P7654 HW1

Due Friday Jan 25, 2013

There are 4 problems here – but the first two should be review. Skip them if they are trivial for you. Also skip the last one if you have seen it before (for example in QFT). If you need extra time, I can give you an extension, but you will find the lectures easier to follow if you do these for Friday.

Problem 1. Second Quantization for Bosons One of the most convenient ways to describe the many-body problem is through field operators. Here is a quick refresher. If you know this stuff cold, then skip this question.

First we need to define a basis for n-particle states. A convenient one for bosons is to specify how many particles have each possible momentum,

$$
|\{n_k\}\rangle = |n_0, n_1, \ldots\rangle.
$$

A convenient way to manipulate these states is to borrow the "ladder" operators from harmonic oscillators. The raising (or creation) operator \hat{a}_k^{\dagger} $\frac{1}{k}$ is defined by

$$
\hat{a}_k^{\dagger}|n_0, n_1, \dots, n_k, \dots\rangle = \sqrt{n_k+1}|n_0, n_1, \dots, n_k+1, \dots\rangle.
$$

Its Hermitian conjugate, the lowering (or annihilation) operator is defined by

$$
\hat{a}_k|n_0, n_1, \dots, n_k, \dots\rangle = \sqrt{n_k}|n_0, n_1, \dots, n_k - 1, \dots\rangle.
$$

- **1.1.** Prove the following relationship for the commutator, $[\hat{a}_k, \hat{a}_k^{\dagger}]$ $_{k}^{[}$] = 1.
- **1.2.** Prove that if $k \neq k'$ that $[\hat{a}_k, \hat{a}_k^{\dagger}]$ $_{k'}^{\dagger}]=0.$
- **1.3.** Show that

$$
\hat{a}_{k}^{\dagger} \hat{a}_{k} | n_{0}, n_{1}, \ldots, n_{k}, \ldots \rangle = n_{k} | n_{0}, n_{1}, \ldots, n_{k}, \ldots \rangle.
$$

In other words, the operator $\hat{n}_k = \hat{a}_k^{\dagger}$ $\bar{k}^{\hat{a}}k$ counts the number of bosons with momentum k.

Next we define the "field operator"

$$
\hat{\psi}(r) = \sum_{k} \frac{e^{ik \cdot r}}{\sqrt{V}} \hat{a}_k,
$$

which removes a particle from position r .

1.4. Show that $[\hat{\psi}(r), \hat{\psi}^{\dagger}(r')] = \delta(r - r')$.

We now introduce the "vacuum state" $|vac\rangle = |0 \cdots \rangle$, which is the state containing no particles. Using our field operators we can then readily define the position basis states:

$$
|r_1 \cdots r_N\rangle = \psi^{\dagger}(r_1) \cdots \psi^{\dagger}(r_N) |vac\rangle,
$$

which is the state with particles at postion r_1, r_2, \ldots, r_N . The wavefunctions of elementary quantum mechanics are $\phi(r_1,\ldots,r_N) = \langle r_1 \cdots r_N | \phi \rangle$.

Problem 2. Second Quantization for Fermions: Again, if you know this stuff cold, then skip this question.

For fermions there are signs to worry about, so we will use a basis $|k_1, k_2, \cdots k_N\rangle$, corresponding to the wavefunction

$$
\phi(r_1, \dots r_N) = \frac{1}{\sqrt{N!}^{N}} \left[e^{ik_1 \cdot r_1} e^{ik_2 \cdot r_2} \cdots e^{ik_N \cdot r_N} - e^{ik_2 \cdot r_1} e^{ik_1 \cdot r_2} \cdots e^{ik_N \cdot r_N} + \dots \right]
$$

where you take all permutations weighted with the signature of the permutation. [We will at first neglect spin.] Clearly if you change the order of the $k's$ you get the same state but with a \pm corresponding to the signature of the permutation.

The ladder operators are now defined by $\psi^{\dagger}(q)|k_1,k_2,\cdots k_N\rangle=|k_1,k_2,\cdots k_N,q\rangle$, and $\psi(q)|k_1,k_2,\cdots k_N,q\rangle=$ $|k_1,k_2,\cdots k_N\rangle$.

