Physics 726: Assignment 3

(to be submitted by Thursday, February 18, 2016)

1. A system of spinless fermions is described by the Hamiltonian

$$\hat{H} = \sum_{m=1}^{\infty} \varepsilon_m c_m^\dagger c_m,$$

where the energy levels $\varepsilon_1 < \varepsilon_2 < \varepsilon_3 < \cdots$ are strictly ordered. The N-fermion ground state is a *Fermi Sea* with all energy levels filled up to ε_N:

$$|F^{(N)}\rangle = c_N^\dagger \cdots c_2^\dagger c_1^\dagger |\text{vac}\rangle.$$

(a) Show explicitly that $|F^{(N)}\rangle$ is an eigenstate of the total number operator $\hat{N} = \sum_{m=1}^{\infty} c_m^\dagger c_m$.

$$\begin{aligned}
\hat{N}|F^{(N)}\rangle &= \hat{N} c_N^\dagger \cdots c_2^\dagger c_1^\dagger |\text{vac}\rangle \\
&= \sum_{m=1}^{\infty} c_m^\dagger c_m c_N^\dagger \cdots c_2^\dagger c_1^\dagger |\text{vac}\rangle \\
&= \sum_{m=1}^{N} c_N^\dagger \cdots c_{m+1}^\dagger \underbrace{c_m^\dagger c_m c_m^\dagger}_{c_m^\dagger(1-c_m^\dagger c_m)} c_{m-1}^\dagger \cdots c_2^\dagger c_1^\dagger |\text{vac}\rangle + \sum_{m=N+1}^{\infty} c_N^\dagger \cdots c_2^\dagger c_1^\dagger c_m^\dagger \underbrace{c_m |\text{vac}\rangle}_{0} \\
&= \sum_{m=1}^{N} c_N^\dagger \cdots c_{m+1}^\dagger c_m^\dagger c_{m-1}^\dagger \cdots c_2^\dagger c_1^\dagger |\text{vac}\rangle = N|F^{(N)}\rangle
\end{aligned}$$

(b) Confirm that $c_4|F^{(5)}\rangle = -c_5^\dagger c_3^\dagger c_2^\dagger c_1^\dagger|\text{vac}\rangle$, and explain why we should view this as the lowest-lying excited state of the four-fermion system.

$$\begin{aligned}
c_4|F^{(5)}\rangle &= c_4 c_5^\dagger c_4^\dagger c_3^\dagger c_2^\dagger c_1^\dagger |\text{vac}\rangle \\
&= -c_5^\dagger \underbrace{c_4 c_4^\dagger}_{1-c_4^\dagger c_4} c_3^\dagger c_2^\dagger c_1^\dagger |\text{vac}\rangle \\
&= -c_5^\dagger c_3^\dagger c_2^\dagger c_1^\dagger |\text{vac}\rangle + c_5^\dagger c_4^\dagger c_4 c_3^\dagger c_2^\dagger c_1^\dagger |\text{vac}\rangle \\
&= -c_5^\dagger c_3^\dagger c_2^\dagger c_1^\dagger |\text{vac}\rangle + (-1)^3 c_5^\dagger c_4^\dagger c_3^\dagger c_2^\dagger c_1^\dagger \underbrace{c_4 |\text{vac}\rangle}_{0}
\end{aligned}$$

$|F^{(5)}\rangle$ is the ground state of the five-particle system, because its energy $\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + \varepsilon_5$ is the lowest of any state with five fermions. Similarly, $|F^{(4)}\rangle = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4$ is the ground state of the four-particle system. $c_4|F^{(5)}\rangle$ is also a state with four fermions, but it differs from $|F^{(4)}\rangle$ in that orbital 4 is empty and orbital 5 is occupied instead. We can view this as the fermion in orbital 4 having been promoted upward to the next available orbital.

(c) Prove that $\langle F^{(N)}|F^{(N')}\rangle = \delta_{N,N'}$, which is to say that the state $|F^{(N)}\rangle$ is (i) properly normalized and (ii) orthogonal to any Fermi Sea with a different number of particles.

