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 $\hat{a}_k^\dagger$ is defined by

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

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

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

1.1. Prove the following relationship for the commutator, $[\hat{a}_k, \hat{a}_k^\dagger] = 1$.

Solution 1.1.

$$\begin{aligned}
\left[a_k, a_k^\dagger\right] |n_0, n_1 \cdots n_k, \cdots\rangle &= \left(a_k a_k^\dagger - a_k^\dagger a_k\right) |n_0, n_1 \cdots n_k, \cdots\rangle \\
&= a_k \sqrt{n_k + 1}\, |n_0, n_1 \cdots n_k + 1, \cdots\rangle - a_k^\dagger \sqrt{n_k}\, |n_0, n_1 \cdots n_k - 1, \cdots\rangle \\
&= (n_k + 1)\, |n_0, n_1 \cdots n_k, \cdots\rangle - n_k\, |n_0, n_1 \cdots n_k, \cdots\rangle \\
&= |n_0, n_1 \cdots n_k, \cdots\rangle \\
\Rightarrow \quad \left[a_k, a_k^\dagger\right] &= 1
\end{aligned} \tag{1}$$

1.2. Prove that if $k \neq k'$ that $[\hat{a}_k, \hat{a}_{k'}^\dagger] = 0$.

Solution 1.2.

$$
\begin{aligned}
\left[a_k, a^\dagger_{(k)}\right] \left|n_0 \cdots n_k, n_{(k)} \cdots\right\rangle &= \left(a_k a^\dagger_{(k)} - a^\dagger_{(k)} a_k\right) \left|n_0 \cdots n_k, n_{(k)} \cdots\right\rangle \\
&= a_k \sqrt{n_{(k)}+1} \left|n_0 \cdots n_k, n_{(k)}+1, \cdots\right\rangle - a^\dagger_{(k)} \sqrt{n_k} \left|n_0 \cdots n_k - 1, n_{(k)} \cdots\right\rangle \\
&= \sqrt{n_k \left(n_{(k)}+1\right)} \left|n_0 \cdots n_k - 1, n_{(k)}+1, \cdots\right\rangle \\
&\quad - \sqrt{n_k \left(n_{(k)}+1\right)} \left|n_0 \cdots n_k - 1, n_{(k)}+1, \cdots\right\rangle \\
&= 0 \\
\Rightarrow \quad \left[a_k, a^\dagger_{(k)}\right] &= 0
\end{aligned} \tag{2}
$$

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 $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ counts the number of bosons with momentum k.

Solution 1.3.

$$
\begin{aligned}
a_k^\dagger a_k \left|n_0, n_1 \cdots n_k, \cdots\right\rangle &= a_k^\dagger \sqrt{n_k} \left|n_0, n_1 \cdots n_k - 1, \cdots\right\rangle \\
&= n_k \left|n_0, n_1 \cdots n_k, \cdots\right\rangle
\end{aligned} \tag{3}
$$

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

Solution 1.4.

$$
\begin{aligned}
\left[\psi(r), \psi^\dagger((r))\right] &= \frac{1}{V} \left[\sum_k e^{ik\cdot r} a_k, \sum_{(k)} e^{-i(k)\cdot(r)} a^\dagger_{(k)}\right] \\
&= \frac{1}{V} \sum_{k,(k)} e^{ik\cdot r - i(k)\cdot(r)} \left[a_k, a^\dagger_{(k)}\right] \\
&= \frac{1}{V} \sum_{k,(k)} e^{ik\cdot r - i(k)\cdot(r)} \delta_{k,(k)} \\
&= \frac{1}{V} \sum_k e^{ik\cdot(r-(r))} \\
&= \delta\left(r - (r)\right)
\end{aligned} \tag{4}
$$

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

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

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

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

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

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

Solution 2.1. Let's start with $k = q$.

$$
\begin{aligned}
a_k a_k^\dagger \left|n_0, \cdots n_k = 0, \cdots\right\rangle = \left|n_0, \cdots n_k = 0, \cdots\right\rangle \text{ and } a_k^\dagger a_k \left|n_0, \cdots n_k = 0, \cdots\right\rangle = 0 \\
\Rightarrow \quad \left\{a_k, a_k^\dagger\right\} \left|n_0, \cdots n_k = 0, \cdots\right\rangle = \left|n_0, \cdots n_k = 0, \cdots\right\rangle \\
a_k a_k^\dagger \left|n_0, \cdots n_k = 1, \cdots\right\rangle = 0 \text{ and } a_k^\dagger a_k \left|n_0, \cdots n_k = 1, \cdots\right\rangle = \left|n_0, \cdots n_k = 0, \cdots\right\rangle \\
\Rightarrow \quad \left\{a_k, a_k^\dagger\right\} \left|n_0, \cdots n_k = 1, \cdots\right\rangle = \left|n_0, \cdots n_k = 1, \cdots\right\rangle \\
\Rightarrow \quad \left\{a_k, a_k^\dagger\right\} = 1
\end{aligned}
\tag{5}
$$

