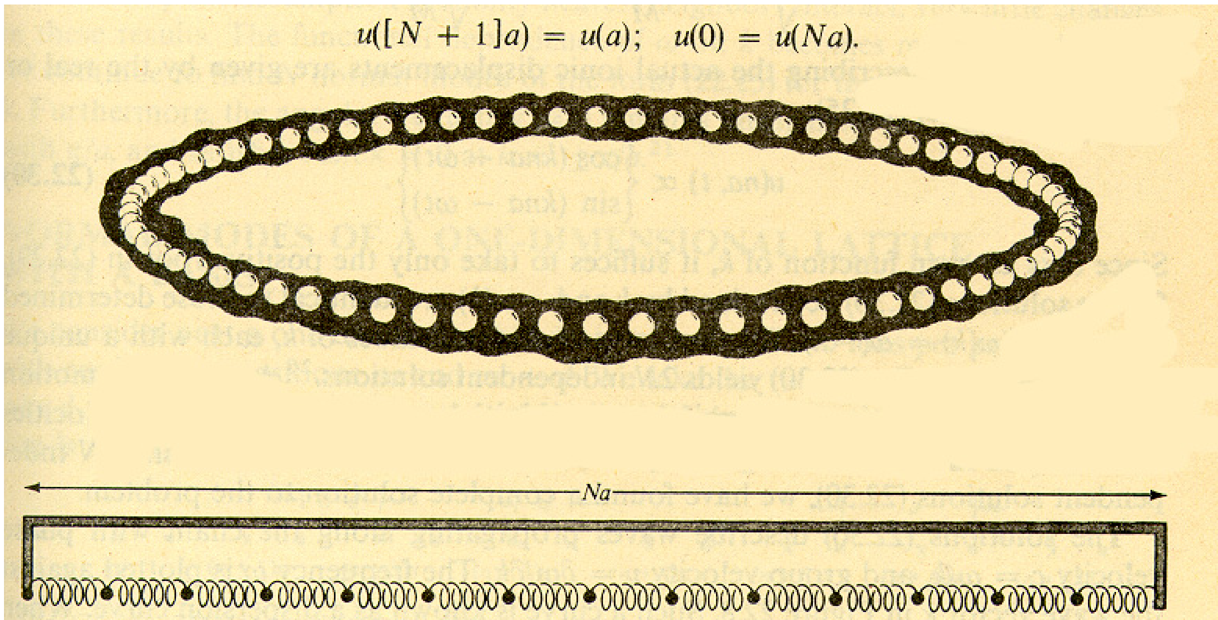
When hearing sounds, how do we distinguish tone, pitch, tune, rhythm, and so on? Could we take an analogy between hearing sounds and measuring the wave motion?

Infinite chain of atoms

1D linear chain of coupled harmonic oscillators



- mass: $M_l = m$
- position: $x_l = la + u_l$
- velocity: $v_l = \dot{x}_l = \dot{u}_l$
- force: $F_l = C(u_{l+1} - u_l) - C(u_l - u_{l-1}) = C(u_{l+1} + u_{l-1} - 2u_l)$
- classical equation of motion: (coupled harmonic oscillators)

$$m\ddot{u}_l = F_l$$

$$\ddot{u}_l = \omega_o^2(u_{l+1} + u_{l-1} - 2u_l) \quad \text{with} \quad \omega_o^2 = \frac{C}{m}$$

Looking for a solution? Use Symmetry!

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(i) mirror symmetry for $N = 2$: ($x_1 \leftrightarrow x_2$)

$\Rightarrow$ normal modes

$$\begin{cases} x_s &= \frac{1}{\sqrt{2}}(x_1 + x_2) \\ x_a &= \frac{1}{\sqrt{2}}(x_1 - x_2) \end{cases}$$

$$P(1 \leftrightarrow 2)x_{s,a} = \pm x_{s,a} = (e^{in\pi})x_{s,a} \qquad (n = 0, 1)$$

where x_s stands for the center-of-mass motion and x_a for the relative motion.

(ii) cyclic symmetry for $N > 2$: $(\ldots \longrightarrow x_1 \longrightarrow x_2 \longrightarrow x_3 \longrightarrow \ldots \longrightarrow x_N \longrightarrow x_1 \ldots)$ In group theory, this symmetry belongs to the Abelian group with 1-dimensional representation:

$$T_a \psi_k = \lambda_k \psi_k \quad \text{with} \quad \psi_k = \psi_k(x)$$

$$(T_a)^N \psi_k = \lambda_k^N \psi_k = \psi_k$$

$$\lambda_k = e^{ika} \quad \text{and} \quad kaN = 2\pi n$$

$$k = \left(\frac{2\pi}{aN}\right) n = \left(\frac{2\pi}{L}\right) n$$

For an example, we can consider

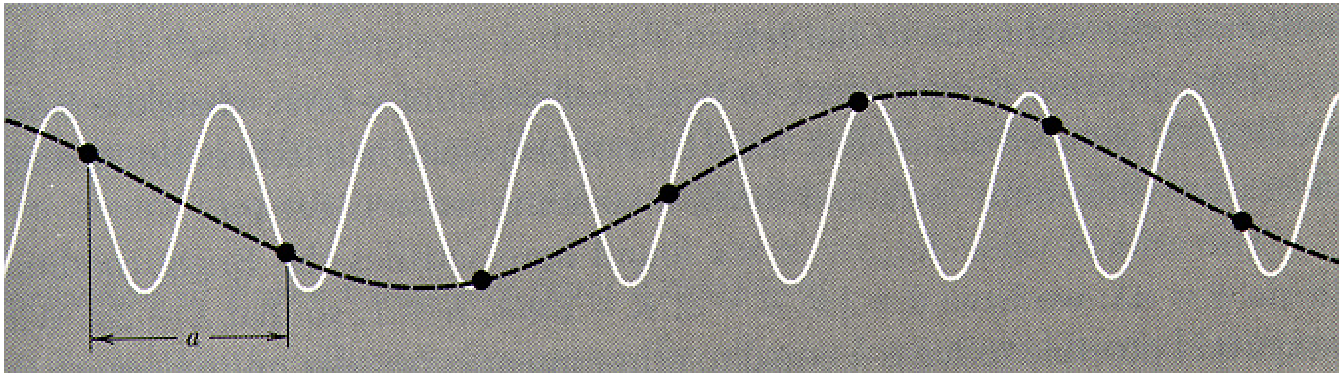
$$\psi_k(x) = u_k(x = x_l) = u_o(k) e^{ikx_l}$$

with $x_l = la$

Nomal modes and dispersion relation

Looking for a normal mode: $u_l(t) \sim e^{-i\omega t}$

All the particles in the chain move coherently, i.e., with the same time-dependence $e^{-i\omega t}$.



For the k-th normal mode with ω_k:

$$u_l(k,t) = \bar{u}_l(k)e^{-i\omega_k t}$$

where $T_a\bar{u}_l(k) = \bar{u}_{l+1}(k) = e^{ika}\bar{u}_l(k)$.

In quantum mechanics, we know that ψ_k satisfies

$$H\psi_k = \varepsilon_k \psi_k$$

when $T_a H T_a^{-1} = H$ and $T_a \psi_k = \lambda_k \psi_k$.

$$-\omega_k^2 \bar{u}_o(k) = \omega_o^2 (e^{ika} + e^{-ika} - 2)\bar{u}_o(k) = -\omega_o^2 \left(2\sin\frac{ka}{2}\right)^2 \bar{u}_o(k)$$

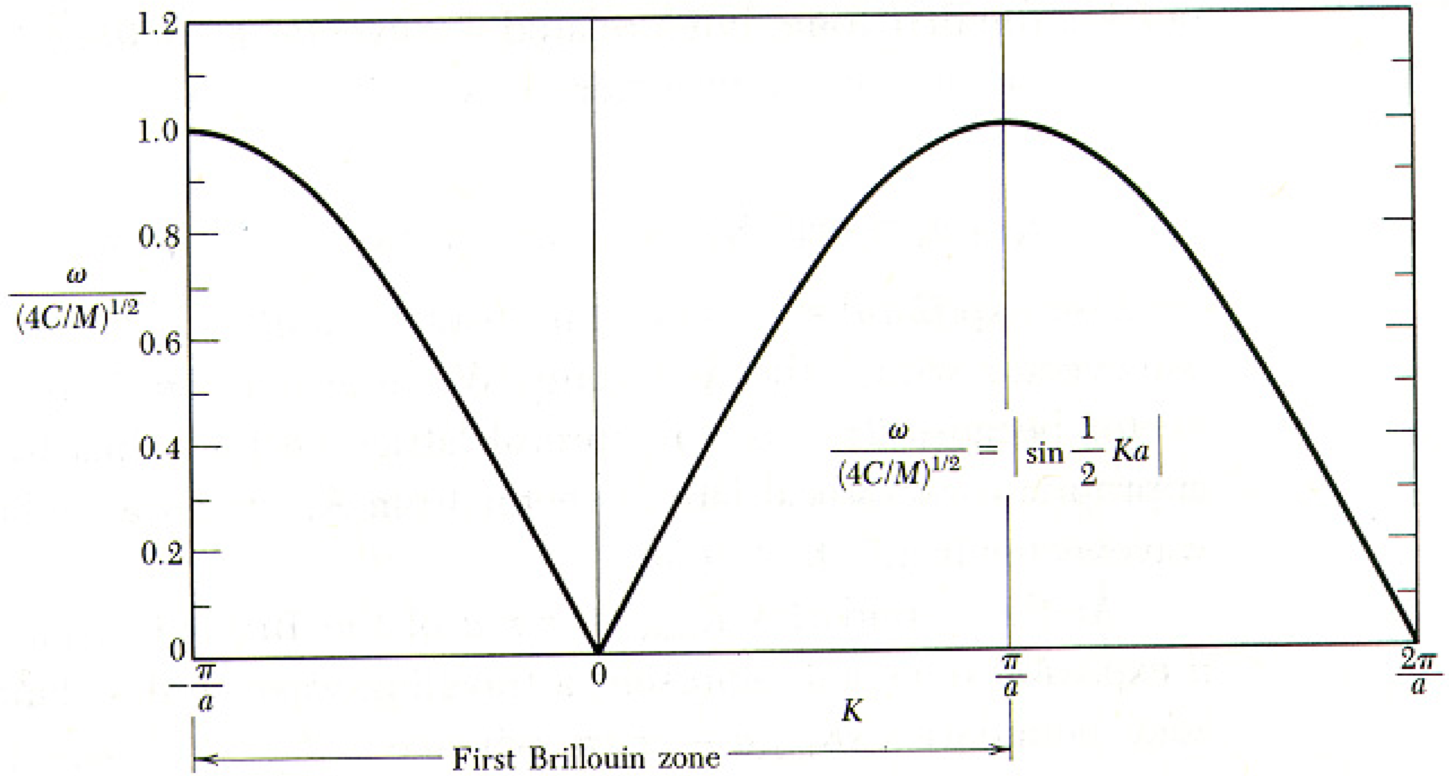
$$\omega_k = 2\omega_o \left|\sin\frac{ka}{2}\right|$$