If $N = N'$, we can proceed by induction. Observe that $\langle F^{(0)}|F^{(0)}\rangle = \langle \text{vac}|\text{vac}\rangle = 1$ and that

$$\begin{aligned}
\langle F^{(N)}|F^{(N)}\rangle &= \langle \text{vac}|c_1 c_2 \cdots c_{N-1} \underbrace{c_N c_N^\dagger}_{1-c_N^\dagger c_N} c_{N-1}^\dagger \cdots c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&= \langle \text{vac}|c_1 c_2 \cdots c_{N-2} \underbrace{c_{N-1} c_{N-1}^\dagger}_{1-c_{N-1}^\dagger c_{N-1}} c_{N-2}^\dagger \cdots c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&\qquad - (-1)^{N-1}\langle \text{vac}|c_1 c_2 \cdots c_{N-1} c_N^\dagger \cdots c_2^\dagger c_1^\dagger \underbrace{c_N|\text{vac}\rangle}_{0} \\
&= \langle F^{(N-1)}|F^{(N-1)}\rangle = 1
\end{aligned}$$

On the other hand, if $N > N'$ then

$$\begin{aligned}
\langle F^{(N)}|F^{(N')}\rangle &= \langle \text{vac}|c_1 c_2 \cdots c_N c_{N'}^\dagger \cdots c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&= (-1)^{N'}\langle \text{vac}|c_1 c_2 \cdots c_{N-1} c_{N'}^\dagger \cdots c_2^\dagger c_1^\dagger \underbrace{c_N|\text{vac}\rangle}_{0} = 0
\end{aligned}$$

The case of $N < N'$ follows in the same way, since $\langle F^{(N)}|F^{(N')}\rangle^* = \langle F^{(N')}|F^{(N)}\rangle = 0$.

(d) Following the logic of question 1(c), demonstrate that

$$\langle F^{(N)}|c_i|F^{(N')}\rangle \sim \delta_{N+1,N'}\,\theta(N \geq 0)\,\theta(N' \geq 1)$$
$$\text{and } \langle F^{(N)}|c_j^\dagger c_k^\dagger c_l|F^{(N')}\rangle \sim \delta_{N,N'+1}\,\theta(N \geq 2)\,\theta(N' \geq 1).$$

The expressions above rely on a modified Heaviside notation in which $\theta(\text{true}) = 1$ and $\theta(\text{false}) = 0$.

So long as $1 \leq i \leq N'$ and $N' > 0$, $c_i|F^{(N')}\rangle$ is an $(N'-1)$-particle state. So the overlap $\langle F^{(N)}|c_i|F^{(N')}\rangle$ is only nonzero if $N' - 1 \geq 0$ and $N \geq 0$ are equal—hence the $\delta_{N+1,N'}$ and the θ factors that follow it.

So long as $1 \leq i \leq N'$ and $1 \leq j < k \leq N$ or $1 \leq k < j \leq N$, the states $c_l|F^{(N')}\rangle$ and $c_k c_j|F^{(N)}\rangle$ describe collections of $N' - 1 \geq 0$ and $N - 2 \geq 0$ particles.

(e) Convince yourself that the first expectation value in question 1(d) vanishes unless $i = N + 1$. List all the possible values of j, k, and l such that the second expectation value is guaranteed to be nonzero.

Consider $c_i|F^{(N')}\rangle$. If $i = N'$, the resulting state is exactly $|F^{(N'-1)}\rangle$, up to a phase. Otherwise, it is an excited $(N'-1)$-particle state that is not a Fermi Sea ground state. The only nonvanishing contribution from $\langle F^{(N)}|c_i|F^{(N')}\rangle$ arises when $i = N' = N + 1$.

For the second expression, we need $N = N' + 1 > 0$, $1 \leq i \leq N'$, and either $j = N$, $k = i$ or $j = i$, $k = N$.