The first line does not have permutation factors like $(-1)^P$ because it takes as many steps to get n_k to the rightmost position as it takes to bring it back to its original position, so the total permutation is always even. On the other hand, if it takes P swaps to get n_k (or k) to the right, then when $k \neq q$,

$$
\begin{aligned}
a_k a_q^\dagger \left|\cdots, k, \cdots\right\rangle &= a_k \left|\cdots, k, \cdots, q\right\rangle = (-1)^{P+1} \left|\cdots, q\right\rangle \\
a_q^\dagger a_k \left|\cdots, k, \cdots\right\rangle &= (-1)^P \left|\cdots\right\rangle = (-1)^P \left|\cdots, q\right\rangle \\
\Rightarrow \quad \left\{a_k, a_q^\dagger\right\} &= 0
\end{aligned}
\tag{6}
$$

The other cases (i.e., when $n_k = 0$ or $n_q = 1$ to start with) can be worked out trivially. Combining the above two, we have

$$\left\{a_k, a_q^\dagger\right\} = \delta_{k,q} \tag{7}$$

The second part is even easier; k has to occur either before or after q in a state ket. That means when annihilating both successively, we either have to swap the two or we don't, depending on the order of annihilation. That is the only difference between acting with $a_k a_q$ and $a_q a_k$. Since a single swap brings one minus sign, and the resulting states are the same (viz., without k *and* q), we have

$$\{a_k, a_q\} = 0 \tag{8}$$

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

Solution 2.2.

$$\begin{aligned}\left\{\psi(r), \psi^\dagger((r))\right\} &= \frac{1}{V}\sum_{k,(k)} e^{ik\cdot r - i(k)\cdot(r)} \left\{a_k, a^\dagger_{(k)}\right\} \\ &= \frac{1}{V}\sum_{k,(k)} e^{ik\cdot r - i(k)\cdot(r)} \delta_{k,(k)} \\ &= \frac{1}{V}\sum_{k} e^{ik\cdot(r-(r))} \\ &= \delta\left(r-(r)\right)\end{aligned} \tag{9}$$

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.

Solution 3.1. The Heisenberg equation of motion for a_k is

$$\frac{d}{dt}a_k = i\left[H, a_k\right] = i\left[\sum_p \epsilon_p a_p^\dagger a_p, a_k\right] = i\epsilon_k\left[a_k^\dagger, a_k\right] a_k. \tag{10}$$

For bosons this is simply

$$\frac{d}{dt}a_k = -i\epsilon_k a_k, \tag{11}$$

while for fermions we can write out explicitly

$$\frac{d}{dt}a_k = i\epsilon_k\left(a_k^\dagger a_k - a_k a_k^\dagger\right) a_k = i\epsilon_k\left(2a_k^\dagger a_k - \left\{a_k, a_k^\dagger\right\}\right) a_k = -i\epsilon_k a_k. \tag{12}$$

In both cases, then

$$a_k\left(t\right) = e^{-i\epsilon_k t} a_k\left(0\right). \tag{13}$$

3.2. Write an explicit expression for

$$\begin{aligned}G_k^>(\omega) &= \int dt\, e^{i\omega t}\left\langle a_k(t) a_k^\dagger(0)\right\rangle \\ G_k^<(\omega) &= \int dt\, e^{i\omega t}\left\langle a_k^\dagger(0) a_k(t)\right\rangle\end{aligned}$$

in terms of $n_k = \langle a_k^\dagger(0) a_k(0)\rangle$. You should use that $\int dt\, e^{i\nu t} = 2\pi\delta(\nu)$.

