INTRODUCTION TO MANY BODY PHYSICS: 620. Fall 2003

Answers to Questions I. Sept 22nd

1. For the Harmonic oscillator $H = \hbar\omega[a^\dagger a + \frac{1}{2}]$, we know that

$$\begin{aligned} \langle a^\dagger a\rangle &= n(\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}, \\ \langle a a^\dagger\rangle &= n(\omega) + 1, \end{aligned} \tag{1}$$

where $\beta = 1/(k_B T)$. Relating the displacement to the creation and annihilation operators,

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}[ae^{-i\omega t} + a^\dagger e^{i\omega t}] \tag{2}$$

and remembering that $\langle a^2\rangle = \langle {a^\dagger}^2\rangle = 0$, we have

$$\begin{aligned} \frac{1}{2}\langle\{x(t),\ x(0)\}\rangle &= \frac{\hbar}{m\omega}(\langle a^\dagger a\rangle + \frac{1}{2})\cos\omega t \\ &= \frac{\hbar}{m\omega}(n(\omega) + \frac{1}{2})\cos\omega t. \end{aligned}$$

We may interpret the first and second terms as the thermal and zero-point fluctuations respectively. Notice how at high temperatures, this result reverts to the classical result

$$\langle x(t)x(0)\rangle = \frac{k_B T}{m\omega^2}\cos\omega t \tag{3}$$

that is expected from the equipartition theorem.

2. (a)Making the transformation

$$\begin{aligned} b &= ua + va^\dagger, \\ b^\dagger &= ua^\dagger + va, \end{aligned} \tag{4}$$

(where u and v are real), we find that

$$[b, b^\dagger] = [ua + va^\dagger,\ ua^\dagger + va] = u^2[a,\ a^\dagger] + v^2[a^\dagger,\ a] = u^2 - v^2, \tag{5}$$

and $[b, b] = [b^\dagger,\ b^\dagger] = 0$ trivially. If $u^2 - v^2 = 1$, then $[b, b^\dagger] = 1$ and the transformation is canonical.

(b) Let us assume that the Hamiltonian can be diagonalized in the form

$$H = \tilde{\omega}(b^\dagger b + \frac{1}{2}). \tag{6}$$

Substituting in the above transformation, we find that

$$H = \omega(a^\dagger a + \frac{1}{2}) + \frac{1}{2}\Delta(a^\dagger a^\dagger + aa), \tag{7}$$

where

$$\omega = \tilde{\omega}(u^2 + v^2), \qquad \Delta = \tilde{\omega}(2uv), \tag{8}$$

Squaring both terms, and subtracting we find

$$\omega^2 - \Delta^2 = \tilde{\omega}^2(u^2 - v^2)^2 = \tilde{\omega}^2 \tag{9}$$

so that $\tilde{\omega} = \sqrt{\omega^2 - \Delta^2}$. Notice that the first condition in (**??**) forces $\tilde{\omega}$ to be formally positive. Physically, we do not expect a negative excitation energy! By substituting $v^2 = u^2 - 1$ into the first equation in (**??**), we obtain

$$\begin{aligned} u^2 &= \frac{1}{2}(1 + \omega/\sqrt{\omega^2 - \Delta^2}), \\ v^2 &= -\frac{1}{2}(1 - \omega/\sqrt{\omega^2 - \Delta^2}). \end{aligned} \tag{10}$$

When $\Delta = \omega$, the frequency of oscillation goes to zero. You might perhaps have spotted that if you write $a = \frac{1}{\sqrt{2}}(x + ip)$, then $(a^\dagger)^2 + a^2 = (x^2 - p^2)$, so that when $\Delta = \omega$, the Hamiltonian takes the form $H = \omega x^2$, i.e the mass of the particle has become infinite, and hence the frequency of oscillation vanishes.

3. (i) To get an approximate estimate of the amplitude of zero-point motion, suppose we treat each site as a simple harmonic oscillator. The amplitude of zero point motion is then

$$\Delta x \sim \sqrt{\frac{\hbar}{2m\omega}} \tag{11}$$

Setting $\Delta x < a/3$, we obtain

$$\frac{\hbar}{m\omega a^2} < \zeta_c \tag{12}$$

In our estimate, $\zeta_c = 2/9$. Actually, this type of relation must hold on purely dimensional grounds, with some value of ζ that needs to be determined.