2.1. Show that the fermionic ladder operators obey the anticommutation relations

$$
\begin{array}{rcl}\n\{\hat{a}_k, \hat{a}_q^{\dagger}\} & = & \delta_{kq} \\
\{\hat{a}_k, \hat{a}_q\} & = & 0\n\end{array}
$$

As with the bosonic case, one again defines an operator which removes a particle from position r ,

$$
\hat{\psi}(r) = \sum_{k} \frac{e^{ik \cdot r}}{\sqrt{V}} \hat{a}_k.
$$

2.2. Show that $\{\hat{\psi}(r), \hat{\psi}^{\dagger}(r')\} = \delta(r - r')$.

Problem 3. Ideal Gas Consider an ideal gas with Hamiltonian

$$
H = \sum_{k} \epsilon_{k} a_{k}^{\dagger} a_{k}
$$

where $\epsilon_k = k^2/2m - \mu$.

3.1. Use the Heisenberg equations of motion for a_k to calculate $a_k(t)$ in terms of $a_k(0)$. Do this for both Bosons and Fermions.

3.2. Write an explicit expression for

$$
G_k^&(\omega) = \int dt e^{i\omega t} \langle a_k(t) a_k^{\dagger}(0) \rangle
$$

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$$

in terms of $n_k = \langle a_k^{\dagger}$ $\int_{k}^{\dagger}(0)a_{k}(0)$. You should use that $\int dt e^{i\nu t} = 2\pi \delta(\nu)$. **3.3.** If the system is in thermal equilibrium at time $t = 0$ we know

$$
n_k = \frac{1}{e^{\beta \epsilon_k} \mp 1}.
$$

Use this to show $G_k^>(\omega) = e^{\beta \omega} G_k^<(\omega)$.

3.4. Find $A_k(\omega) = G_k^>(\omega) - G_k^<(\omega)$

Problem 4. Wick's Theorem: In class we introduced "Wick's Theorem." Here you will convince yourself that it is right. I won't walk you through the full proof – there are lots of great books on it.

Wick's theorem is a theorem about expectation values of linear operators (ie. Matrices) in a Gaussian ensemble. It says that the expectation value of a product of operators is the sum of all pairwise contractions. For fermionic operators the contractions are weighted by $(-1)^s$ where s is the signature of the permutation which brings the pairs together. For bosonic operators, all contractions are equally weighted.

Consider a system with Hamiltonian

$$
H = \sum_{k} \epsilon_{k} a_{k}^{\dagger} a_{k}.
$$

We will think about k being momentum states, and $\epsilon_k = k^2/2m - \mu$, but formally any quadratic Hamiltonian can be written in this form. The operators a_k can be either Bosonic or Fermionic. We wish to calculate expectation values of the form

$$
\langle a_{k_1}^{\dagger} \cdots a_{k_n}^{\dagger} a_{q_n} \cdots a_{q_1} \rangle = \frac{1}{Z} \text{Tr} e^{-\beta H} a_{k_1}^{\dagger} \cdots a_{k_n}^{\dagger} a_{q_n} \cdots a_{q_1}.
$$

The trace can be done using any complete set of states: we will use momentum number states, where there are a definite number of particles in each momentum.

4.1. We will first do a calculation you are familiar with from Statistical Mechanics. Find $n_k = \langle a_k^{\dagger} \rangle$ $_{k}^{\dagger}a_{k}\rangle$. Do it for both Bosons and Fermions. Hint: note that the mode k decouples from the others, so this is either just a sum of two terms (Fermi), or a geometric series (Bose).

4.2. Using the same elementary argument (ie. not Wick's theorem), find $\langle n_k^2 \rangle$ $\langle k \rangle = \langle a_k^{\dagger} \rangle$ $_{k}^{\dagger}a_{k}a_{k}^{\dagger}$ $_k^{\dagger}a_k$. [You can do this by summing the series again, or by differentiating with respect to ϵ_k]. Verify that this agrees with the Wick's theorem result \pm $\mathbf{r}=\mathbf{r}$

$$
\langle a_k^{\dagger} a_k a_k^{\dagger} a_k \rangle = \langle a_k^{\dagger} a_k \rangle \langle a_k a_k^{\dagger} \rangle + \langle a_k^{\dagger} a_k \rangle \langle a_k^{\dagger} a_k \rangle.
$$

What do you conclude about the fluctuations in the occupation of a mode $\langle \hat{n}_k^2 \rangle$ $\langle k \rangle - \langle n_k \rangle^2$? How does this compare to what you would expect classically?

4.3. Now, use the same elementary argument to analyze $\langle a_k^{\dagger} \rangle$ ${}_{k}^{\dagger}a_{k}a_{q}^{\dagger}a_{q}$ where $k \neq q$. Does this agree with Wick's theorem?