Long wavelength limit:

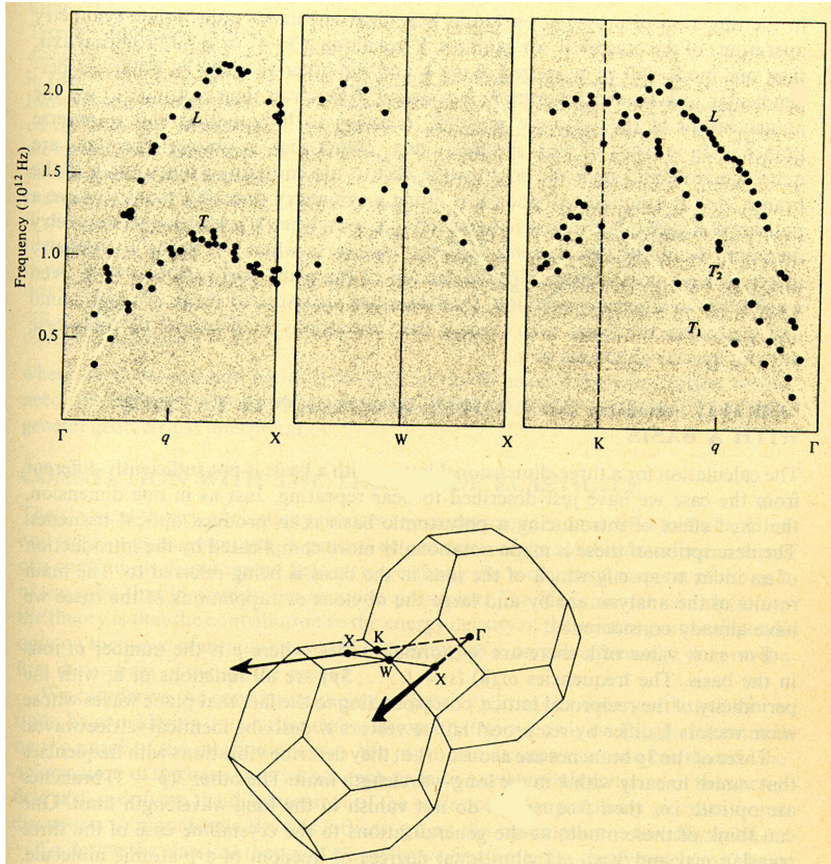
When $ka \ll 1$, we can approximate the dispersion as

$$\omega_k = \left(\frac{C}{m}\right)^{1/2} ka = v_s k$$

where $v_s = (Ca^2/m)^{1/2}$: sound velocity.