(ii) If we evaluate the amplitude of oscillation for the 3D crystal, we obtain

$$\begin{aligned} \langle 0|\Phi_j^2|0\rangle &= 3\frac{1}{N_s}\sum_q \frac{\hbar}{2m\omega_q} \\ &= 3a^3 \int \frac{d^3q}{(2\pi)^3}\frac{\hbar}{2m\omega_q} \\ &= \frac{3\hbar}{4m\omega} I_3 \end{aligned} \tag{13}$$

where the factor of three derives from the three directions of oscillation and

$$\begin{aligned} I_3 &= \int_0^\pi \frac{du^3}{\pi^3}\frac{1}{\sqrt{\sum_{l=1,3}\sin^2(u_l)}} \\ &= 0.91 \end{aligned} \tag{14}$$

The final condition is

$$\frac{\hbar}{m\omega a^2} < \zeta_c = \frac{4}{27 I_3} = 0.16 \tag{15}$$

If you had ignored the three directions of motion, you would have obtained a value that is three times larger.

(iii)Since the frequency increases more rapidly than a^{-2}, zero-point motion will become smaller when a is smaller, so the crystal is liquid when $a > a_c$, and solid for $a < a_c$. Putting in the numbers, we obtain :

$$\begin{aligned} a_c &= \left(\frac{\hbar}{m\omega\zeta_c}\right)^{\frac{1}{2}} = \left(\frac{\hbar^2}{m(\hbar\omega/k_B)k_B\zeta_c}\right)^{\frac{1}{2}} = \left[\frac{(10^{-34})^2}{4 \times 1.7 \times 10^{-27} \times 300 \times 1.34 \times 10^{-23} \times 0.16}\right]^{\frac{1}{2}} \\ &= 4.8 \times 10^{-11}\mathrm{m} \end{aligned} \tag{16}$$

or half an angstrom.

4. To transform the Hamiltonian

$$H = \sum_j \left\{ J_1({a^\dagger}_{i+1} a_i + H.c) + J_2({a^\dagger}_{i+1}{a^\dagger}_i + H.c) \right\} \tag{17}$$

we first transform to momentum space, writing $a_j = \frac{1}{N^{1/2}} \sum_q e^{iqR_j} a_q$, whereupon

$$H = \frac{1}{2}\sum_q \left[2J_1 \cos(qa)({a^\dagger}_q a_q + a_{-q}{a^\dagger}_{-q}) + 2J_1 \cos(qa)({a^\dagger}_q {a^\dagger}_{-q} + a_{-q} a_q) \right]. \tag{18}$$

(Note that each operator in brackets is symmetric under $q \rightleftharpoons -q$, so that if you obtained expressions of the form e^{iqa} they would automatically be symmetrized to $\cos(qa)$.) This is of the form found in 3., so we may carry out a Boguilubov transformation

$$\begin{aligned} b_q &= u_q a_q + v_q {a^\dagger}_{-q}, \\ {b^\dagger}_q &= u_q {a^\dagger}_q + v_q a_{-q}, \end{aligned} \tag{19}$$

(notice the minus signs which are needed to conserve momentum), to obtain

$$H = \sum_q \omega_q ({b^\dagger}_q b_q + \frac{1}{2}) \tag{20}$$

where

$$\omega_q = 2[J_1^2 - J_2^2]^{1/2} \cos(qa). \tag{21}$$

In terms of the original operators,

$$a_i = \frac{1}{\sqrt{N}} \sum_q (u b_q - v {b^\dagger}_{-q}) e^{iqR_j}. \tag{22}$$

The coefficients are momentum independent:

$$\begin{pmatrix} u^2 \\ v^2 \end{pmatrix} = \frac{1}{2}\left(\frac{J_1}{\sqrt{J_1^2 - J_2^2}} \pm 1\right). \tag{23}$$

When $J_1 = J_2$, the spectrum is zero at all values of momentum.

