ECE215A/MAT206A, Winter 2009
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HW 4 Solutions

1. Monotomic linear lattice, mass m, spacing a, nearest neighbor interaction (spring constant) C.

   a) 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 $\dfrac{du_s}{dt} = -\omega u\sin(\omega t - ska)$ 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

$$\cos(\alpha - \beta) = \cos\alpha\cos\beta + \sin\alpha\sin\beta$$

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

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

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

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

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

So,

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

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

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

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

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

3. 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

$\Rightarrow$.
$$m^2\omega^4 + \left(C_1 + C_2\right)^2 - 2m\left(C_1 + C_2\right)\omega^2 - \left(C_1^2 + C_2^2 + 2C_1C_2\cos ka\right) = 0$$

$$\omega^2 = \frac{C_1 + C_2}{m} \pm \frac{1}{m}\sqrt{\left(C_1 + C_2\right)^2 - 2C_1C_2\left(1 - \cos ka\right)} \begin{cases} + \ \ optical \ \ branch \\ - \ \ acoustical \ \ branch \end{cases}$$

(a) At ka = 0

$$\omega^2 = \frac{C_1 + C_2}{m} \pm \frac{C_1 + C_2}{m} = 0 \quad \left(- \ \ sign, acoustical \ \ branch\right)$$

$$\omega^2 = \frac{2\left(C_1 + C_2\right)}{m} = \frac{22C}{m} \quad for \ C_2 = 10 \cdot C_1 \equiv 10C$$

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

(b) At ka = π, cos ka = -1

$$\omega^2 = \frac{C_1 + C_2}{m} \pm \frac{1}{m}\sqrt{\left(C_1 + C_2\right)^2 - 4C_1C_2}$$

$$or \ \omega = \sqrt{\frac{C_1 + C_2}{m} \pm \frac{1}{m}\sqrt{\left(C_2 - C_1\right)^2}} = \sqrt{\frac{2C_1}{m}} \equiv \sqrt{\frac{2C}{m}} \quad \left(-sign, \ \ acoustical \ \ branch\right)$$

$$\omega = \sqrt{\frac{2C_2}{m}} \equiv \sqrt{\frac{20C}{m}} \quad \left(+sign, \ \ optical \ \ branch\right)$$

4. Acoustical phonons in a two-dim lattice

(a) Excluding zero point term, and assuming the two acoustic waves have the same velocity,

$$\left\langle U \right\rangle = 2\int_0^{\omega_D} < n_k > \hbar\omega_k D\left(\omega\right) = 2\int_0^{\omega_D} \frac{\hbar\omega_k D\left(\omega\right) d\omega}{e^{\hbar\omega/k_B T} - 1}$$

2 polarizations, one longitudinal, one transverse

For each polarization $D\left(\omega\right) = \frac{dN\left(k\right)}{dk}\frac{dk}{d\omega}d\omega = \frac{d}{dk}\left[\left(\frac{L}{2\pi}\right)^2 \pi k^2\right]\frac{d\omega}{\mathrm{v}} = \frac{A}{2\pi}\frac{\omega}{\mathrm{v}^2}d\omega$

where we have $\omega = k\mathrm{v} \rightarrow velocity \ of \ sound$ and ω_D is defined by

$N_C = \int_0^{\omega_D} D(\omega) d\omega = \int_0^{\omega_D} \frac{A\omega}{2\pi v^2} d\omega = \frac{A\omega_D{}^2}{4\pi v^2}$. Thus, $\langle U \rangle = \frac{A}{\pi v^2} \int_0^{\omega_D} \frac{\hbar\omega^2 d\omega}{e^{\hbar\omega/k_BT} - 1}$.

Define $x = \hbar\omega/k_BT \Rightarrow \langle U \rangle = \frac{A(k_BT)^3}{\pi v^2 \hbar^2} \int_0^{x_D} \frac{x^2 dx}{e^x - 1}, x_D \equiv \frac{\hbar\omega_D}{k_BT}$.

