Quantum Mechanics III
HW 7

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6.4 Starting from equations (6.9) and (6.10), show that the creation and annihilation operators are hermitian conjugates, and verify equations (6.11), (6.13), and (6.15). To avoid inessential complications, assume one boson mode only.

To show the creation/annihilation operators are hermitian conjugates, denote a single boson mode of n particles as the orthonormal states $\{|n\rangle\}$, along with the annihilation operator b

$$b\,|n\rangle = \sqrt{n}\,|n-1\rangle\,.$$

Now form the inner product

$$\begin{aligned}\langle n-1|b|n\rangle &= (n-1, bn) = (b^\dagger(n-1), n)\\ &= \sqrt{n}.\end{aligned}$$

Since the states are orthonormal, this must imply

$$\begin{aligned}b^\dagger\,|n-1\rangle &= \sqrt{n}\,|n\rangle\\ \Rightarrow b^\dagger\,|n\rangle &= \sqrt{n+1}\,|n+1\rangle\,.\end{aligned}$$

The operator equation above, equivalent to the hermitian conjugate of the annihilation operator, is the definition of the creation operator (6.10).

For a single mode, we have

$$[b, b^\dagger]\,|n\rangle = (n+1)\,|n\rangle - n\,|n\rangle = |n\rangle \Rightarrow [b, b^\dagger] = 1,$$

thus

$$[b, b] = [b^\dagger, b^\dagger] = 0, \quad [b, b^\dagger] = 1.$$

As for the number operator

$$\hat{n}\,|n\rangle = b^\dagger b\,|n\rangle = b^\dagger\sqrt{n}\,|n-1\rangle = n\,|n\rangle\,.$$

Lastly, we may form any n particle state $|n\rangle$ of a single boson mode by acting $b^\dagger$ on the vacuum:

$$(b^\dagger)^n\,|0\rangle = (b^\dagger)^{n-1}\,|1\rangle = (b^\dagger)^{n-2}\sqrt{2}\,|2\rangle = (b^\dagger)^{n-3}\sqrt{3}\sqrt{2}\,|3\rangle = ... = \sqrt{n!}\,|n\rangle$$

So to get just the state $|n\rangle$ we divide by $\sqrt{n!}$

$$\frac{(b^\dagger)^n}{\sqrt{n!}} = |n\rangle\,.$$

6.6 Show by direct calculation of the relevant commutator that the particle number $\hat{N} = \sum_{\mathbf{k}\sigma} \hat{n}_{\mathbf{k}\sigma}$ is a constant of motion for our interacting electron gas, Eq. (6.47).

From the Heisenberg equation of motion for the number operator $\hat{N}$,

$$-i\hbar\frac{d}{dt}\hat{N} = [H, \hat{N}] \stackrel{!}{=} 0.$$

In computing the commutator

$$[H, \hat{N}] = \left[\left(\sum_{\mathbf{k},\sigma} \epsilon_k c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{e^2}{2\epsilon_0 V} \sum_{\mathbf{kpq},\lambda\sigma} \frac{1}{q^2} c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}\right), \sum_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'}\right].$$

we must make use of the anti-commutation relations

$$[c_k, c_l]_+ = [c^\dagger_k, c^\dagger_l]_+ = 0 \Rightarrow c_k c_l = -c_l c_k, \quad c^\dagger_k c^\dagger_l = -c^\dagger_l c^\dagger_k$$

$$[c_k, c^\dagger_l]_+ = \delta_{kl} \Rightarrow c_k c^\dagger_l = \delta_{kl} - c^\dagger_l c_k$$

along with the commutator of the number operator

$$[\hat{n}_{\mathbf{k}\sigma}, \hat{n}_{\mathbf{k}'\sigma'}] = [c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'}] = 0.$$

The kinetic term in the Hamiltonian consists of number operators (multiplied by associated energies), so

$$\begin{aligned}\left[\sum_{\mathbf{k},\sigma} \epsilon_k c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \hat{N}\right] &= \sum_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \epsilon_k \left[c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'}\right] \\ &= \sum_{\mathbf{k}\sigma\mathbf{k}'\sigma'} \epsilon_k \left[\hat{n}_{\mathbf{k}\sigma}, \hat{n}_{\mathbf{k}'\sigma'}\right] = 0.\end{aligned}$$