5. (i) Newton's laws of motion for the one-dimensional chain are

$$\begin{aligned} \ddot{x}_j &= -\Omega_1^2(2x_j - x_{j+1} - x_{j-1}), && \text{(j odd)} \\ \ddot{x}_j &= -\Omega_2^2(2x_j - x_{j+1} - x_{j-1}), && \text{(j even)} \end{aligned}$$

where $\Omega_1^2 = k/M$ and $\Omega_2^2 = k/m$. We seek normal mode solutions of the form

$$x_j = \frac{1}{\sqrt{N}} \sum_q e^{i(qR_j - \omega_q t)} x_{q\eta}^{(\pm)} \tag{24}$$

where $\pm$ refers to even and odd numbered sites, respectively and $\eta = \pm$ will refer to the two bands of excitation- one optic, one acoustic. (There are N heavy and light atoms.) Substituting this into the equations of motion, we obtain

$$\omega^2 \begin{pmatrix} x_{q\eta}^{(+)} \\ x_{q\eta}^{(-)} \end{pmatrix} = 2 \begin{bmatrix} \Omega_1^2 & -\Omega_1^2 \cos(qa) \\ -\Omega_2^2 \cos(qa) & \Omega_2^2 \end{bmatrix} \begin{pmatrix} x_{q\eta}^{(+)} \\ x_{q\eta}^{(-)} \end{pmatrix}. \tag{25}$$

Subtracting the left from the right, taking the determinant of the resulting matrix and solving for the roots we obtain

$$\omega_{q\eta}^2 = (\Omega_1^2 + \Omega_2^2) + \eta\sqrt{(\Omega_1^2 - \Omega_2^2)^2 + 4\Omega_1^2\Omega_2^2 \cos^2 qa}, \qquad (\eta = \pm 1) \tag{26}$$

corresponding to two normal modes- one acoustic ($\eta = -1$), one "optic" ($\eta = +1$). The dispersion of these modes is sketched beneath.

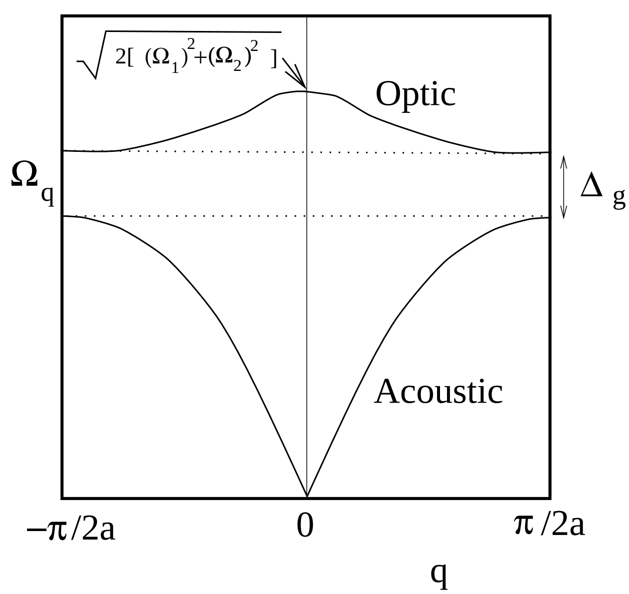

Figure 1:

(ii) The gap between the two modes is minimum for $qa = \pi/2$, and is given by $\Delta_g = \sqrt{2}|\Omega_1 - \Omega_2|$.

(iii)The second-quantized Hamiltonian will involve two types of phonon- one optic ($\eta = +$) and one acoustic ($\eta = -$), and can be written

$$H = \sum_{q,\eta=\pm} \omega_{q\eta}[a^{\dagger}{}_{q\eta} a_{q\eta} + \frac{1}{2}] \tag{27}$$

Second-quantization is a question of first finding the canonically conjugate normal co-ordinates, then rewriting the normal co-ordinates in terms of creation and annihilation operators. The canonical commutation relations between the normal co-ordinates will guarantee that the creation and annihilation operators satisfy canonical bosonic commutation relations.

