ECE215A/Materials206A Winter 2008
Prof. Brown/ECE Dept/UCSB

Homework 4 Solutions (first four problems only, for Quiz#1)

(1) Energy of lattice wave

a) Monotomic linear lattice, mass m, spacing a, nearest neighbor interaction (spring constant) C. Consider longitudinal wave: $\Delta r_s \equiv u_s = u\cos(\omega t - ska)$. The total energy of the wave is the sum over all atoms of the energy of each atom. From mechanics, we know that the instantaneous energy of a harmonic oscillator has a kinetic energy term and a potential energy term. The potential term depends only on the force constant and the displacement of the oscillator from equilibrium. Thus the linear lattice can be repeated as a series of springs with masses (atoms) attached.

The potential energy associated with the *sth* spring is

$$PE_s \to \frac{1}{2}C\left(u_{s+1}-u_s\right)^2 = \frac{1}{2}C\left(u_s-u_{s+1}\right)^2$$

The kinetic energy associated with the *sth* mass is

$$KE_s \to \frac{1}{2}M\upsilon_s{}^2 = \frac{1}{2}M\left(\frac{du_s}{dt}\right)^2$$

By summing over all atoms we get the total energy:

$$U(t) = \frac{1}{2}M\sum_s\left(\frac{du_s}{dt}\right)^2 + \frac{1}{2}C\sum_s\left(u_s-u_{s+1}\right)^2 \quad \text{(instantaneous)}$$

b) For longitudinal wave $u_s = u\cos(\omega t - ska)$, we have $\frac{du_s}{dt} = -\omega u\sin(\omega t - ska)$ and

$$U(t) = \sum_S\left\{\frac{1}{2}M\omega^2u^2\sin^2(\omega t - ska) + \frac{1}{2}Cu^2\left[\cos(\omega t - ska) - \cos(\omega t - ska - ka)\right]^2\right\}$$

The last term has the form $\left[\cos(\alpha-\beta)-\cos\alpha\right]^2$ *with* $\alpha = \omega t - ska,\ \ \beta = ka$. So we can use the trigonometric identity $\cos(\alpha-\beta) = \cos\alpha\cos\beta + \sin\alpha\sin\beta$ to write

$$U(t) = \sum_S\left[\frac{1}{2}M\omega^2u^2\sin^2\alpha + \frac{1}{2}Cu^2\left(\cos\alpha(\cos\beta-1)+\sin\alpha\sin\beta\right)\right]^2$$

$$= \sum_s \left[\frac{1}{2} M\omega^2 u^2\right] \sin^2\alpha + \frac{1}{2} Cu^2 \left(\cos^2\alpha(\cos\beta-1)^2 + 2\cos\alpha(\cos\beta-1)\sin\alpha\sin\beta + \sin^2\alpha\sin^2\beta\right)$$

To get the average, we integrate over the period of wave, τ

$$\bar{U} = \int_o^\tau U(t)dt \qquad \tau = \frac{2\pi}{\omega} = \frac{1}{f}$$

$$\int_o^\tau \sin^2\alpha dt = \frac{\tau}{2}; \int_2^\tau \cos^2\alpha dt = \frac{\tau}{2}; \int_o^\tau 2\sin\alpha\cos\alpha dt = \int_o^\tau \sin 2\alpha dt = 0$$

So,

$$\bar{U} = \frac{1}{2} M\omega^2 u^2 \frac{\tau/2}{\tau} + \frac{1}{2} Cu^2 \left[\frac{\tau/2}{\tau}(\cos\beta-1)^2 + \frac{\tau/2}{\tau}\sin^2\beta\right]$$

$$\bar{U} = \frac{1}{4} M\omega^2 u^2 + \frac{1}{4} Cu^2 \left[\cos^2\beta - 2\cos\beta + 1 + \sin^2\beta\right] = \frac{1}{4} M\omega^2 u^2 + \frac{1}{2} Cu^2 \left[1-\cos\beta\right]$$

