Ph135 - Problem Set 4

November 9, 2018

Problem 1

(a) Denote by $x_{A,n}$ ($x_{B,n}$) the displacement of the n-th atom A (B) from the equilibrium. The potential energy takes the form

$$V = \frac{k}{2}\sum_n \left[(x_{B,n} - x_{A,n})^2 + (x_{A,n+1} - x_{B,n})^2\right]. \tag{1}$$

After a Fourier transformation

$$\begin{aligned} x_{A,n} &= \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dq e^{iqna} x_{A,q}, \\ x_{B,n} &= \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dq e^{iqna} x_{B,q}, \end{aligned} \tag{2}$$

the potential energy takes the form

$$V = \frac{k}{2}\sum_n \left|\frac{a}{2\pi}\int dq e^{iqna}(x_{B,q} - x_{A,q})\right|^2 + \sum_n \left|\frac{a}{2\pi}\int dq e^{iqna}(x_{A,q}e^{iqa} - x_{B,q})\right|^2 \tag{3}$$

Since

$$\begin{aligned} \left|\frac{a}{2\pi}\int dq e^{iqna}(x_{B,q} - x_{A,q})\right|^2 &= \left(\frac{a}{2\pi}\right)^2 \int dq \int dq' \sum_n e^{i(q-q')na}(x_{A,q} - x_{B,q})(x_{A,q'} - x_{B,q'})^* \\ &= \left(\frac{a}{2\pi}\right)^2 \int dq \int dq' \frac{2\pi}{a}\delta(q-q')(x_{A,q} - x_{B,q})(x_{A,q'} - x_{B,q'})^* \\ &= \frac{a}{2\pi}\int dq |x_{A,q} - x_{B,q}|^2, \end{aligned} \tag{4}$$

and

$$\begin{aligned} \left|\frac{a}{2\pi}\int dq e^{iqna}(x_{A,q}e^{iqa} - x_{B,q})\right|^2 &= \left(\frac{a}{2\pi}\right)^2 \int dq \int dq' \sum_n e^{i(q-q')na}(x_{A,q}e^{iqa} - x_{B,q})(x_{A,q'}e^{iq'a} - x_{B,q'})^* \\ &= \left(\frac{a}{2\pi}\right)^2 \int dq \int dq' \frac{2\pi}{a}\delta(q-q')(x_{A,q}e^{iqa} - x_{B,q})(x_{A,q'}e^{iq'a} - x_{B,q'})^* \\ &= \frac{a}{2\pi}\int dq |x_{A,q}e^{iqa} - x_{B,q}|^2. \end{aligned} \tag{5}$$

We thus have

$$\begin{aligned} V &= \frac{k}{2}\frac{a}{2\pi}\int dq |x_{A,q} - x_{B,q}|^2 + \frac{k}{2}\frac{a}{2\pi}\int dq |x_{A,q}e^{iqa} - x_{B,q}|^2 \\ &= \frac{k}{2}\frac{a}{2\pi}\int dq (2|x_{A,q}|^2 + 2|x_{B,q}|^2 - (1+e^{iqa})x_{A,q}x_{B,q}^* - (1+e^{-iqa})x_{B,q}x_{A,q}^*), \end{aligned} \tag{6}$$

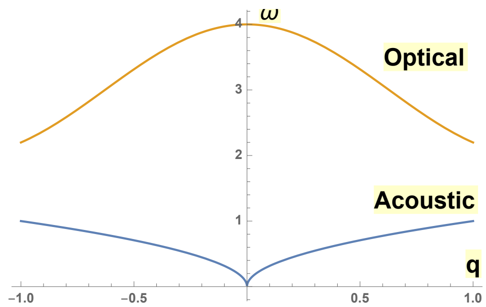

Figure 1: Dispersion relation of phonons in the chain

and the Hamiltonian is given by

$$H = \frac{a}{2\pi}\int dq\left(\frac{|p_{A,k}|^2}{2m_A} + \frac{|p_{B,k}|^2}{2m_B} + 2|x_{A,q}|^2 + 2|x_{B,q}|^2 - (1+e^{iqa})x_{A,q}x^*_{B,q} - (1+e^{-iqa})x_{B,q}x^*_{A,q}\right). \tag{7}$$

The equations of motion are given by

$$\begin{aligned}
\frac{dp_{A,q}}{dt} &= -\frac{i}{\hbar}[p_{A,q}, H] \\
&= -\frac{i}{\hbar}\frac{a}{2\pi}\int dq\left(2[p_{A,q}, x_{A,q}x^*_{A,q}] - (1+e^{iqa})[p_{A,q}, x_{A,q}x^*_{B,q}] - (1+e^{-iqa})[p_{A,q}, x_{B,q}x^*_{A,q}]\right) \\
&= -\frac{k}{2}\left(4x_{A,q} - 2(1+e^{-iqa})x_{B,q}\right) \\
&= -k\left(2x_{A,q} - (1+e^{-iqa})x_{B,q}\right), \qquad (8)\\
\frac{dx_{A,q}}{dt} &= -\frac{i}{\hbar}[x_{A,q}, H] = \frac{p_{A,q}}{m_A}, \qquad (9)
\end{aligned}$$