Here's how you can derive canonically conjugate normal co-ordinates. First, rescale the momenta and displacements at each site to absorb the difference in masses, writing

$$P_i = p_i/\sqrt{m_i}, \qquad Q_i = x_i\sqrt{m_i}, \tag{28}$$

The Hamiltonian can now be written in the form

$$H = \sum_i \left\{ \frac{P_i^2}{2} + \frac{1}{2}[2\Omega_i^2\ Q_i^2 - \Omega_1\Omega_2\ Q_i(Q_{i+1} + Q_{i-1})] \right\} \tag{29}$$

where $\Omega_i^2 = (\Omega_1)^2 = k/M$ on odd sites and $\Omega_i^2 = (\Omega_2)^2 = k/m$ on even sites. Now writing

$$\begin{aligned} P_j &= \frac{1}{\sqrt{N}} \sum_q P_q^{(\pm)} e^{-iqR_j}, \\ Q_j &= \frac{1}{\sqrt{N}} \sum_q Q_q^{(\pm)} e^{iqR_j}, \end{aligned} \tag{30}$$

where + refers to odd and (-) refers to even sites. In terms of these variables, the Hamiltonian is diagonal.

$$H = \frac{1}{2} \sum_q \left[P_q^T P_{-q} + Q_{-q}^T \underline{\Omega}^2(q) Q_q \right] \tag{31}$$

where

$$\underline{\Omega}^2(q) = 2 \begin{bmatrix} \Omega_1^2 & -\Omega_1\Omega_2\cos(qa) \\ -\Omega_1\Omega_2\cos(qa) & \Omega_2^2 \end{bmatrix}, \tag{32}$$

and $P_q^T = (P_q^{(+)}, P_q^{(-)})$, $Q_q^T = (Q_q^{(+)}, Q_q^{(-)})$.

The eigenvectors of $\underline{\Omega}^2(q)$ satisfy $\underline{\Omega}^2(q)\xi_{q\eta} = \omega_{q\eta}^2 \xi_{q\eta}$, where $\eta = \mp$ refers to the acoustic and optic modes. They are real and orthonormal. Consequently, if we write

$$\begin{aligned} P_q^{(\pm)} &= \sum_{\eta=\pm} \xi_{q\eta} p_{q\eta}, \\ Q_q^{(\pm)} &= \sum_{\eta=\pm} \xi_{q\eta} x_{q\eta}, \end{aligned} \tag{33}$$

then it follows that

$$H = \sum_{q,\eta} \frac{1}{2} \left[p_{q\eta} p_{-q\eta} + \omega_{q\eta}^2 x_{q\eta} x_{-q\eta} \right] \tag{34}$$

is diagonal. We may write the momentum and position in terms of the normal co-ordinates, as follows

$$\begin{aligned}
p_j &= \frac{\sqrt{M}}{\sqrt{N}} \sum_{q\eta} p_{q\eta} \xi_{\eta q}^{(+)} e^{-iqR_j}, && \text{(odd sites)} \\
p_j &= \frac{\sqrt{m}}{\sqrt{N}} \sum_{q\eta} p_{q\eta} \xi_{\eta q}^{(-)} e^{-iqR_j} && \text{(even sites)} \\
x_j &= \frac{1}{\sqrt{MN}} \sum_{q\eta} x_{q\eta} \xi_{\eta q}^{(+)} e^{-iqR_j}, && \text{(odd sites)} \\
x_j &= \frac{1}{\sqrt{mN}} \sum_{q\eta} x_{q\eta} \xi_{\eta q}^{(-)} e^{-iqR_j} && \text{(even sites)}
\end{aligned} \tag{35}$$

Up to this point, classical and quantum mechanics are identical! As a last step, we rewrite the normal co-ordinates in terms of creation and annihilation operators:

$$x_{q\eta} = \sqrt{\frac{\hbar}{2\omega_{q\eta}}} [a_{q\eta} + a^\dagger{}_{-q\eta}] \tag{36}$$

and

$$\pi_{q\eta} = -i\sqrt{\frac{\hbar\omega_{q\eta}}{2}} [a_{q\eta} - a^\dagger{}_{-q\eta}] \tag{37}$$

where $[a_{q\eta},\ a^\dagger{}_{q'\eta'}] = \delta_{\eta\eta'} \delta_{qq'}$ are canonically conjugate.