For linear monatomic lattice we have $\omega^2 = \frac{2C}{M}(1-\cos\beta)$. So finally

$$\bar{U} = \frac{1}{4} M\omega^2 u^2 + \frac{1}{4} M\omega^2 u^2 = \frac{1}{2} M\omega^2 u^2$$

(2) Continuum wave equation

For nearest neighbor-interaction, the force on a given atom (labeled by s) is given by $F = C(\Delta r_{s+1} - \Delta r_s) - C(\Delta r_s - \Delta r_{s-1})$ where we also assume spring constants are equal to C. For long wavelength lattice waves, we know Δr_{S+1} will nearly in phase and nearly equal amplitude to Δr_S. Also, Δr_{S-1} will be nearly in phase and equal amplitude to Δr_S. So we can Taylor expand Δr_{S+1} and Δr_{S-1}, thinking of each as a function of the atom average position r. Thus we can write

$$\Delta r_{s+1} \equiv \Delta r(r_{s+1}); \quad \Delta r_s \equiv \Delta r(r_s); \quad \Delta r_{s-1} \equiv \Delta r(r_{s-1}).$$

And by Taylor expansion (to 2nd order)

$$\Delta r_{s+1} \equiv \Delta r(r_{s+1}) = \Delta r(r_s) + \left.\frac{d\Delta r}{dr}\right|_{r=r_s} (r_{s+1} - r_s) + \frac{1}{2}\left.\frac{d^2\Delta r}{dr^2}\right|_{r=r_s} (r_{s+1} - r_s)^2$$

But for uniform lattice constant d, $r_{S+1} - r_S = a$. And for lattice oriented along x axis, $r \to x$ (without loss of generality). Thus,

$$\Delta r_{s+1} = \Delta r_s + \left.\frac{d\Delta r}{dx}\right|_{x=r_s}(a) + \frac{1}{2}\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s}(a)^2 + \ldots \qquad *$$

Similarly, we can deduce

$$\Delta r_{s-1} \equiv \Delta r\left(r_{s-1}\right) = \Delta r_s + \left.\frac{d\Delta r}{dx}\right|_{x=r_s}(-a) + \frac{1}{2}\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s}(-a)^2 + \ldots \qquad **$$

So, $$F = C\left(\Delta r_{s+1} - \Delta r_s\right) + C\left(\Delta r_{s-1} - \Delta r_s\right)$$

and we substitute in * and **

$$= C\left(\left.\frac{d\Delta r}{dx}\right|_{x=r_s}(a) + \frac{1}{2}\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s}(a)^2 + \left.\frac{d\Delta r}{dx}\right|_{x=r_s}(-a) + \frac{1}{2}\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s}(-a)^2\right)$$

$$= C\left(\frac{1}{2}\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s}(a)^2 + \frac{1}{2}\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s}(-a)^2\right) = Ca^2\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s}$$

So using Newton's law $F = \frac{md^2\Delta r_s}{dt^2}$, we get the wave equation

$$\frac{d^2\Delta r_s}{dt^2} = \frac{ca^2}{m}\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s} \equiv \upsilon^2\frac{d^2\Delta r_s}{dx^2}$$

where $$\left.\frac{d^2\Delta r}{dx^2}\right|_{x=r_s} \equiv \frac{d^2\Delta r_s}{dx^2}$$

(3) Lattice waves for crystal having basis of two different atoms

At $k = \pi/a$ the solutions for the two branches are $\omega^2 = 2C/M_1$ (acoustical) and $\omega^2 = 2C/M_2$ (optical) where it is assumed $M_1 > M_2$. We substitute these back into the connection equations:

$$\left(2C-M_1\omega^2\right)u - C\left[1+\exp(-jka)\right]v = 0 \quad (a)$$

$$-C\left[1+\exp(jka)\right]u + \left[2C-M_2\omega^2\right]v = 0 \quad (b)$$

$$(a)\ leads\ to\ \ \frac{u}{v} = \frac{C\left[1+\exp(-jka)\right]}{2C-M_1\omega^2} \qquad (c)$$

$$(b)\ leads\ to\ \ \frac{u}{v} = \frac{2C-M_2\omega^2}{C\left[1+\exp(jka)\right]} \qquad (d)$$

