Phy 240B HW 2 Solutions

1. (i) $\omega = c\tilde{\nu} = 2\pi \cdot 3\times 10^{10}\,\text{cm/s} \cdot 1330\,\text{cm}^{-1} = 2.51\times 10^{14}\,\text{s}^{-1}$

$E = \hbar\omega = 165\,\text{meV}$. $\lambda = \infty$ since $q = 0$

(ii) $x_0 = \sqrt{\frac{\hbar}{M\omega}}$

$M = \frac{0.012\,\text{kg/mol}}{N_A} = 1.99\times 10^{-26}\,\text{kg}$

$\therefore x_0 = \sqrt{\frac{1.055\times 10^{-34}\,\text{Js}}{1.99\times 10^{-26}\,\text{kg}\cdot\omega}} \simeq 0.046\,\text{Å}$. ← Length of oscillation.

$p_0 = \sqrt{\hbar M\omega} = \sqrt{1.055\times 10^{-27}\,\text{erg s}\cdot 1.99\times 10^{-23}\,\text{g}\cdot\omega} = 2.3\times 10^{-18}\,\text{g cm/s}$

In a.u., $p_0 = \frac{1}{x_0} = \left(\frac{0.046\,\text{Å}}{0.529\,\text{Å}/a_B}\right)^{-1} = 11.5$ a.u.

2. For nonlinear molecules, such as the triangular Z_3, there are $3N-6$ vibrations. N = # of atoms = 3 in our case, so there are 3 vibrations. One set of normal modes of vibration may be

The latter 2 have the same frequency; linear combinations of the two can also be normal modes.

3. (i) Use eq 13.120 in Marder (p. 334):

$$2W = \sum_{k\nu} \frac{1}{N} \frac{\hbar^2 (\vec{E}_{k\nu} \cdot \vec{q})^2}{2M\hbar\omega_{k\nu}}$$

$$\to \frac{V}{8\pi^3} \int \frac{d\vec{k}}{N} \frac{\hbar^2 q^2}{2M\hbar\omega}$$

$$= \frac{V}{8\pi^3} \frac{1}{N} \int \frac{4\pi k^2 dk \cdot \hbar^2 q^2}{2M\hbar\omega}$$

Debye model:

$$\frac{N}{V} = \frac{\omega_D^3}{6\pi^2 c^3} = \frac{k_D^3}{6\pi^2} \qquad (\omega_D \equiv \text{Debye freq.})$$

So

$$2W = \frac{1}{2\pi^2} \frac{6\pi^2}{k_D^3} \int_0^{k_D} \frac{k^2 dk \cdot \hbar^2 q^2}{2M\hbar c k}$$

$$= \frac{3}{2} \frac{1}{k_D^3} \frac{1}{2} k_D^2 \frac{\hbar^2 q^2}{2M\hbar c}$$

$$= \frac{3}{4} \frac{\hbar^2 q^2}{M\hbar c k_D}$$

(ii) In 2D at $T=0$,

$$2W \sim \int_0^{k_D} \frac{d\vec{k}}{k} = \int_0^{k_D} dk,$$

so the DW factor does not diverge.

At $T > 0$, however, the $2n_{k\nu}+1$ factor in eq. 13.119 will go like $1/k$ at low enough k, in which case the DW factor indeed diverges.

In 1D, it diverges at any T.

(iii) We need to take into account anharmonic contributions & long-range order.

4.

$$\cdots \quad M_1 \quad M_2 \quad \cdots$$

$C_1 \quad C_2 \quad C_1$

$u_2((n-1)a) \quad u_1(na) \quad u_2(na) \quad u_1((n+1)a)$

(i) The displacements of atoms is denoted as such:

$$u_i = \alpha_i e^{i(kx-\omega t)}, \quad i = 1, 2.$$

Newton's law:

$$\begin{cases} M_1 \ddot{u}_1(na) = C_2[u_2(na) - u_1(na)] - C_1[u_1(na) - u_2((n-1)a)] \\ M_2 \ddot{u}_2(na) = C_1[u_1((n+1)a) - u_2(na)] - C_2[u_2(na) - u_1(na)] \end{cases}$$

$$\begin{cases} -M_1\omega^2\alpha_1 = C_2(\alpha_2 - \alpha_1) - C_1(\alpha_1 - \alpha_2 e^{-ika}) \\ -M_2\omega^2\alpha_2 = C_1(\alpha_1 e^{ika} - \alpha_2) - C_2(\alpha_2 - \alpha_1) \end{cases}$$

$$\begin{vmatrix} M_1\omega^2 - C_1 - C_2 & C_1 e^{-ika} + C_2 \\ C_1 e^{ika} + C_2 & M_2\omega^2 - C_1 - C_2 \end{vmatrix} = 0$$

$\vdots$

$$\therefore \omega^2 = \frac{(M_1+M_2)(C_1+C_2) \pm \sqrt{(M_1+M_2)^2(C_1+C_2)^2 - 8M_1M_2C_1C_2(1-\cos ka)}}{2M_1M_2}$$

If we let $M_1 = M_2$,

$$\omega^2 = \frac{C_1+C_2}{M} \pm \frac{\sqrt{(C_1+C_2)^2 - 2C_1C_2(1-\cos ka)}}{M}$$

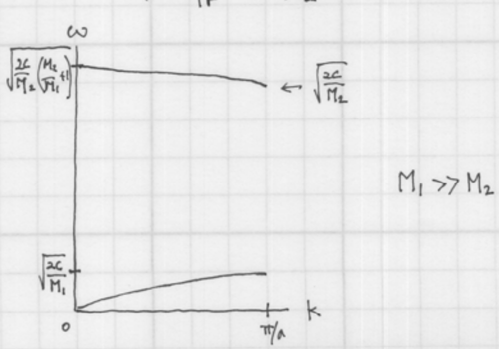
$$= \frac{C_1+C_2}{M} \pm \frac{\sqrt{C_1^2+C_2^2 + 2\cos ka \cdot C_1C_2}}{M} \quad \checkmark$$

If we let $C_1 = C_2$,

$$\omega^2 = \frac{C(M_1+M_2)}{M_1M_2} \pm \frac{C\sqrt{M_1^2+M_2^2+2M_1M_2\cos ka}}{M_1M_2} \quad \checkmark$$

(ii) Using the last expression of part (i),

$$\omega^2 = \begin{cases} 0,\ 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) & ; \quad k = 0 \\ \frac{2C}{M_1},\ \frac{2C}{M_2} & ; \quad k = \frac{\pi}{a} \end{cases}$$



Sound velocity:

$$v = \frac{\omega}{k} = \frac{1}{k}\sqrt{\frac{C(M_1+M_2) - C\sqrt{M_1^2+M_2^2+2M_1M_2\cos ka}}{M_1M_2}}$$

(iii) The lower branch is the acoustic branch, characteristic of sound waves at small k ($\omega \propto k$); atoms in a unit cell are in phase with one another. The upper branch is the optical branch; the lighter the lighter atom, the higher is its frequency. When $M_1 \gg M_2$, the optical branch is virtually linear.