1. (a) $m\ddot{S}_n + f(2S_n - S_{n-1} - S_{n+1}) = 0$

设 $S_n = u(q)\exp[i(qna - wt)]$，代入上面方程，得：

$-mw^2 + f(2 - e^{-iqa} - e^{iqa}) = 0$

$-mw^2 + f(2 - 2\cos qa) = 0$

$w^2 = \frac{4f}{m}\sin^2(\frac{qa}{2})$

当 $M_1 = M_2$ 时，双原子链色散回归单原子链形式。

当 $q = 0$ 时，单原子链只有声学支，双原子链 w 可不为 0，有光学支。

(b) $\sum_{n=1}^{N} m\dot{S}_n(t) = \sum_{n=1}^{N} -iwm\,u(q)\exp[i(qna - wt)]$

$= -imw\,u(q)e^{-iwt}\sum_{n=1}^{N}\exp(iqna)$

由周期性边界条件可得：$q = \frac{2\pi m}{Na}$

∴ 声子总动量为 0.

(c) $m\ddot{S}_n + f(2S_n - S_{n-1} - S_{n+1}) = 0$

$m\ddot{S}_x + f(2S_x - S_{x-\Delta x} - S_{x+\Delta x}) = 0$

将 $S_{x-\Delta x}$、$S_{x+\Delta x}$ 在 ~~x~~ x 处做泰勒展开，可得：

$m\ddot{S}_x = f\Delta x\left(\frac{ds}{dx}\Big|_{x+\Delta x} - \frac{ds}{dx}\Big|_x\right)$

$= f\Delta x\frac{d^2s}{dx^2}\Delta x$

∴ $\rho\ddot{S} = f\Delta x\, d^2s/dx^2$ 为弹性波波动方程.

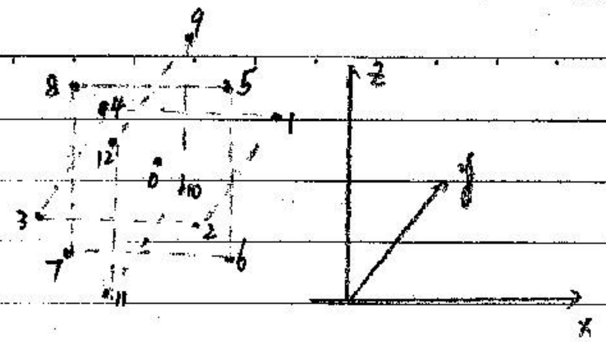
(d) 令 $S = u\cos(qx - wt)$ 代入波动方程

$w = q\sqrt{f\Delta x/\rho}$

$v = \frac{dw}{dq} = \sqrt{f\Delta x/\rho}$

∴ 有效弹性模量为 $f\Delta x = fa$

2.



以图示方示定义坐标轴

x方向为(100)方向，1~12为最近邻原子

则：

$$\phi_1 = \phi_3 = -\frac{f}{2}\begin{pmatrix}1 & 1 & 0\\ 1 & 1 & 0\\ 0 & 0 & 0\end{pmatrix} \qquad \phi_2 = \phi_4 = -\frac{f}{2}\begin{pmatrix}1 & -1 & 0\\ -1 & 1 & 0\\ 0 & 0 & 0\end{pmatrix}$$

$$\phi_5 = \phi_7 = -\frac{f}{2}\begin{pmatrix}1 & 0 & 1\\ 0 & 0 & 0\\ 1 & 0 & 1\end{pmatrix} \qquad \phi_6 = \phi_8 = -\frac{f}{2}\begin{pmatrix}1 & 0 & -1\\ 0 & 0 & 0\\ -1 & 0 & 1\end{pmatrix}$$

$$\phi_9 = \phi_{11} = -\frac{f}{2}\begin{pmatrix}0 & 0 & 0\\ 0 & 1 & 1\\ 0 & 1 & 1\end{pmatrix} \qquad \phi_{10} = \phi_{12} = -\frac{f}{2}\begin{pmatrix}0 & 0 & 0\\ 0 & 1 & -1\\ 0 & -1 & 1\end{pmatrix}$$

$$\phi_0 = -\sum_{L=1}^{12}\phi(L) = 4f\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}$$

$\therefore D = \frac{1}{M}\sum_{R_L}\phi(R_L)e^{-i\vec{k}\vec{R}_L}$ 令 $\vec{k} = k_x$，(100)方向

则 $$D = \frac{2f}{M}\begin{pmatrix}2-2\cos\frac{k_x a}{2} & 0 & 0\\ 0 & 1-\cos\frac{k_x a}{2} & 0\\ 0 & 0 & 1-\cos\frac{k_x a}{2}\end{pmatrix}$$