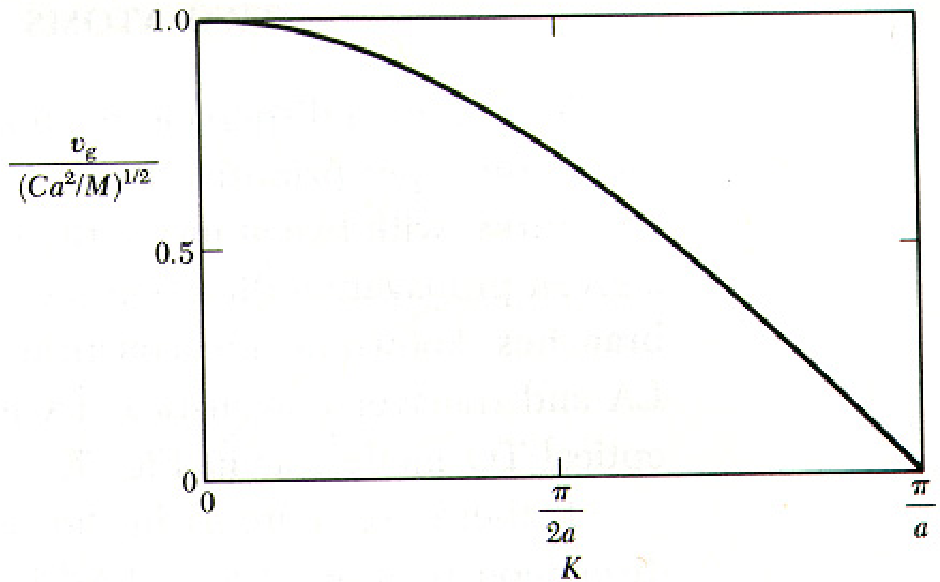

1.2
1.0
0.8
0.6
0.4
0.2
0
$\frac{\omega}{(4C/M)^{1/2}}$
$\frac{\omega}{(4C/M)^{1/2}} = \left|\sin \frac{1}{2} Ka\right|$
$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
$\frac{2\pi}{a}$
K
First Brillouin zone

Phonon dispersion curves for fcc Pb



Group velocity:

$$v_g = \frac{d\omega_k}{dk} = \left(\frac{Ca^2}{m}\right)^{1/2} \cos\frac{ka}{2}$$



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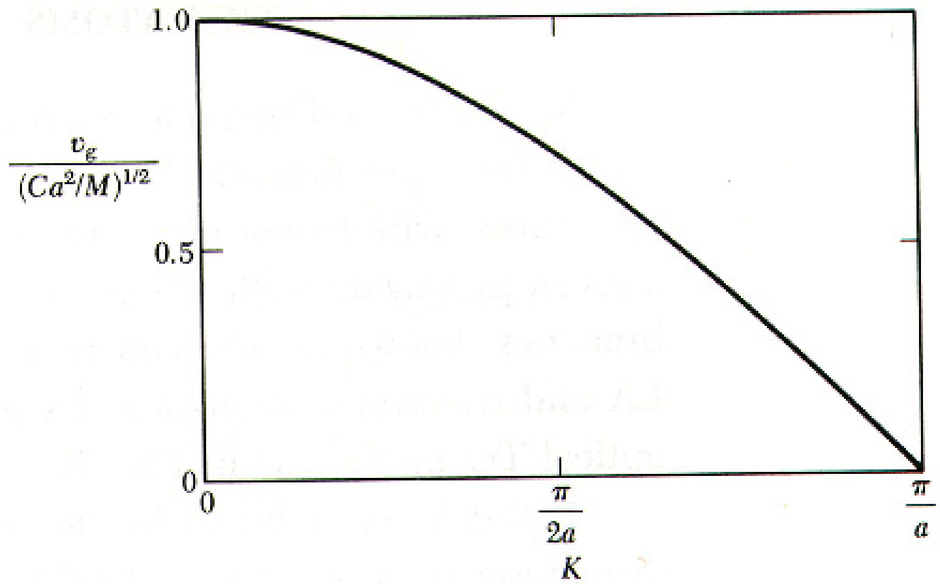

It is noted that $v_g = 0$ at $k = \frac{\pi}{a}$. Could you explain this result in terms of Bragg reflection at the zone boundary?

Two atoms per unit cell

When there are two atoms per unit cell, we can assign two variables u_1 and u_2 such that:

- $u_{1,l} \rightarrow$ atom 1 in the l-th unit cell
- $u_{2,l} \rightarrow$ atom 2 in the l-th unit cell

The equation of motion:

$$m_1 \ddot{u}_{1,l} = C(u_{2,l} + u_{2,l-1} - 2u_{1,l})$$

$$m_2 \ddot{u}_{2,l} = C(u_{1,l+1} + u_{1,l} - 2u_{2,l})$$

Looking for a normal mode solution with:

$$u_{1,l}(k,t) = u_1(k)e^{i(kal-\omega_k t)}$$

$$u_{2,l}(k,t) = u_2(k)e^{i(kal-\omega_k t)}$$

$$\begin{pmatrix} -\omega_k^2 m_1 & 0 \\ 0 & -\omega_k^2 m_2 \end{pmatrix} \begin{pmatrix} u_1(k) \\ u_2(k) \end{pmatrix} = \begin{pmatrix} -2C & C(1+e^{-ika}) \\ C(1+e^{ika}) & -2C \end{pmatrix} \begin{pmatrix} u_1(k) \\ u_2(k) \end{pmatrix}$$

$$m_1 m_2 \omega_k^4 - 2C(m_1 + m_2)\omega_k^2 + 2C^2(1 - \cos ka) = 0$$

$$\omega_k^2 = \frac{C(m_1 + m_2)}{m_1 m_2} \pm \sqrt{\left[\frac{C(m_1 + m_2)}{m_1 m_2}\right]^2 - 4C^2(1 - \cos ka)^2}$$