As for the interaction term, we cut it down to the form

$$\begin{aligned}\left[\left(\sum_{\mathbf{kpq},\lambda\sigma} \frac{1}{q^2} c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}\right), \sum_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'}\right] &= \sum_{\mathbf{kpq},\lambda\sigma,\mathbf{k}'\sigma'} \frac{1}{q^2} \left[c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}, c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'}\right] \\ &\sim c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} - c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}.\end{aligned}$$

Before we go further, it will be helpful to use the following relation between operators

$$\begin{aligned}c_i c_j c^\dagger_k &= c_i(-c^\dagger_k c_j + \delta_{jk}) \\ &= -c_i c^\dagger_k c_j + c_i \delta_{jk} \\ &= -(-c^\dagger_k c_i + \delta_{ik}) c_j + c_i \delta_{jk} \\ &= c^\dagger_k c_i c_j - \delta_{ik} c_j + \delta_{jk} c_i\end{aligned}$$

and similarly

$$c_i c^\dagger_j c^\dagger_k = c^\dagger_j c^\dagger_k c_i - \delta_{ik} c^\dagger_j + \delta_{ij} c^\dagger_k.$$

Now put it to use

$$\begin{aligned}&c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} - c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} \\ &= \{c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} (c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} - \delta_{\mathbf{p}\sigma,\mathbf{k}'\sigma'} c_{\mathbf{k}\lambda} + \delta_{\mathbf{k}\lambda,\mathbf{k}'\sigma'} c_{\mathbf{p}\sigma}) c_{\mathbf{k}'\sigma'}\} \\ &\quad - \{c^\dagger_{\mathbf{k}'\sigma'} (c^\dagger_{\mathbf{k+q}\lambda} c^\dagger_{\mathbf{p-q}\sigma} c_{\mathbf{k}'\sigma'} - \delta_{\mathbf{p-q}\sigma,\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k+q}\lambda} + \delta_{\mathbf{k+q}\lambda,\mathbf{k}'\sigma'} c^\dagger_{\mathbf{p-q}\sigma}) c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}\}.\end{aligned}$$

By virtue of $[c_k, c_l]_+ = [c_k^\dagger, c_l^\dagger]_+ = 0$, we can commute operators in the terms without any delta functions to find that they both cancel. We are then left with

$$\begin{aligned}
&\{-\delta_{\mathbf{p}\sigma,\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{k}\lambda} c_{\mathbf{k}'\sigma'} + \delta_{\mathbf{k}\lambda,\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}'\sigma'}\} \\
&\quad - \{-\delta_{\mathbf{p}-\mathbf{q}\sigma,\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} + \delta_{\mathbf{k}+\mathbf{q}\lambda,\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}\} \\
&= \{-c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{k}\lambda} c_{\mathbf{p}\sigma} + c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}\} \\
&\quad - \{-c^\dagger_{\mathbf{p}-\mathbf{q}'\sigma} c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} + c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}\} \\
&= \{-c^\dagger_{\mathbf{p}-\mathbf{q}'\sigma} c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} + c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}\} \\
&\quad - \{-c^\dagger_{\mathbf{p}-\mathbf{q}'\sigma} c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} + c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda}\} \\
&= 0.
\end{aligned}$$

Now that my eyes hurt, we can confirm that

$$\frac{d}{dt}\hat{N} = \frac{i}{\hbar}[H, \hat{N}] = 0$$

and so $\hat{N}$, the total number of particles, is a constant of motion.

6.12 The boson-fermion model is specified by the Hamiltonian

$$H/\hbar = \omega a^\dagger a + \omega_0 c^\dagger c + (\Omega c^\dagger a + \Omega^* a^\dagger c),$$

where a and c are boson and fermion operators and ω, ω_0, Ω are appropriate constants. Show that the number of excitations $\hat{N} = a^\dagger a + c^\dagger c$ is a constant of the motion.

