Emergent States of Matter

Second Quantisation Worksheet

Due 5pm Fri 2 Feb, 2018 in the ESM 569 box
NOT FOR CREDIT

The purpose of this worksheet is to bring you up to speed with second quantisation notation. You have met it before but not all of you will be comfortable using it. We will use it later in the course, so it is important that you have had some practice with it. This worksheet will be marked, for your benefit, but it will not count as a homework assignment. Nevertheless, I strongly urge you to do your best on these "five-finger exercises." Please attempt these questions without looking at textbooks, if you can. You will learn more by thinking about these problems yourself.

Question QM–1.
Verify the following results for the one-dimensional harmonic oscillator with Hamiltonian $H = p^2/2m + \frac{1}{2}m\omega^2 q^2$, where p is momentum and q is position, and $[p, q] = -i\hbar$. Define annihilation and creation operators

$$a^+ = (2m\hbar\omega)^{-1/2}(p + im\omega q)$$
$$a = (2m\hbar\omega)^{-1/2}(p - im\omega q).$$

Let the eigenfunctions and eigenvalues of H satisfy $H|n\rangle = E_n|n\rangle$. Denote the ground state by $|0\rangle$ so that $a|0\rangle = 0$.
(1) $[a, a^+] = 1$
(2) $H = \hbar\omega(a^+a + 1/2)$
(3) $[H, a^+] = \hbar\omega a^+$; $[H, a] = -\hbar\omega a$
(4) $Ha^+|n\rangle = (E_n + \hbar\omega)a^+|n\rangle$
$Ha|n\rangle = (E_n - \hbar\omega)a|n\rangle$
$i.e. a^+|n\rangle$ and $a|n\rangle$ are eigenstates of H with energies $E_n \pm \hbar\omega$.
(5) Show that $E_0 = \frac{1}{2}\hbar\omega; E_n = (n + \frac{1}{2})\hbar\omega$
(6) $|n\rangle = \frac{1}{\sqrt{n!}}(a^+)^n|0\rangle$

Question QM–2.
Bosons are particles or quanta of integer spin, with any number of particles or quanta being allowed to occupy a given quantum state. Consider a system with energy levels $E_0, E_1, E_2, \ldots E_k$ into which can be put a system with an integral number n_0, n_1, n_2, $\ldots n_k \ldots$ of *non-interacting* bosons. (n_k is the occupation number of the k^{th} energy level). A state with n_0 bosons in eigenstate E_0, n_1 bosons in eigenstate E_1, $\ldots$ is written as

$$|n_0, n_1, n_2, \ldots n_k \ldots\rangle.$$

Define the creation operators b_k^+ and annihilation operators b_k by:

$$b_k^+|n_0, n_1, n_2 \ldots n_k \ldots\rangle = \sqrt{n_k + 1}\,|n_0, n_1, \ldots n_k + 1 \ldots\rangle$$
$$b_k|n_0 \ldots n_k \ldots\rangle = \sqrt{n_k}\,|n_0 \ldots n_k - 1 \ldots\rangle.$$

Verify the following properties of the b_k^+, b_k and the total number operator $N = \sum_k b_k^+ b_k$

(1) $[b_k, b_{k'}^+] = \delta_{kk'}$
(2) $[b_k, b_{k'}] = [b_{k'}^+ b_{k'}^+] = 0$
(3) $b_k^+ b_k \left|n_0, \ldots n_k \ldots\right\rangle = n_k \left|n_0 \ldots n_k \ldots\right\rangle$
(4) $N \left|n_0 \ldots n_k \ldots\right\rangle = (\sum_k n_k) \left|n_0 \ldots n_k \ldots\right\rangle$
(5) $\left|n_0, n_1, \ldots n_k \ldots\right\rangle = \frac{(b_k^+)^{n_k}}{(n_k!)^{1/2}} \cdots \frac{(b_1^+)^{n_1}}{(n_1!)^{1/2}} \frac{(b_0^+)^{n_0}}{(n_0)^{1/2}} \left|000 \ldots 0 \ldots\right\rangle$
(6) $H = \sum_k E_k b_k^+ b_k$ is the Hamiltonian of the system.
(7) $[H, b_k^+] = E_k b_k^+$
$[H, b_k] = -E_k b_k$
(8) $e^{-\beta H} b_k^+ e^{\beta H} = e^{-\beta E_k} b_k^+$

(Hint: define $f(\lambda) = e^{-\lambda H} b_k^+ e^{\lambda H}$ and find $\frac{df}{d\lambda}$).

Question QM–3.