(b) In the limit of low temperature, $x_D \equiv \hbar\omega_D/k_BT \to \infty$. And using the fact $\int_0^{\infty} \frac{x^2 dx}{e^x - 1} \approx 2.40$, we find $\langle U \rangle \cong \frac{(2.40) A (k_BT)^3}{\pi v^2 \hbar^2} = \frac{(2.40)(4N_C)(k_BT)^3}{\omega_D{}^2 \hbar^2} = \frac{9.6 N_C (k_BT)^3}{\omega_D{}^2 \hbar^2}$

$$C_V \approx \frac{d\langle U \rangle}{dT} = \frac{7.20 \cdot A \cdot k_B{}^3 T^2}{\pi v^2 \hbar^2}$$

(c) In the limit high temperature $\frac{1}{e^x - 1} \approx \frac{1}{x}$

So, $\langle U \rangle \approx \frac{A(k_BT)^3}{\pi v^2 \hbar^2} \int_0^{x_D} x dx = \frac{A(k_BT)^3}{\pi v^2 \hbar^2} \frac{x_D{}^2}{2} = \frac{A(k_BT)\omega_D{}^2}{2\pi v^2}$. But from definition of ω_D in two dim in (a), we have $\omega_D{}^2 = \frac{4\pi N_C v^2}{A} \Rightarrow \langle U \rangle = 2N_C k_B T$ and $C_v \approx \frac{d\langle U \rangle}{dT} = 2N_C k_B$ (no surprise; this is just 2/3 of Dulong-Petit law in 3 dim).

6. A 3-dim lattice with four atoms per primitive cell

(a) The number of acoustical lattice waves is 3. The number of optical lattice waves is 9 . Of all the optical waves, 3 are longitudinal and 6 are transverse.

(b) From Chapter 4, the total energy of acoustical phonons according to the Debye model is

$\langle U_{tot} \rangle = \sum_{p=1}^{3} \frac{\hbar V}{2\pi^2 v_{s,p}^3} \left(\frac{k_BT}{\hbar}\right)^4 \int_0^{x_{D,p}} \frac{x^3 dx}{e^x - 1} = \sum_{p=1}^{3} 3N_C k_B T \left(\frac{k_BT}{\hbar\omega_D}\right)^3 \int_0^{x_{D,p}} \frac{x^3 dx}{e^x - 1}$ subject to the constraint $\omega_{D,p}{}^3 = \frac{6\pi^2 v_{s,p}{}^3 N_C}{V}$ where N_C is the number of unit cells, V is the volume of the crystal sample, and $v_{s,p}$ is the speed of sound for the pth wave type (i.e., polarization). In the limit of low temperature, $x_D = T_D/T$ gets very large so we can approximate $\int_0^{\infty} \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15}$. And we get

$<U_{tot}> = \sum_{p=1}^{3} \frac{\pi^4}{5} N_C k_B T \left(\frac{k_BT}{\hbar\omega_D}\right)^3$. The heat capacity is $C_V \approx d<U_{tot}>/dT = = \sum_{p=1}^{3} \frac{4\pi^4}{5} N_C k_B \left(\frac{k_BT}{\hbar\omega_D}\right)^3$

(c) The Debye frequency is given by $\omega_{D,p}{}^3 = \dfrac{6\pi^2 v_{s,p}{}^3 N_C}{V}$ where N_C/V is the inverse volume of a primitive cell. Substitution of the sample parameters leads to $\omega_D = 6.3\text{x}10^{13}$ s^{-1}. Application of the relation $(k_B T_D / \hbar)^3 = \omega_{D,p}{}^3$ then yields T_D = 479 K.

(d) At 77 K we have $T < T_D$ so the low-temperature expression in (b) should be a good approximation, and the sum over polarizations p leads to a factor of 3 since all acoustic waves are assume to have the same speed of sound, 5000 m/s. This leads to the result $C_V{}' \equiv \dfrac{C_V}{V} \approx \dfrac{12\pi^4}{5}\dfrac{N_C}{V}\cdot k_B\left(\dfrac{T}{T_D}\right)^3$ = 4.5x10^5 J/K.

(e) The classical (Dulong-Petit) heat capacity is given by $3N_c k_B$, and the specific heat capacity by $3(N_C/V)k_B$ = 1.38x10^6 J/K – 3 times larger than the 77-K value.