Since the spin space of bosons and fermions are fundamentally different (integer vs half integer), it should follow that boson operators and fermion operators commute

$$[a, c] = [a^\dagger, c^\dagger] = [a, c^\dagger] = [a^\dagger, c] = 0.$$

Boson operators a obey the commutation relation

$$[a, a^\dagger] = 1 \tag{1}$$

while the fermion operators c obey anti-commutation relation

$$[c, c^\dagger]_+ = 1. \tag{2}$$

To find the time dependence of $\hat{N}$, we commute with the Hamiltonian as before

$$\begin{aligned}
[H, \hat{N}] &= \left[\omega a^\dagger a + \omega_0 c^\dagger c + (\Omega c^\dagger a + \Omega^* a^\dagger c), a^\dagger a + c^\dagger c\right] \\
&= \left[\Omega c^\dagger a + \Omega^* a^\dagger c, a^\dagger a + c^\dagger c\right] \\
&= \Omega c^\dagger [a, a^\dagger a] + \Omega a [c^\dagger, c^\dagger c] + \Omega^* c [a^\dagger, a^\dagger a] + \Omega^* a^\dagger [c, c^\dagger c].
\end{aligned}$$

The commutations with the number operator are solved using (1) and (2)

$$[a, a^\dagger a] = [a, N_a] = a, \qquad [a^\dagger, a^\dagger a] = [a^\dagger, N_a] = -a^\dagger$$

while for fermions

$$[c, c^\dagger c] = [c, N_c] = c, \qquad [c^\dagger, c^\dagger c] = [c^\dagger, N_c] = -c^\dagger.$$

Altogether then, we have

$$[H, \hat{N}] = \Omega c^\dagger a + \Omega a(-c^\dagger) + \Omega^* c(-a^\dagger) + \Omega^* a^\dagger c = 0$$

Thus $\hat{N}$ is a constant of motion.

6.15 Let us study the electron gas. As we know from statistical mechanics, if there were no electron-electron interactions, at zero temperature the thermal equilibrium would be the Fermi sea: one-particle states with the wave number k less than the Fermi wave number k_F are occupied and the rest of the states are empty. Of course, the ground state energy of the noninteracting gas is $\frac{3}{5}N\epsilon_F$.

(a) Regarding the electron-electron interactions as a perturbation, find the leading correction to the energy in integral form.

The integral can be done analytically, but you do not need to do it to answer the following questions:

(b) In the perturbative limit, do the repulsive electron-electron interactions increase or decrease the energy?

(c) The interaction energy per electron is obviously a function of density n, and at $T = 0$ there is no other independent intensive thermodynamic variable. How does the interaction energy scale as a function of density?

Finally:

(d) Find the interaction energy explicitly, including the dimensionless multiplicative constant.

(a) Recall that the first order correction to the energy due to perturbation H^1 is

$$E_n^1 = \langle n^0 | H^1 | n^0 \rangle$$

where $|n^0\rangle$ is the unperturbed eigenstate of H^0 with energy E_n^0. In this case, the ground state ($T = 0$) is the fermi sea, where all states are occupied up to

$$k_F = \left(\frac{6\pi^2 n}{g} \right)^{1/3}$$

with particle density n and degeneracy $g = 2s + 1 = 2$. We denote the ground state as

$$|GS\rangle = \prod_{\sigma, \mathbf{k}: |\mathbf{k}| < k_F} c^\dagger_{\mathbf{k}\sigma} |0\rangle \, .$$

The first order contribution is then the expectation of the electron-electron interaction potential V

$$E^1 = \langle GS | V | GS \rangle = \frac{e^2}{2\epsilon_0 V} \sum_{\mathbf{kpq}, \lambda\sigma} \frac{1}{q^2} \langle GS | c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} | GS \rangle \, .$$

Focusing on the inner product term,

$$\langle GS | c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} | GS \rangle \, ,$$

all first order perturbations are zero unless

$$c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} |GS\rangle = a \, |GS\rangle$$

for some eigenvalue a. This is due to the $\langle GS | \psi \rangle = \delta_{GS,\psi}$ where $|\psi\rangle$ is a single state in the Fock space. Since $\mathbf{q} \neq 0$, the above may only be satisfied given

$$\begin{aligned}
c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} |GS\rangle &\to \delta_{\lambda,\sigma} \delta_{\mathbf{k}+\mathbf{q},\mathbf{p}} c^\dagger_{\mathbf{k}+\mathbf{q}\lambda} c^\dagger_{\mathbf{p}-\mathbf{q}\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}\lambda} |GS\rangle \\
&= c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma} |GS\rangle \\
&= -c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} |GS\rangle \\
&= -\hat{n}_{\mathbf{k}+\mathbf{q}\sigma} \hat{n}_{\mathbf{k}\sigma} |GS\rangle
\end{aligned}$$