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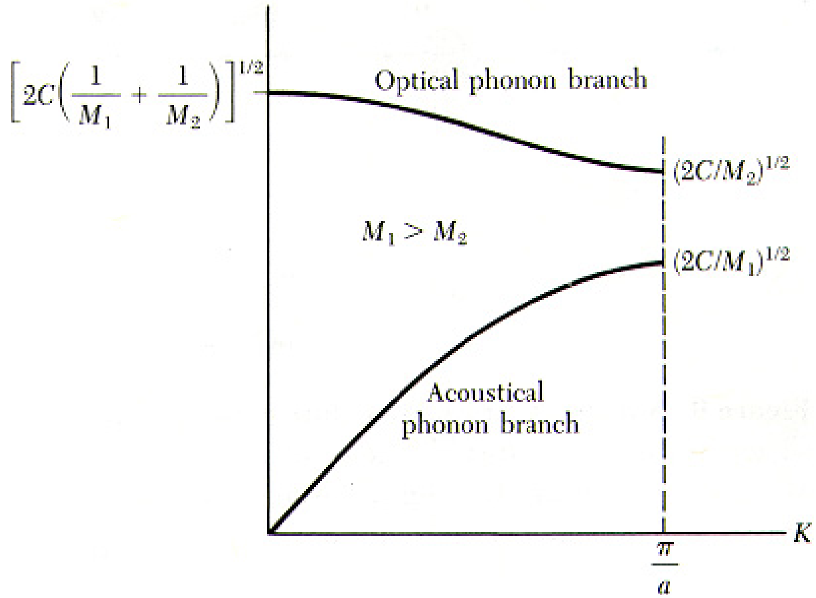
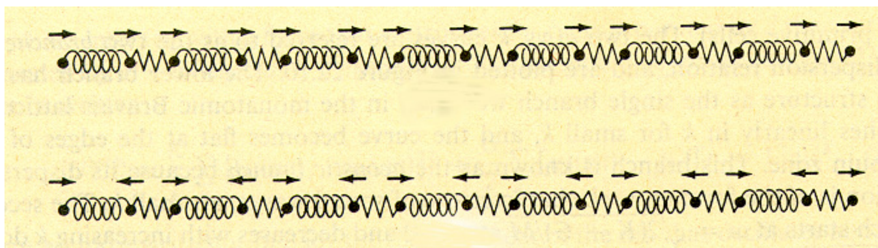
Long wavelength limit:

When $ka \ll 1$,

$$\omega_{a,k} = \sqrt{\frac{Ca^2}{2(m_1 + m_2)}}k \qquad \text{acoustic branch}$$

$$\omega_{o,k} = \sqrt{\frac{2C(m_1 + m_2)}{m_1 m_2}} \qquad \text{optic branch}$$


$\left[2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)\right]^{1/2}$
Optical phonon branch
$(2C/M_2)^{1/2}$
$M_1 > M_2$
$(2C/M_1)^{1/2}$
Acoustical phonon branch
K
$\frac{\pi}{a}$



Homework #2

(due: Tuesday, 16 March 2004)

Impurity Problem: What if there is an impurity in the system? Suppose that the mass of the impurity atom is *much heavier* or *lighter* than that of the lattice atoms, describe the motion of the impurity atom. What is the normal mode for the motion of such impurity atom?

Phonons — quantum of elastic waves

Instead of $\{\mathbf{x}_i, \mathbf{p}_i\}$, the amplitude $u_l(t)$ and its velocity $\dot{u}_l(t)$ should be considered as dynamic variables.

From the equation of motion for the k-th normal modes:

$$\ddot{\bar{u}}_o(k,t) = -\omega_k^2 \bar{u}_o(k,t),$$

the Hamiltonian for the elastic waves can be written by

$$\mathcal{H} = \sum_k \frac{\pi_k^2}{2m} + \frac{1}{2} m\omega_k^2 u_k^2$$

with the conjugate momentum $\pi_k = m\dot{u}_k$ and $u_k \equiv \bar{u}_o(k,t)$.