Similarly,

$$\begin{aligned}
\frac{dp_{B,q}}{dt} &= -\frac{k}{2}\left(4x_{B,q} - 2(1+e^{iqa})x_{A,q}\right), \qquad (10)\\
\frac{dx_{B,q}}{dt} &= \frac{p_{B,q}}{m_B}. \qquad (11)
\end{aligned}$$

In matrix form,

$$\begin{aligned}
\frac{d}{dt}\begin{pmatrix} x_{A,q} \\ x_{B,q}\end{pmatrix} &= -\begin{pmatrix} 2k/m_A & -k(1+e^{-iqa})/m_A \\ -k(1+e^{iqa})/m_B & 2k/m_B \end{pmatrix}\begin{pmatrix} x_{A,q} \\ x_{B,q}\end{pmatrix} \\
&\equiv -\Omega\begin{pmatrix} x_{A,q} \\ x_{B,q}\end{pmatrix} \qquad (12)
\end{aligned}$$

The normal mode frequencies are given by the eigenvalues of the matrix Ω, which are

$$\omega^2_\pm = k\left(\frac{m_A+m_B}{m_Am_B} \pm \sqrt{\left(\frac{m_A+m_B}{m_Am_B}\right)^2 - \frac{4}{m_Am_B}\sin^2(\frac{qa}{2})}\right). \tag{13}$$

Since $\omega_-(q=0)=0$, it corresponds to the acoustic branch, and ω_+ corresponds to the optical branch.

(b) As $q \to 0$,

$$\omega_-(q) = aq\sqrt{\frac{k}{2(m_A+m_B)}} + O(q^2). \tag{14}$$

Thus the speed of sound is given by

$$\begin{aligned} c &= \frac{\partial \omega_-}{\partial q}\bigg|_{q\to 0} \\ &= a\sqrt{\frac{k}{2(m_A+m_B)}}. \end{aligned} \tag{15}$$

(c) At low temperature, the optical branch isn't excited, so we only need to consider the contribution of the acoustic branch to the total energy, which is given by

$$\begin{aligned} U &= 2L\int_0^{\pi/a}\frac{dq}{2\pi}\hbar\omega_-(q)\frac{1}{e^{\beta\hbar\omega_-(q)}-1} \\ &\approx 2L\int_0^{\pi/a}\frac{dq}{2\pi}\hbar cq\frac{1}{e^{\beta\hbar cq}-1} \\ &= \frac{k_B^2T^2L}{\pi\hbar c}\int_0^{\frac{\pi\hbar c\beta}{a}} dx\frac{x}{e^x-1} \\ &= \frac{k_B^2T^2L}{\pi\hbar c}\frac{\pi^2}{6} = \frac{k_B^2T^2\pi L}{6\hbar c}. \end{aligned} \tag{16}$$

The heat capacity is then given by

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{k_B^2T\pi L}{3\hbar c}. \tag{17}$$

Problem 2

Let $|\psi\rangle$ be a trial wave function of the form

$$|\psi\rangle = \sum_{i=1}^{N}\alpha_i|i\rangle \tag{18}$$

We try to minimize

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{i,j}\alpha_i\alpha_j^*h_{ji}}{\sum_{i,j}\alpha_i\alpha_j^*M_{ji}}. \tag{19}$$

Therefore,

$$\begin{aligned} &\frac{\partial}{\partial\alpha_k^*}\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \\ =&\frac{\partial}{\partial\alpha_k^*}\frac{\sum_{i,j}\alpha_i\alpha_j^*h_{ji}}{\sum_{i,j}\alpha_i\alpha_j^*M_{ji}} \\ =&\frac{(\sum_i\alpha_ih_{ki})(\sum_{i,j}\alpha_i\alpha_j^*M_{ji}) - (\sum_{i,j}\alpha_i\alpha_j^*h_{ji})(\sum_i\alpha_iM_{ki})}{(\sum_{i,j}\alpha_i\alpha_j^*M_{ji})^2} = 0, \end{aligned} \tag{20}$$

which implies that

$$(h\alpha)(\alpha^\dagger M\alpha) = (\alpha^\dagger h\alpha)(M\alpha). \tag{21}$$

Since $\alpha^\dagger M\alpha$ and $\alpha^\dagger h\alpha$ are just numbers,

$$h\alpha = EM\alpha, \tag{22}$$

and

$$M^{-1/2}hM^{-1/2}(M^{1/2}\alpha) = E(M^{1/2}\alpha). \tag{23}$$

Hence the best lowest-energy N solutions that are superpositions of the form $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |i\rangle$ have energies that given by the eigenvalues of the matrix:

$$H_{\text{eff}} = M^{-1/2}hM^{1/2}. \tag{24}$$

Denote by $\alpha' = M^{1/2}\alpha$ the corresponding eigenstate of H_{eff},

$$M^{-1/2}hM^{-1/2}\alpha' = E\alpha', \tag{25}$$

then

$$|\psi\rangle = \sum_{i=1}^{N}(M^{-1/2}\alpha')|i\rangle. \tag{26}$$