At ka = π, exp(-jka) = exp(jka) = -1. So for acoustical branch, ω^2=2C/M_1,

$$(c) \Rightarrow \frac{u}{v} = \frac{0}{0} \qquad (d) \Rightarrow \frac{u}{v} = \frac{2C\left(1-\frac{M_2}{M_1}\right)}{0} \to \infty$$

u/v →∞ means that u is arbitrarily non-zero for v = 0. This means that all the motion is in u (main atom). For optical branch, ω^2=2C/M_2,

$$(c) \Rightarrow \frac{u}{v} = \frac{0}{2C\left(1-\frac{M_1}{M_2}\right)} = 0 \quad (d) \Rightarrow \frac{u}{v} = \frac{0}{0}(undefined)$$

u/v → 0 means that v is arbitrary non-zero for u = 0 , so that all the motion in v (satellite atom).

(4) Diatomic Chain

From assumptions of nearest neighbor-interaction, equal masses but unequal spring constants, C_1 and C_2 derived in lecture, the force equations on the atoms in the ***sth*** unit cell

$$m\frac{d^2\Delta r_1}{dt^2} = C_1\left(\Delta r_{2,s}-\Delta r_{1,s}\right) - C_2\left(\Delta r_{1,s}-\Delta r_{2,s-1}\right)$$

$$m\frac{d^2\Delta r_{2,s}}{dt^2} = C_2\left(\Delta r_{1,s+1}-\Delta r_{2,s}\right) - C_1\left(\Delta r_{2,s}-\Delta r_{1,s}\right)$$

Assuming the discrete wave solutions

$$\Delta r_{1,s} = \Delta r_1 e^{j(ksa-\omega t)}, \quad \Delta r_{2,s} = \Delta r_2 e^{j(ksa-\omega t)}$$

We found the coupled algebraic equations for the amplitudes Δr_1 *and* Δr_2

$$\begin{pmatrix} m\omega^2 - C_1 - C_2 & C_1 + C_2 e^{-jka} \\ C_1 + C_2 e^{jka} & m\omega^2 - C_1 - C_2 \end{pmatrix} \begin{pmatrix} \Delta r_1 \\ \Delta r_2 \end{pmatrix} = 0$$

A non-trivial solution for Δr_1 and Δr_2 requires that the 2x2 matrix be non-invertible $\Rightarrow$ det{ } = 0

$$\Rightarrow \quad m^2\omega^4 + (c_1 + c_2)^2 - 2m(c_1 + c_2)\omega^2 - \left(c_1^2 + c_2^2 + 2c_1c_2\cos ka\right) = 0$$

$$\omega^2 = \frac{c_1 + c_2}{m} \pm \frac{1}{m}\sqrt{(c_1 + c_2)^2 - 2c_1c_2(1 - \cos ka)} \begin{cases} + & optical\ \ branch \\ - & acoustical\ \ branch \end{cases}$$

(a) At ka = 0

$$\omega^2 = \frac{c_1 + c_2}{m} \pm \frac{c_1 + c_2}{m} = 0 \quad (-\ \ sign, acoustical\ \ branch)$$

$$\omega^2 = \frac{2(c_1 + c_2)}{m} = \frac{22c}{m} \quad for\ \ c_2 = 10 \cdot c_1 \equiv 10c$$

$$or\ \ \omega = \sqrt{\frac{22c}{m}} \quad (+\ \ sign, optical\ \ branch)$$

(b) At ka = π, cos ka = -1

$$\omega^2 = \frac{c_1 + c_2}{m} \pm \frac{1}{m}\sqrt{(c_1 + c_2)^2 - 4c_1c_2}$$

$$or\ \ \omega = \sqrt{\frac{c_1 + c_2}{m} \pm \frac{1}{m}\sqrt{(c_2 - c_1)^2}} = \sqrt{\frac{2c_1}{m}} \equiv \sqrt{\frac{2c}{m}} \quad (-sign, acoustical\ \ branch)$$

$$\omega = \sqrt{\frac{2c_2}{m}} \equiv \sqrt{\frac{20c}{m}} \quad (+sign, optical\ \ branch)$$