In quantum mechanics, the Hamiltonian for the harmonic oscillators can be described by

$$\mathcal{H} = \sum_k \hbar\omega_k (a_k^+ a_k + \frac{1}{2})$$

and the quantum states are

$$\mathcal{H}|\Psi(n_1, n_2, ..., n_N)\rangle = E_{n_1, n_2, ..., n_N}|\Psi(n_1, n_2, ..., n_N)\rangle$$

$$|\Psi(n_1, n_2, ..., n_N)\rangle = |n_{k=1}\rangle \otimes |n_{k=2}\rangle \otimes ... \otimes |n_{k=N}\rangle$$

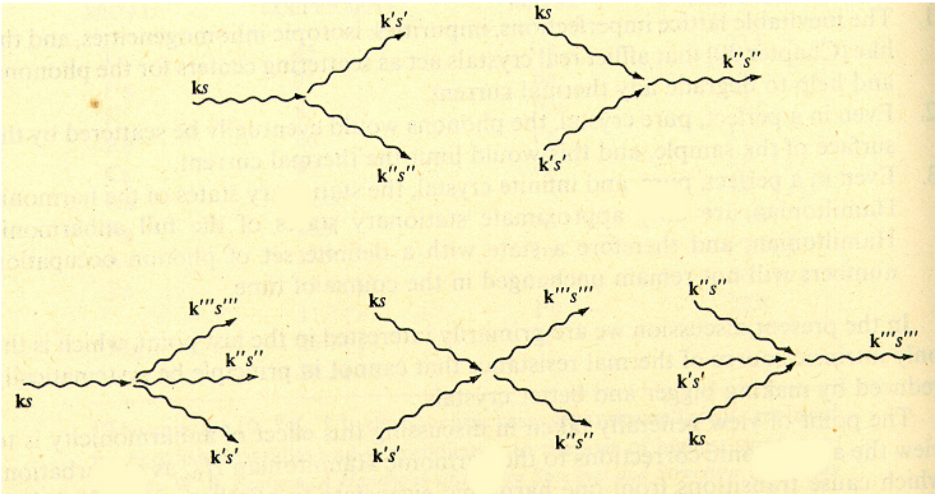
Anharmonicity

When there are anharmonic coupling between atoms, it appears as

$$V(u_1, u_2, ..., u_N) = ... + A_i(u_l - u_{l+1})^3 + ...$$

Which then induce the phonon-phonon scattering such as

$$\mathcal{H}_1 = ... + \sum_{k_1,k_2,k_3} V_{k_1,k_2,k_3} a^+_{k_1} a^+_{k_2} a_{k_3} + ...$$



Energy and momentum

Phonon energy:

$\varepsilon_k = \hbar\omega_k$ where the energy is determined by the factor

$$\omega_o = \sqrt{\frac{C}{m}}$$

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Question: Try to make an order-of-magnitude estimate of ω_o in solids. Here it is a key to make a reasonable guess on the scale of C, the effective force constant? Any good idea?

Often the force constant is give as a function of k. In some cases, it becomes *negative*, i.e., $C(k_o) < 0$ for some values of k_o. In other words, $\omega_o < 0$! What will happen if $\omega_o^2 < 0$, i.e., $\omega_k^2 < 0$?

If $\omega_k^2 < 0$, then $\omega_k \sim \pm i|\omega_k|$.

$$\psi_k \sim e^{-i\omega_k t} = e^{\pm|\omega_k|t}$$

: **Unstable** $\longrightarrow$ lattice distortion for the mode **k**.

Phonon momentum:

The crystal momentum of the k-th normal mode

$$P_k = m\frac{d}{dt}\sum_l u_l(k,t) = m\frac{du_o(k,t)}{dt}\sum_{l=0}^{N-1} e^{ikal}$$

$$P_k = m\frac{du_o(k,t)}{dt}\frac{1-e^{ikaN}}{1-e^{ika}}$$

(i) $k \neq 0$ and $k \neq G_n = (2\pi/a)n$

$$P_k = 0$$

Why? Because relative coordinates do not carry the total momentum.

