1) Let $C(1) = -C$, $C(2) = -\frac{1}{2}C$

$$H = \sum_n \left\{ \frac{p_n^2}{2M} + \frac{1}{2}|C(1)|\,(x_n - x_{n-1})^2 + \frac{1}{2}|C(2)|\,(x_n - x_{n-2})^2 \right\}$$

$$C(0) = -2C(1) - 2C(2) = 3C$$

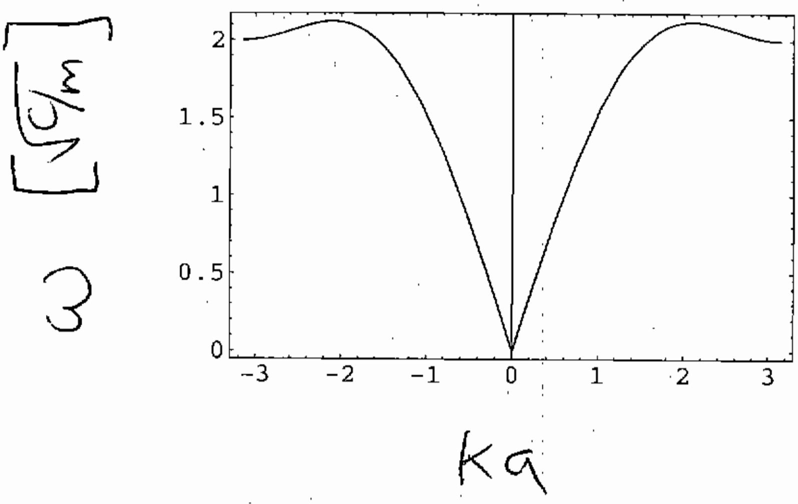
$$\tilde{C}(k) = C\left(3 - e^{ika} - e^{-ika} - \frac{1}{2}e^{i2ka} - \frac{1}{2}e^{-2ika}\right)$$

$$= C\left(2 - 2\cos ka + 1 - \cos 2ka\right)$$

$$= C\left(4\sin^2\frac{ka}{2} + 2\sin^2 ka\right)$$

$$\omega(k) = \sqrt{\frac{\tilde{C}(k)}{m}} = \sqrt{\frac{2C}{m}\left(2\sin^2\frac{ka}{2} + \sin^2 ka\right)}$$

$$\omega(k) \underset{ka \ll 1}{\approx} \sqrt{\frac{3Ca^2}{m}}\,k \qquad \omega\left(\frac{\pi}{a}\right) = \sqrt{\frac{4C}{m}}$$



The speed of sound is higher than for nearest-neighbor interactions only, but the frequency at the Brillouin Zone boundary is the same.

Physics 460 Problem Set # 9

Solutions (cont.)

2) a) $$E = \sum_k \hbar\omega_k \left(n_k + \frac{1}{2}\right)$$

$$\underset{L\to\infty}{=} \frac{La}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \; \hbar\omega_k \left(\frac{1}{e^{\beta\hbar\omega_k}-1} + \frac{1}{2}\right)$$

$$= \frac{La}{\pi}\int_0^{\omega_D} \frac{d\omega}{\frac{d\omega}{dk}} \; \hbar\omega \left(\frac{1}{e^{\beta\hbar\omega}-1} + \frac{1}{2}\right)$$

$\omega_D = \sqrt{4C/m}$

b) $C_V = \left.\frac{\partial E}{\partial T}\right|_V$ involves only

$$E - E_0 = \frac{La}{\pi}\int_0^{\omega_D} \frac{d\omega}{d\omega/dk} \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}$$

For $k_B T \ll \hbar\omega_D$, the integrand is exponentially small except for $\omega \ll \omega_D$. In this limit $ka \ll 1$, and one can approximate

$$\omega(k) \simeq \sqrt{\frac{Ca^2}{m}}\, k \equiv V_s k$$

$$E - E_0 \simeq \frac{La}{\pi V_s}\int_0^{\omega_D} \frac{\hbar\omega\, d\omega}{e^{\beta\hbar\omega}-1}$$

let $\beta\hbar\omega = x$

$$E - E_0 \cong \frac{La}{\pi\hbar V_s}\beta^{-2}\int_0^{\beta\hbar\omega_D}\frac{x\,dx}{e^x-1}$$

$$\simeq \frac{La k_B^2 T^2}{\pi\hbar V_s}\int_0^{\infty}\frac{x\,dx}{e^x-1}$$

3

$$I = \int_0^\infty \frac{x\,dx}{e^x - 1} = \frac{\pi^2}{6}$$

$$E - E_0 \simeq \frac{\pi}{6} \frac{La\, k_B^2 T^2}{\hbar v_s}$$

$$\boxed{C_V = \left.\frac{\partial E}{\partial T}\right|_V = \frac{\pi}{3} \frac{La\, k_B^2 T}{\hbar v_s}}$$

c) $$\lim_{T\to\infty} \frac{1}{e^{\beta\hbar\omega} - 1} = \frac{1}{\beta\hbar\omega}$$

$$\lim_{T\to\infty} E - E_0 = \sum_k \frac{\hbar\omega_k}{\beta\hbar\omega_k} = k_B T \sum_k 1$$

$$\sum_k 1 = L \quad , \quad E - E_0 \underset{T\to\infty}{=} L k_B T$$

$$\lim_{T\to\infty} C_V = L k_B$$

The equipartition theorem states that each quadratic term in the Hamiltonian has an expectation value of $\frac{k_B T}{2}$ at high temperatures.

$$H = \sum_{n=1}^{L} \left[\frac{p_n^2}{2m} + \frac{c}{2}(x_n - x_{n-1})^2 \right]$$

Kinetic energy gives $L \frac{k_B T}{2}$,

potential energy gives $\frac{L k_B T}{2}$.