$\omega(\vec{k})$ 由 $D(\vec{k})$ 代入久期方程：

$$\det\|D(\vec{k}) - m\omega^2 I\| = 0$$

$\omega_1^2 = \frac{4f}{m}\left(1-\cos\frac{k_x a}{2}\right) = \omega_l^2$ 纵向

$\omega_2^2 = \omega_3^2 = \frac{2f}{m}\left(1-\cos\frac{k_x a}{2}\right) = \omega_t^2$ 横向

横向声子是简并的

(010)(001)(111)三个方向都适用上面的结论。

这些声子都可用线性链运动方程描述。

考虑BZ边界上的声子 $k_x = \frac{\pi}{a}$，则

0, 9, 10, 11, 12 相位为 e^{i0}

1, 2, 5, 6 原子相位为 $e^{i\frac{\pi}{2}}$

3, 4, 7, 8 原子相位为 $e^{-i\frac{\pi}{2}}$

3. a) 双谐振子系统，谐振子能量为

$$(n+\frac{1}{2})\hbar\omega_1 \quad , \quad (m+\frac{1}{2})\hbar\omega_2$$

则几率 $P_{nm} \propto \exp\left[\frac{-(n+\frac{1}{2})\hbar\omega_1+(m+\frac{1}{2})\hbar\omega_2}{kT}\right]$

$$\sum_{m,n=0}^{\infty} P_{nm} \propto \sum_{n,m=0}^{\infty} e^{-\frac{(n+\frac{1}{2})\hbar\omega_1}{kT}} \cdot e^{-\frac{(m+\frac{1}{2})\hbar\omega_2}{kT}}$$

$$= \frac{e^{-\frac{\hbar\omega_1}{2kT}}}{(1-e^{-\frac{\hbar\omega_1}{kT}})} \cdot \frac{e^{-\frac{\hbar\omega_2}{2kT}}}{(1-e^{-\frac{\hbar\omega_2}{kT}})}$$

$\because \sum_{m,n=0}^{\infty} P_{nm} = 1$

$$\therefore P_{nm} = e^{-\frac{n\hbar\omega_1}{kT}}(1-e^{-\frac{\hbar\omega}{kT}})e^{-\frac{m\hbar\omega_2}{kT}}(1-e^{-\frac{\hbar\omega_2}{kT}})$$

$$\therefore U(T) = \sum_{m,n=0}^{\infty} E_{nm}\cdot P_{nm}$$

$$= \hbar\omega_1\left(\frac{1}{2}+\frac{1}{e^{\frac{\hbar\omega_1}{kT}}-1}\right) + \hbar\omega_2\left(\frac{1}{2}+\frac{1}{e^{\frac{\hbar\omega_2}{kT}}-1}\right)$$

$$C = \frac{dU}{dT} = \frac{(\hbar\omega_1)^2}{kT^2}\frac{e^{\frac{\hbar\omega_1}{kT}}}{(e^{\frac{\hbar\omega_1}{kT}}-1)^2} + \frac{(\hbar\omega_2)^2}{kT^2}\frac{e^{\frac{\hbar\omega_2}{kT}}}{(e^{\frac{\hbar\omega_2}{kT}}-1)^2}$$

b) 对于双能级系统，

$$U = \frac{E_1 e^{-E_1/kT} + E_2 e^{-E_2/kT}}{e^{-E_1/kT} + e^{-E_2/kT}}$$

$$C = \frac{E_1 e^{\frac{E_1-E_2}{kT}}\cdot\frac{(E_1-E_2)}{kT^2}}{(1+e^{\frac{E_1-E_2}{kT}})^2} + \frac{E_2\frac{(E_2-E_1)}{kT^2}\cdot e^{\frac{E_2-E_1}{kT}}}{(1+e^{\frac{E_2-E_1}{kT}})^2}$$

NO.

Date

4. 双原子链质量比为 1:5，则 $5M_1 = M_2$

$\therefore \omega^2 = f \cdot \frac{6}{5M} [1 \pm (1 - \frac{5}{9}\sin^2\frac{qa}{2})^{\frac{1}{2}}]$

则相速度为：

$$\frac{\omega}{q} = \sqrt{f \frac{6}{5M} [1 \pm (1 - \frac{5}{9}\sin^2\frac{qa}{2})^{\frac{1}{2}}]} \Big/ q$$

群速度为：

$$\frac{d\omega}{dq} = \frac{1}{2} \frac{\pm f \frac{6}{5M} \cdot \frac{1}{2} \cdot \frac{\frac{5}{9} 2\sin\frac{qa}{2} \cos\frac{qa}{2} \cdot \frac{a}{2}}{\sqrt{1 - \frac{5}{9}\sin^2\frac{qa}{2}}}}{\sqrt{f \cdot \frac{6}{5M} [1 \pm (1 - \frac{5}{9}\sin^2\frac{qa}{2})^{1/2}]}}$$

对于热导，主要是群速度提供贡献，光学模色散较缓，所以群速度相对于声学模较小，所以其对热导贡献较小。