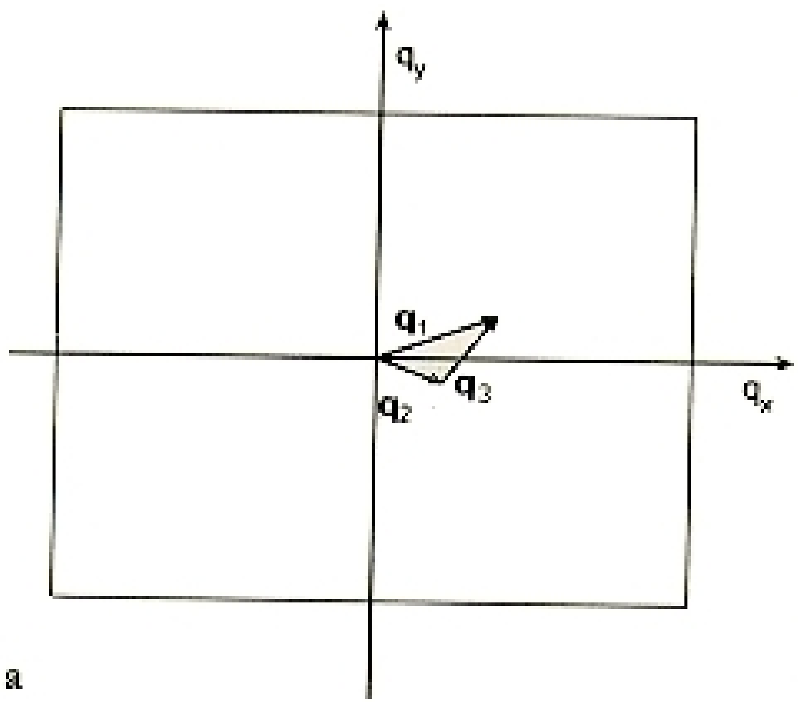
(ii) $k = 0$ or G_n

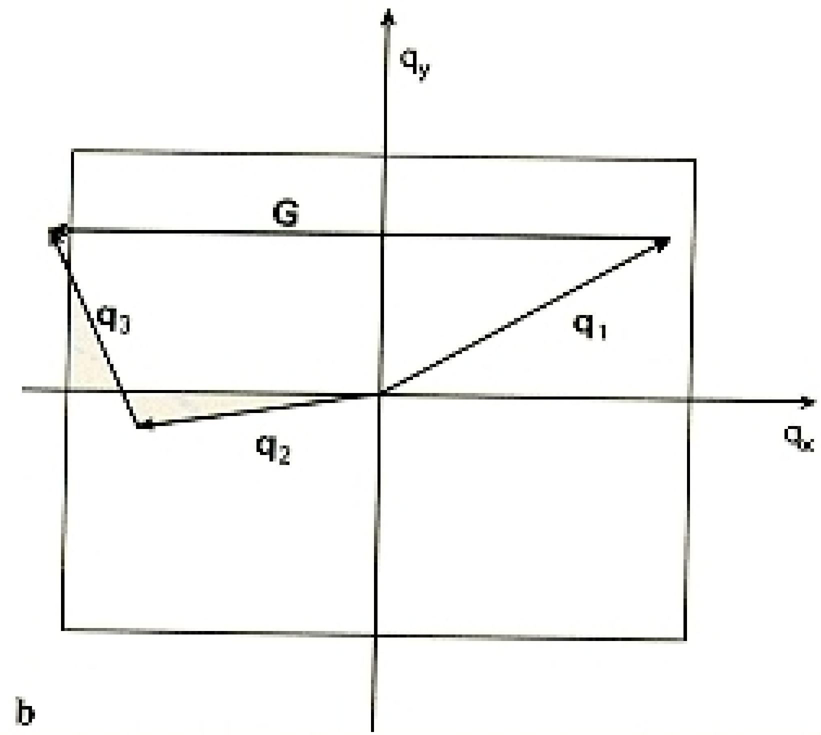
$$P_k = Nm\frac{du_o(k,t)}{dt}$$

(iii) Two crystal momenta k and $k + G_n$ are equivalent!

Umklapp Process: phonon scattering

$$\mathbf{k} + \mathbf{G} = \mathbf{k}' + \mathbf{G}'$$





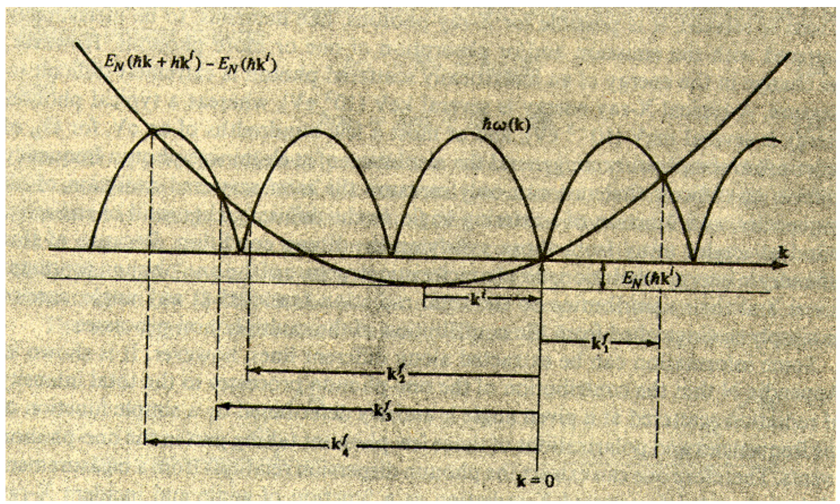
Electron-phonon or neutron-phonon scattering:

- momentum conservation:

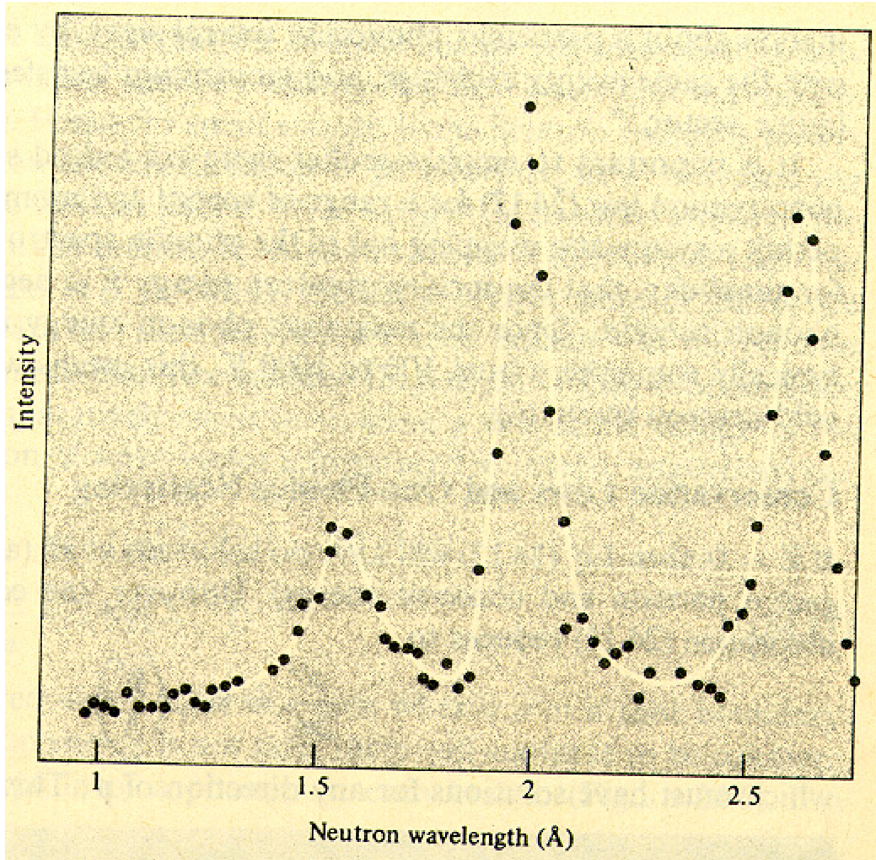
$$\mathbf{k} = \mathbf{k}' + \mathbf{K} + \mathbf{G}$$

- energy conservation:

$$\frac{k^2}{2m} = \frac{{k'}^2}{2m} \pm \omega_{\mathbf{K}}$$



Neutron Scattering for Cu



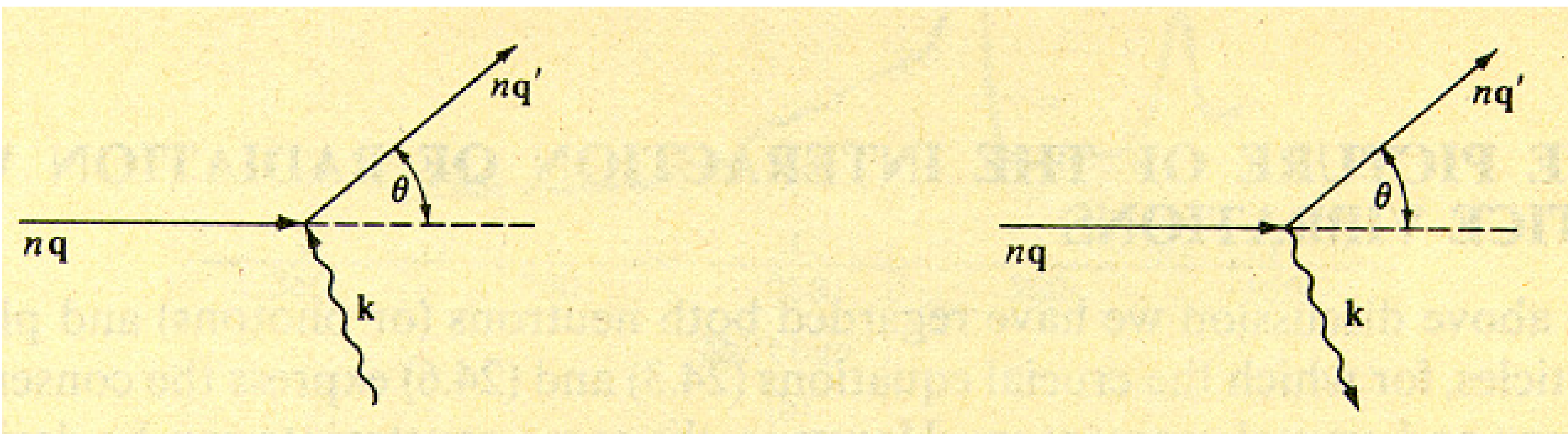
phonon-photon scattering:

- momentum conservation:

$$\mathbf{k} = \mathbf{k}' + \mathbf{K} + \mathbf{G}$$

- energy conservation:

$$kc = k'c \pm \omega_{\mathbf{K}}$$



Characteristic structure of Brillouin spectrum