Total energy

$$E \underset{T \to \infty}{=} L k_B T.$$

Physics 460 Homework #9

Solutions (cont.)

S.H.O. $x^2 = \frac{\hbar}{2m\omega}(a+a^\dagger)(a+a^\dagger)$

$$= \frac{\hbar}{2m\omega}\left[a^2 + a^\dagger a + a a^\dagger + (a^\dagger)^2\right]$$

$$\langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega}\langle 0|a a^\dagger|0\rangle$$

$$= \frac{\hbar}{2m\omega}\langle 0|1 + a^\dagger a|0\rangle = \frac{\hbar}{2m\omega}$$

3a) $X_n - X_{n-\ell} = \frac{1}{\sqrt{L}}\sum_k Q_k \left(e^{ikna} - e^{ik(n-\ell)a}\right)$

$$= \frac{1}{\sqrt{L}}\sum_k \sqrt{\frac{\hbar}{2m\omega_k}}\,(a_k + a^\dagger_{-k})\,e^{ikna}\left(1 - e^{-ik\ell a}\right)$$

$\langle 0|(x_n - x_{n-\ell})^2|0\rangle =$

$$\frac{1}{L}\sum_{kk'}\frac{\hbar}{2M\sqrt{\omega_k\omega_{k'}}}\,e^{i(k+k')na}\left(1-e^{-ik\ell a}\right)\left(1-e^{-ik'\ell a}\right)\underbrace{\langle 0|a_k a^\dagger_{-k'}|0\rangle}_{\delta_{k,-k'}}$$

$\langle 0| (x_n - x_{n-\ell})^2 |0\rangle$

$$= \frac{1}{L} \sum_k \frac{\hbar}{2m\omega_k} \left(1 - e^{-ik\ell a}\right)\left(1 - e^{ik\ell a}\right)$$

$$= \frac{1}{L} \sum_k \frac{2\hbar}{m\omega_k} \sin^2 \frac{k\ell a}{2}$$

$$= \frac{1}{L} \sum_k \frac{\hbar}{\sqrt{mC}} \frac{\sin^2 \frac{k\ell a}{2}}{\left|\sin \frac{ka}{2}\right|} ,$$

using $\omega_k = \sqrt{\frac{4C}{m}} \left|\sin \frac{ka}{2}\right|$.

For large L, $\frac{1}{L}\sum_k \to \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk$:

$$\langle 0| (x_n - x_{n-\ell})^2 |0\rangle \underset{L\to\infty}{=} \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk \, \frac{\hbar}{\sqrt{mC}} \frac{\sin^2(k\ell a/2)}{\left|\sin \frac{ka}{2}\right|}$$

$$= \frac{2\hbar}{\pi\sqrt{mC}} \int_0^{\pi/2} dx \, \frac{\sin^2(\ell x)}{\sin x}$$

This integral can be evaluated.
One finds:

$$\boxed{\langle 0|(x_n - x_{n-\ell})^2|0\rangle = \begin{cases} \dfrac{\hbar}{\pi\sqrt{mc}} \ln \ell, & \ell \to \infty \\[2ex] \dfrac{2\hbar}{\pi\sqrt{mc}}, & \ell = 1 \end{cases}}$$

The nearest-neighbor bond length is well defined provided

$$\langle 0|(x_n - x_{n-1})^2|0\rangle \ll a^2$$

$$\Rightarrow \quad a \gg \frac{\hbar}{mv},$$

where $v = \sqrt{\frac{ca^2}{m}}$ is the speed of sound

3b) $$\langle 0| x_n^2 |0\rangle = \frac{1}{L}\sum_{kk'} \frac{\hbar}{2m\sqrt{\omega_k \omega_{k'}}} e^{ina(k-k')}$$

$$\times \underbrace{\langle 0| a_k a^\dagger_{k'} |0\rangle}_{\delta_{kk'}}$$

$$= \frac{1}{L}\sum_k \frac{\hbar}{2m\omega_k}$$

$$\xrightarrow[L\to\infty]{} \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dk \frac{\hbar}{2m\,\omega(k)}$$

(omitting the term $k=0$, which describes the center of mass of the crystal).

$$= \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \frac{\hbar}{4\sqrt{CM}\,|\sin\frac{ka}{2}|}$$

$$= \frac{\hbar}{2\sqrt{CM}}\int_0^{\frac{\pi}{2}} \frac{dx}{\sin x}$$

$$\longrightarrow \infty \quad !$$

Thus the nth atom is totally delocalized! This suggests that crystalline order is destroyed by quantum fluctuations in one dimension. Indeed, <u>Mermin & Wagner</u> proved that quantum fluctuations always destroy long range order in one dimension.

What we thought was the Hamiltonian of a 1D crystal really describes a <u>fluid</u>. This "harmonic fluid" is ubiquitous in 1D systems.