Fermions are particles or quanta with half-integral spin, with a possible occupation number 0 or 1 for any single particle quantum state. The interchange of two fermions in a state causes the wavefunction to change sign. Define creation and annihilation operators c_j^+, c_j respectively, where

$$c_j^+ \left|n_0, n, \ldots n_j \ldots\right\rangle = \left|n_0, n, \ldots n_j + 1 \ldots\right\rangle$$
$$c_j \left|n_0, n, \ldots n_j \ldots\right\rangle = \left|n_0, n, \ldots n_j - 1 \ldots\right\rangle$$
$$(c_j^+)^2 = (c_j)^2 = 0$$

Show that

(1) $c_j^+ c_j \left|n_0, n, \ldots n_j \ldots\right\rangle = n_j \left|n_0 \ldots n_j \ldots\right\rangle$ where the n_j's are 0 or 1.
(2) Now let us see how the antisymmetry of the wavefunction gets reflected in the algebra obeyed by the creation and annihilation operators. The spatial wavefunction for the state $c_k^+ c_j^+ \left|0, 0, \ldots,\right\rangle$ is the symmetrised form of $\phi_j(1)\phi_k(2)$, where $\phi_j(1)$ is the wavefunction when particle 1 is placed in state j, etc. For fermions, this means $(\phi_j(1)\phi_k(2) - \phi_j(2)\phi_k(1))/\sqrt{2}$. Note that the ordering of the particles is defined by reading the order of the operators from right to left. Interchange the particles to form the state whose wavefunction is SYM$[\phi_k(1)\phi_j(2)]$. HINT: You should do this in several steps: remove particle 1 from state j; remove particle 2 from state k and then add it to state j; finally add particle 1 to state k. Hence, or otherwise, show that

$$\{c_j^+, c_k^+\} = \{c_j, c_k\} = 0 \quad \text{for all } j, k$$
$$\{c_j, c_k^+\} = \delta_{jk}$$

where $\{u, v\} = uv + vu$ (the "anticommutator"). For the last identity, you may find it helpful to consider the effect of the operator $c_j c_k^+ c_k$ acting on a state.
(3) $H = \sum_j E_j c_j^+ c_j$; $N = \sum_j c_j^+ c_j$. H is the Hamiltonian and N is the number operator of the system of non-interacting particles.
(4)
$$[H, c_k^+] = E_k c_k^+$$
$$[H, c_k] = -E_k c_k$$
(5) $e^{-\beta H} c_k^+ e^{\beta H} = e^{-\beta E_k} c_k^+$

Question QM–4.

By considering the grand canonical ensemble density matrix $\rho = \frac{1}{Z}e^{-\beta(H-\mu N)}$, where the partition function is $Z = \text{Tr}\ e^{-\beta(H-\mu N)}$ or otherwise, show that the thermal equilibrium expectation value of the occupation number operator for the k^{th} level is (μ = chemical potential):

$$\langle N_k \rangle_{\text{bosons}} = \langle b_k^+ b_k \rangle = \frac{1}{e^{\beta(E_k-\mu)} - 1}$$
$$\langle N_k \rangle_{\text{fermions}} = \langle c_k^+ c_k \rangle = \frac{1}{e^{\beta(E_k-\mu)} + 1}$$

[*Hint: write* $H' = H - \mu N$ *and use Q.2(8) and Q.3(5).*]

Question QM–5.

Now we are all set to see how the normal modes of a one-dimensional harmonic chain of equal masses and springs can be described by independent particle excitations. Note that, *a priori*, this is definitely a system with interactions. Consider N masses M joined by springs of spring constant k, separated by a distance a in equilibrium. Let q_i be the displacement of the i^{th} mass from its equilibrium position R_i and p_i its momentum. Assume periodic boundary conditions.

(1) Write down the classical Hamiltonian, and in terms of the normal coordinates

$$\tilde{p}_k = \frac{1}{\sqrt{N}} \sum_i p_i e^{ikR_i}$$
$$\tilde{q}_k = \frac{1}{\sqrt{N}} \sum_i q_i e^{ikR_i}$$

and show that the quantum Hamiltonian H_0 is

$$H_0 = \sum_k \left(\frac{1}{2M} \tilde{p}_k \tilde{p}_{-k} + \frac{1}{2} M \omega_k^2 \tilde{q}_k \tilde{q}_{-k} \right)$$
$$\omega_k^2 = \frac{4k}{M} \sin^2 \left(\frac{ka}{2} \right)$$

(2) Use the quantization condition $[p_i, q_j] = -i\hbar\delta_{ij}$ to find the commutator $[\tilde{p}_k, \tilde{q}_k]$.

(3) Show that $\tilde{p}_k$ and $\tilde{q}_k$ are not Hermitian, but instead satisfy

$$\tilde{q}_k^+ = \tilde{q}_{-k}$$
$$\tilde{p}_k^+ = \tilde{p}_{-k}$$

(4) Using the ideas of Q.1 define annihilation and creation operators in terms of $\tilde{q}_k$, $\tilde{q}_k^+$, $\tilde{p}_k$, $\tilde{p}_k^+$, which allow the Hamiltonian to be transformed into $H = \sum_k \hbar\omega_k (a_k^+ a_k + \frac{1}{2})$ *i.e.*a set of independent oscillators, one for each k value. From Q.1 this shows that a_k^+ creates a *non-interacting* boson with wavenumber k and energy $\hbar\omega_k$. This free particle or elementary excitation is called a phonon.