Solution 3.2. Inserting the previous result we find

$$G_k^<(\omega) = \int dt\, e^{i(\omega-\epsilon_k)t} \langle a_k^\dagger(0) a_k(0)\rangle = 2\pi\delta\left(\omega-\epsilon_k\right) n_k \tag{14}$$

while

$$\begin{aligned} G_k^>(\omega) &= \int dt\, e^{i(\omega-\epsilon_k)t} \langle a_k(0) a_k^\dagger(0)\rangle = \pi\delta\left(\omega-\epsilon_k\right) \langle a_k(0) a_k^\dagger(0)\rangle \\ &= \begin{cases} 2\pi\delta\left(\omega-\epsilon_k\right) \langle a_k(0) a_k^\dagger(0) + \left[a_k^\dagger(0), a_k(0)\right]\rangle & Bosons \\ 2\pi\delta\left(\omega-\epsilon_k\right) \langle -a_k(0) a_k^\dagger(0) + \left\{a_k^\dagger(0), a_k(0)\right\}\rangle & Fermions \end{cases} \\ &= 2\pi\delta\left(\omega-\epsilon_k\right)\left(1 \pm n_k\right) \end{aligned} \tag{15}$$

where the plus sign is for bosons and the minus for fermions.

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 $G_k^>(\omega) = e^{\beta\omega} G_k^<(\omega)$.

Solution 3.3. Plugging in the Bose-Einstein and Fermi-Dirac distributions we find

$$\begin{aligned} G_k^>(\omega) &= 2\pi\delta\left(\omega-\epsilon_k\right)\left(1 \pm n_k\right) = 2\pi\delta\left(\omega-\epsilon_k\right) \frac{e^{\beta\epsilon_k} \mp 1 \pm 1}{e^{\beta\epsilon_k} \mp 1} \\ &= 2\pi\delta\left(\omega-\epsilon_k\right) e^{\beta\epsilon_k} n_k = e^{\beta\epsilon_k} G_k^<(\omega). \end{aligned} \tag{16}$$

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

Solution 3.4.

$$A_k(\omega) = G_k^>(\omega) - G_k^<(\omega) = \left(e^{\beta\epsilon_k} - 1\right) G_k^<(\omega) = 2\pi\delta\left(\omega-\epsilon_k\right) \frac{e^{\beta\epsilon_k} - 1}{e^{\beta\epsilon_k} \mp 1}. \tag{17}$$

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

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

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 $n_k = \langle a^\dagger_k a_k \rangle$. 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).

Solution 4.1. Let's begin by reminding ourselves that

$$\mathrm{Tr}\, A = \sum_{\{\psi\}} \langle \psi | A | \psi \rangle \tag{18}$$

where ψ is a complete set of the states describing the system. In this case, we can use the set of states $|\{n_k\}\rangle = \prod_k \frac{\left(a^\dagger_k\right)^{n_k}}{\sqrt{n_k!}} |\mathrm{vac}\rangle$ to expand

$$\mathrm{Tr}\, A = \sum_{\{n_k\}} \langle \{n_k\} | A | \{n_k\} \rangle . \tag{19}$$

For fermions, we sum over $n_k = 0, 1$ while for bosons we sum over all non-negative integers.
Finally, we can also make use of the fact that operators relating to different momenta commute to expand $e^{-\beta H} = e^{-\sum_q \beta \epsilon_q} a^\dagger_q a_q = \prod_q e^{-\beta \epsilon_q a^\dagger_q a_q}$. The trace then cancels out with the partition function in the denominator for all $q \neq k$.
Taking all this into account, we find

$$\begin{aligned} n_k = \langle a^\dagger_k a_k \rangle = \frac{\sum_n \langle n_k | e^{-\beta \epsilon_k a^\dagger_k a_k} a^\dagger_k a_k | n_k \rangle}{\sum_n \langle n_k | e^{-\beta \epsilon_k a^\dagger_k a_k} | n_k \rangle} &= \frac{\sum_n e^{-\beta \epsilon_k n} n}{\sum_n e^{-\beta \epsilon_k n}} \\ &= -\frac{1}{\beta} \frac{\partial}{\partial \epsilon_k} \log \left[\sum_n e^{-\beta \epsilon_k n} \right] . \end{aligned} \tag{20}$$

For fermions we find

$$n^f_k = -\frac{1}{\beta} \frac{\partial}{\partial \epsilon_k} \log \left[1 + e^{-\beta \epsilon_k} \right] = \frac{e^{-\beta \epsilon_k}}{1 + e^{-\beta \epsilon_k}} = \frac{1}{e^{\beta \epsilon_k} + 1} \tag{21}$$

while for bosons we have

$$n^b_k = -\frac{1}{\beta} \frac{\partial}{\partial \epsilon_k} \log \left[\frac{1}{1 - e^{-\beta \epsilon_k}} \right] = \frac{e^{-\beta \epsilon_k}}{1 - e^{-\beta \epsilon_k}} = \frac{1}{e^{\beta \epsilon_k} - 1} . \tag{22}$$

