

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

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

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

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

Squaring both terms, and subtracting we find

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

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

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

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

$$\Delta x \sim \sqrt{\frac{\hbar}{2m\omega}} \quad (11)$$

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

$$\frac{\hbar}{m\omega a^2} < \zeta_c \quad (12)$$

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

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

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

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

The final condition is

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

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 :

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

or half an angstrom.

4. To transform the Hamiltonian

$$H = \sum_j \left\{ J_1(a^\dagger_{i+1}a_i + H.c) + J_2(a^\dagger_{i+1}a^\dagger_i + H.c) \right\} \quad (17)$$

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

$$H = \frac{1}{2} \sum_q \left[2J_1 \cos(qa)(a^\dagger_q a_q + a_{-q} a^\dagger_{-q}) + 2J_2 \cos(qa)(a^\dagger_q a^\dagger_{-q} + a_{-q} a_q) \right]. \quad (18)$$

(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

$$\begin{aligned} b_q &= u_q a_q + v_q a^\dagger_{-q}, \\ b^\dagger_q &= u_q a^\dagger_q + v_q a_{-q}, \end{aligned} \quad (19)$$

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

$$H = \sum_q \omega_q (b^\dagger_q b_q + \frac{1}{2}) \quad (20)$$

where

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

In terms of the original operators,

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

The coefficients are momentum independent:

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

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

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

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

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

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

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

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

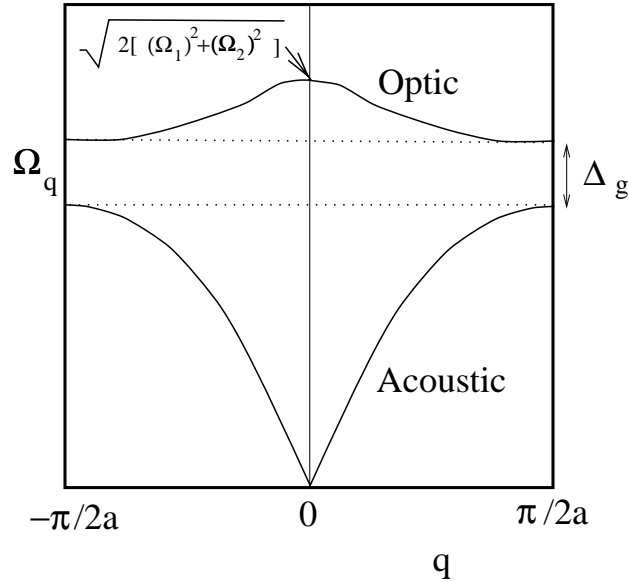


Figure 1:

(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

$$H = \sum_{q, \eta = \pm} \omega_{q\eta} [a_{q\eta}^\dagger a_{q\eta} + \frac{1}{2}] \quad (27)$$

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

$$P_i = p_i / \sqrt{m_i}, \quad Q_i = x_i \sqrt{m_i}, \quad (28)$$

The Hamiltonian can now be written in the form

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

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

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

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

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

where

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

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

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

then it follows that

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

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

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

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:

$$x_{q\eta} = \sqrt{\frac{\hbar}{2\omega_{q\eta}}} [a_{q\eta} + a_{-q\eta}^\dagger] \quad (36)$$

and

$$\pi_{q\eta} = -i\sqrt{\frac{\hbar\omega_{q\eta}}{2}} [a_{q\eta} - a_{-q\eta}^\dagger] \quad (37)$$

where $[a_{q\eta}, a_{q'\eta'}^\dagger] = \delta_{\eta\eta'} \delta_{qq'}$ 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

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

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

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

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

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

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

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

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

Expanding this to leading order in f gives

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

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

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

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

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

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

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