Questions I. (Due Fri, Sept 18th.)

These questions can all be done with a minimum of algebra. They will familiarize you with the method of second-quantization, as applied to free bosonic fields. Please choose one of the three harder questions. If you do more than one, I will grade the others as extra credit.

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

$$\langle \hat{n} \rangle = n(\omega) = \frac{1}{e^{\beta \hbar \omega} - 1},$$

(1)

where $\beta = 1/(k_B T)$ and $\hat{n} = a^\dagger a$ is the number operator. In the ground-state, using the equations of motion for the creation and annihilation operators, we showed that the zero-point fluctuations in position were described by the correlation function

$$\frac{1}{2} \langle \{x(t), x(0)\} \rangle = \frac{\hbar}{2m\omega} \cos \omega t.$$  

(2)

Generalize this result to finite temperatures. You should find that there are two terms in the correlation function. Please give them a physical interpretation.

2. (a) Show that if $a$ is a canonical bose operator, the canonical transformation

$$b = ua + va^\dagger, 
\quad b^\dagger = ua^\dagger + va,$$

(3)

(where $u$ and $v$ are real), preserves the canonical commutation relations, provided $u^2 - v^2 = 1$.

(b) Using the results of (a), diagonalize the Hamiltonian

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

(4)

by transforming it into the form $H = \tilde{\omega}(b^\dagger b + \frac{1}{2})$. Find $\tilde{\omega}$, $u$ and $v$ in terms of $\omega$ and $\Delta$. What happens when $\Delta = \omega$?

3. (Harder) According to the “Lindeman” criterion, a crystal melts when the rms displacement of its atoms exceeds a third of the average separation of the atoms. Consider a three dimensional crystal with separation $a$, atoms of mass $m$ and a nearest neighbor quadratic interaction $V = \frac{m\omega^2}{2}(\Phi_R - \Phi_{R+a})^2$.

(i) Estimate the amplitude of zero point fluctuations using the uncertainty principle, to show that if

$$\frac{\hbar}{m\omega a^2} > \zeta_c$$

(5)

where $\zeta_c$ is a dimensionless number of order one, the crystal will be unstable, even at absolute zero, and will melt due to zero-point fluctuations. (Hint... what would the answer be for a simple harmonic oscillator?)
(ii) Calculate ζc in the above model. If you like, to start out, imagine that the atoms only move in one direction, so that Φ is a scalar displacement at the site with equilibrium position R. Calculate the rms zero-point displacement of an atom \( \sqrt{\langle 0|\Phi(x)^2|0\rangle} \). Now generalize your result to take account of the fluctuations in three orthogonal directions.

(iii) Suppose \( \hbar\omega/k_B = 300K \), and the atom is a Helium atom. Assuming that \( \omega \) is independent of atom separation \( a \), estimate the critical atomic separation \( a_c \) at which the solid becomes unstable to quantum fluctuations. Note that in practice \( \omega \) is dependent on \( a \), and rises rapidly at short distances, with \( \omega \sim a^{-\alpha} \), where \( \alpha > 2 \). Is the solid stable for \( a < a_c \) or for \( a > a_c \)?

4. (Harder) Find the transformation that diagonalizes the Hamiltonian

\[
H = \sum_j \left\{ J_1(a_j^{\dagger}a_j + H.c) + J_2(a_j^{\dagger}a_j^{\dagger} + H.c) \right\}
\]

where \( a_j^{\dagger} \) creates a boson located at the jth site. The position of the jth-site is located at \( R_j = aj \). You may find it helpful to (i) transform to momentum space, writing \( a_j = \frac{1}{\sqrt{N}} \sum_q e^{iqR_j}a_q \), using periodic boundary conditions on a ring of n-sites. After this, carry out a canonical transformation of the form \( b_q = u_qa_q + v_qa_q^{\dagger}, \) where \( u^2 - v^2 = 1 \). What happens when \( J_1 = J_2 \)?

5. (Harder) Find the classical normal mode frequencies and normal co-ordinates for the one dimensional chain with Hamiltonian

\[
H = \sum_j \left[ \frac{p_j^2}{2m_j} + \frac{k}{2}(x_j - x_{j-1})^2 \right]
\]

where at even sites \( m_{2j} = m \) and at odd sites \( m_{2j+1} = M \). Please sketch the dispersion curves.

(ii) What is the gap in the excitation spectrum?

(iii) Write the diagonalized Hamiltonian in second quantized form and discuss how you might arrive at your final answer. You will now need two types of creation operator.

6. (Harder) This problem sketches the proof that the displacement of the quantum Harmonic oscillator, originally in its ground-state (in the distant past), is given by

\[
\langle x(t) \rangle = \int_0^\infty R(t - t')f(t')dt',
\]

where

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

is the “response function” and \( x(t) \) is the position operator in the Heisenberg representation of \( H_0 \). A more detailed discussion can be found in chapter 10.

An applied force \( f(t) \) introduces an additional forcing term to the harmonic oscillator Hamiltonian

\[
\hat{H}(t) = H_0 + V(t) = \hat{H}_0 - f(t)\hat{x},
\]

where \( H_0 = \hbar\omega(a^{\dagger}a + \frac{1}{2}) \) is the unperturbed Hamiltonian. To compute the displacement of the Harmonic oscillator, it is convenient to work in the “interaction representation”, which is the
Heisenberg representation for $H_0$. In this representation, the time-evolution of the wavefunction is due to the force term. The wavefunction of the harmonic oscillator in the interaction representation $|\psi_I(t)\rangle$ is related to the Schrodinger state $|\psi_S(t)\rangle$ by the relation $|\psi_I(t)\rangle = e^{iH_0 t/\hbar}|\psi_S(t)\rangle$.

(a) By using the equation of motion for the Schrodinger state $i\hbar \partial_t |\psi_S(t)\rangle = (H_0 + V(t))|\psi_S(t)\rangle$, show that the time evolution of the wavefunction in the interaction representation is
\[ i\hbar \partial_t |\psi_I(t)\rangle = V_I(t)|\psi_I(t)\rangle = -f(t)\hat{x}(t)|\psi_I(t)\rangle, \]
where $V_I(t) = e^{iH_0 t/\hbar}\hat{V}(t)e^{-iH_0 t/\hbar} = -x(t)f(t)$ is the force term in the interaction representation.

(b) Show that if $|\psi(t)\rangle = |0\rangle$ at $t = -\infty$, then the leading order solution to the above equation of motion is then
\[ |\psi_I(t)\rangle = |0\rangle + \frac{i}{\hbar} \int_{-\infty}^{t} dt' f(t')\hat{x}(t')|0\rangle + O(f^2), \]
so that
\[ \langle \psi_I(t)| = \langle 0| - \frac{i}{\hbar} \int_{-\infty}^{t} dt' f(t')\langle 0|\hat{x}(t') + O(f^2). \]

(c) Using the results just derived expand the expectation value $\langle \psi_I(t)|x(t)|\psi_I(t)\rangle$ to linear order in $f$, obtaining the above cited result.