where in the third line, we note that $\mathbf{k} \neq \mathbf{k}+\mathbf{q}$ for the anti-commutation. Thus our summation is now only over three indices

$$E^1 = \langle GS|V|GS\rangle = \frac{e^2}{2\epsilon_0 V}\sum_{\sigma,\mathbf{kq}} -\frac{1}{q^2}\langle GS|\hat{n}_{\mathbf{k+q}\sigma}\hat{n}_{\mathbf{k}\sigma}|GS\rangle$$

The number operators will return a 1 if $|\mathbf{k}+\mathbf{q}|, |\mathbf{k}| < k_F$ and zero otherwise, and the so the expectation may be expressed as step functions. In the thermodynamic limit, as we take the length of our box $L \to \infty$, the lattice spacing of our quantized $\mathbf{k}$ values becomes infinitesimal and we may perform an integration

$$\frac{e^2}{2\epsilon_0 V}\sum_{\sigma,\mathbf{kq}} -\frac{1}{q^2}\langle GS|\hat{n}_{\mathbf{k+q}\sigma}\hat{n}_{\mathbf{k}\sigma}|GS\rangle \to -\frac{e^2}{2\epsilon_0 V}\left(\frac{V}{(2\pi)^3}\right)^2 \int d^3k\ d^3q\ \frac{1}{q^2}\theta(k_F-|\mathbf{k}|)\theta(k_F-|\mathbf{k}+\mathbf{q}|)$$

For each direction of $\mathbf{q}$, we vary $\mathbf{k}$ over all space. Under integration over k, the term $|\mathbf{k}+\mathbf{q}|$ does not depend on the *direction* of $\mathbf{q}$, but rather on the magnitude. So we write the following integral

$$E^1 = -\frac{e^2}{2\epsilon_0 V}\left(\frac{V}{(2\pi)^3}\right)^2 8\pi^2 \int dq\ dk\ d(\cos\theta_k)\ k^2\ \theta(k_F - \sqrt{k^2+q^2+2kq\cos\theta_k})\theta(k_F-|\mathbf{k}|)$$

Note that k is bound to a maximum of k_F, so $k < k_F$. From this we deduce that $0 < q < 2k_F$. Moreover

$$\begin{aligned}
k^2+q^2+2kq\cos\theta_k &\leq k_F^2 \\
q\cos\theta_k &\leq \frac{k_F^2-k^2-q^2}{2k} \\
q\cos\theta_k &\leq -\frac{q^2}{2k_F} \\
\cos\theta_k &\leq -\frac{q}{2k_F} \\
1 \geq \cos\theta_k &\geq \frac{q}{2k_F}
\end{aligned}$$

where we have added the upper bound of unity. Thus $\frac{q}{2\cos\theta_k} < k < k_F$. The integral may then be formed as

$$\begin{aligned}
E^1 &= -\frac{e^2}{2\epsilon_0 V}\left(\frac{V}{(2\pi)^3}\right)^2 8\pi^2 \int_0^{2k_F} dq \int_{\frac{q}{2k_F}}^1 d(\cos\theta_k) \int_{\frac{q}{2\cos\theta_k}}^{k_F} dk\ k^2 \\
&= -\frac{e^2}{4\pi\epsilon_0} V \frac{k_F^4}{4\pi^3} \\
&= -\frac{e^2}{4\pi\epsilon_0}\frac{V}{4\pi^3}\left(3\pi^2 n\right)^{4/3}
\end{aligned}$$

(b) From the integration over $\mathbf{q}$ and $\mathbf{k}$, we see that the integrand is positive and the overall sign of the perturbation due to e-e interaction is negative (can also be seen by explicit evaluation of integral). So the interaction energy decreases the total energy in the limit of first order perturbation.

(c),(d) The interaction energy per particle can be found from part (a) as

$$\begin{aligned}
\frac{E^1}{N} &= -\frac{e^2}{4\pi\epsilon_0}\frac{1}{4\pi^3}\left(3\pi^2\right)^{4/3} n^{1/3} \\
&\sim -n^{1/3}
\end{aligned}$$