6. (a) To derive the linear response, let us begin in the Schrodinger representation, where $H_S(t) = H_0 + V_S(t)$ and

$$\begin{aligned}
H_0 &= \hbar\omega(a^\dagger a + \frac{1}{2}), \\
V_S(t) &= -f(t)x.
\end{aligned} \tag{38}$$

We now transform to the "interaction representation", which removes the time evolution of the states due to H_0, so that

$$\begin{aligned}
|\psi_I(t)\rangle &= e^{iH_0 t/\hbar} |\psi_S(t)\rangle \\
V_I(t) &= e^{iH_0 t/\hbar} V_S(t) e^{-iH_0 t/\hbar}
\end{aligned} \tag{39}$$

The equation of motion for $|\psi_I(t)\rangle$ is then

$$\begin{aligned}
i\hbar\partial_t |\psi_S(t)\rangle &= i\hbar\partial_t \left(e^{iH_0 t/\hbar} \right) |\psi_S(t)\rangle + e^{iH_0 t/\hbar} i\hbar\partial_t |\psi_S(t)\rangle \\
&= -H_0 e^{iH_0 t/\hbar} |\psi_S(t)\rangle + e^{iH_0 t/\hbar} (H_0 + V_S(t)) |\psi_S(t)\rangle \\
&= -e^{iH_0 t/\hbar} H_0 |\psi_S(t)\rangle + e^{iH_0 t/\hbar} (H_0 + V_S(t)) |\psi_S(t)\rangle \\
&= e^{iH_0 t/\hbar} (V_S(t)) |\psi_S(t)\rangle = e^{iH_0 t/\hbar} (V_S(t)) e^{-iH_0 t/\hbar} |\psi_I(t)\rangle
\end{aligned}$$

$$= \quad (V_I(t))|\psi_I(t)\rangle. \tag{40}$$

(b) The general solution solution to (**??**) is

$$|\psi_I(t)\rangle = \mathrm{T}\exp\left(-i\frac{1}{\hbar}\int_{-\infty}^{t} V_I(t')dt'\right). \tag{41}$$

Expanding this to leading order in f gives

$$|\psi_I(t)\rangle = \left(1 + i\int_{-\infty}^{t} dt' f(t')x_I(t')\right) + O(f^2) \tag{42}$$

where $x_I = e^{iH_0 t/\hbar} x e^{-iH_0 t/\hbar}$ is in the "interaction" representation. The complex conjugate of this expression is

$$\langle\psi_I(t)| = \langle\psi_I(t)|\left(1 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' x_I(t')f(t')\right) + O(f^2) \tag{43}$$

(c) Finally, we may evaluate the expectation of the displacement at time t. This is given by

$$\begin{aligned}
\langle x(t)\rangle &= \langle\psi_I(t)|x_I(t)|\psi_I(t)\rangle \\
&= \langle\psi_I(t)|\left(1 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' x_I(t')f(t')\right) x_I(t) \left(1 + \frac{i}{\hbar}\int_{-\infty}^{t} dt' f(t')x_I(t')\right)|\psi_I(t)\rangle + O(f^2) \\
&= \overbrace{\langle 0|x_I(t)|0\rangle}^{=0} + \int_{-\infty}^{t} dt' \overbrace{\frac{i}{\hbar}\langle 0|[x_I(t), x_I(t')]|0\rangle}^{R(t-t')} f(t') + O(f^2) \\
&= \int_{-\infty}^{t} dt' R(t-t')f(t').
\end{aligned} \tag{44}$$

By convention, we drop the subsripts "I" on the x, implicitly assuming that they are in the Heisenberg representation of the undriven Hamiltonian H_0, so

$$R(t-t') = \frac{i}{\hbar}\langle 0|[x_I(t), x_I(t')]|0\rangle.$$