4.2. Using the same elementary argument (ie. not Wick's theorem), find $\langle n^2_k \rangle = \langle a^\dagger_k a_k a^\dagger_k a_k \rangle$. [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

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

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

Solution 4.2. Similar to the previous calculation,

$$\langle \hat{n}_k^2 \rangle = \frac{\sum_n e^{-\beta \epsilon_k n} n^2}{\sum_n e^{-\beta \epsilon_k n}} = \frac{1}{\sum_n e^{-\beta \epsilon_k n}} \left(-\frac{1}{\beta} \frac{\partial}{\partial \epsilon_k} \right)^2 \sum_n e^{-\beta \epsilon_k n}. \tag{23}$$

For fermions we see

$$\langle \left(\hat{n}_k^f \right)^2 \rangle = \frac{1}{1 + e^{-\beta \epsilon_k}} \left(-\frac{1}{\beta} \frac{\partial}{\partial \epsilon_k} \right)^2 \left(1 + e^{-\beta \epsilon_k} \right) = \frac{e^{-\beta \epsilon_k}}{1 + e^{-\beta \epsilon_k}} = \frac{1}{e^{\beta \epsilon_k} + 1}, \tag{24}$$

matching

$$\begin{aligned} \langle a_k^\dagger a_k a_k^\dagger a_k \rangle &= \langle a_k^\dagger a_k \rangle \langle a_k a_k^\dagger \rangle + \langle a_k^\dagger a_k \rangle \langle a_k^\dagger a_k \rangle \\ &= \langle a_k^\dagger a_k \rangle \langle -a_k^\dagger a_k + \left\{ a_k, a_k^\dagger \right\} \rangle + \langle a_k^\dagger a_k \rangle \langle a_k^\dagger a_k \rangle = \langle a_k^\dagger a_k \rangle. \end{aligned} \tag{25}$$

This is as expected because of course for fermions the $\hat{n}_k^2 = \hat{n}_k$.
For bosons

$$\langle \left(n_k^f \right)^2 \rangle = \left(1 - e^{-\beta \epsilon_k} \right) \left(-\frac{1}{\beta} \frac{\partial}{\partial \epsilon_k} \right)^2 \left(\frac{1}{1 - e^{-\beta \epsilon_k}} \right) = \frac{1 + e^{\beta \epsilon_k}}{\left(e^{\beta \epsilon_k} - 1 \right)^2}, \tag{26}$$

matching

$$\begin{aligned} \langle a_k^\dagger a_k a_k^\dagger a_k \rangle &= \langle a_k^\dagger a_k \rangle \langle a_k a_k^\dagger \rangle + \langle a_k^\dagger a_k \rangle \langle a_k^\dagger a_k \rangle \\ &= \langle a_k^\dagger a_k \rangle \langle a_k^\dagger a_k + \left[a_k, a_k^\dagger \right] \rangle + \langle a_k^\dagger a_k \rangle \langle a_k^\dagger a_k \rangle \\ &= 2 \langle n_k \rangle^2 + \langle n_k \rangle = \frac{1 + e^{\beta \epsilon_k}}{\left(e^{\beta \epsilon_k} - 1 \right)^2}. \end{aligned} \tag{27}$$

It's easy to see that the fluctuation in particle number is given by

$$\langle \hat{n}_k \rangle^2 - \langle \hat{n}_k \rangle = e^{\beta \epsilon_k} \langle \hat{n}_k \rangle^2. \tag{28}$$

We see that as $\beta \epsilon_k \gg 1$, i.e. when the temperature scale is large enough to wash out the discreteness of energy levels, we approach the classical result of $\langle \hat{n}_k \rangle^2$.

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

Solution 4.3. This is easy to calculate since k, q are uncoupled. For the direct calculation we have simply

$$\langle a_k^\dagger a_k a_q^\dagger a_q \rangle = \langle a_k^\dagger a_k \rangle \langle a_q^\dagger a_q \rangle = n_k n_q. \tag{29}$$

Wick's theorem, on the other hand, tells us

$$\langle a_k^\dagger a_k a_q^\dagger a_q \rangle = \langle a_k^\dagger a_k \rangle \langle a_q^\dagger a_q \rangle + \langle a_k^\dagger a_q \rangle \langle a_k a_q^\dagger \rangle, \tag{30}$$

and again since k, q are uncoupled the last term drops out and we have the same result.