(f) Show that $\langle F^{(1)}|c_i^\dagger c_j|F^{(1)}\rangle = \delta_{i,1}\delta_{j,1}$ and $\langle F^{(2)}|c_i^\dagger c_j|F^{(2)}\rangle = \delta_{i,1}\delta_{j,1} + \delta_{i,2}\delta_{j,2}$ and that, more generally,

$$\langle F^{(N)}|c_i^\dagger c_j|F^{(N)}\rangle = \sum_{m=1}^{N} \delta_{i,m}\delta_{j,m} = \delta_{i,j}\,\theta(1 \leq i \leq N) = \delta_{i,j}\langle F^{(N)}|\hat{n}_i|F^{(N)}\rangle \equiv \delta_{i,j}\langle \hat{n}_i\rangle.$$

The one-particle Fermi sea:

$$\begin{aligned}
\langle F^{(1)}|c_i^\dagger c_j|F^{(1)}\rangle &= \langle \text{vac}|c_1 c_i^\dagger c_j c_1^\dagger|\text{vac}\rangle \\
&= \langle \text{vac}|(\delta_{i,1} - c_i^\dagger c_1)(\delta_{j,1} - c_1^\dagger c_j)|\text{vac}\rangle \\
&= \delta_{i,1}\delta_{j,1}
\end{aligned}$$

The two-particle Fermi sea:

$$\begin{aligned}
\langle F^{(2)}|c_i^\dagger c_j|F^{(2)}\rangle &= \langle \text{vac}|c_1 c_2 c_i^\dagger c_j c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&= \langle \text{vac}|c_1 (\delta_{i,2} - c_i^\dagger c_2)(\delta_{j,2} - c_2^\dagger c_j) c_1^\dagger|\text{vac}\rangle \\
&= \langle \text{vac}|c_1 (\delta_{i,2} - c_i^\dagger c_2)(\delta_{j,2} - c_2^\dagger c_j) c_1^\dagger|\text{vac}\rangle \\
&= \langle \text{vac}|c_1 (\delta_{i,2}\delta_{j,2} - \delta_{i,2} c_2^\dagger c_j - \delta_{j,2} c_i^\dagger c_2 + c_i^\dagger c_2 c_2^\dagger c_j) c_1^\dagger|\text{vac}\rangle \\
&= \delta_{i,2}\delta_{j,2}\langle \text{vac}|c_1 c_1^\dagger|\text{vac}\rangle - \delta_{i,2}\langle \text{vac}|c_1 c_2^\dagger c_j c_1^\dagger|\text{vac}\rangle \\
&\qquad - \delta_{j,2}\langle \text{vac}|c_1 c_i^\dagger c_2 c_1^\dagger|\text{vac}\rangle + \langle \text{vac}|c_1 c_i^\dagger c_2 c_2^\dagger c_j c_1^\dagger|\text{vac}\rangle \\
&= \delta_{i,2}\delta_{j,2} - \delta_{i,2}\langle \text{vac}|(-c_2^\dagger c_1)(\delta_{j,1} - c_1^\dagger c_j)|\text{vac}\rangle \\
&\qquad - \delta_{j,2}\langle \text{vac}|(\delta_{i,1} - c_i^\dagger c_1)(-c_1^\dagger c_2)|\text{vac}\rangle \\
&\qquad + \langle \text{vac}|(\delta_{i,1} - c_i^\dagger c_1)(1 - c_2^\dagger c_2)(\delta_{j,1} - c_1^\dagger c_j)|\text{vac}\rangle \\
&= \delta_{i,1}\delta_{j,1} + \delta_{i,2}\delta_{j,2}
\end{aligned}$$

The N-particle Fermi sea, solved by recursion:

$$\begin{aligned}
\langle F^{(N)}|c_i^\dagger c_j|F^{(N)}\rangle &= \langle \text{vac}|c_1 c_2 \cdots c_{N-1} c_N c_i^\dagger c_j c_N^\dagger c_{N-1}^\dagger \cdots c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&= \langle \text{vac}|c_1 c_2 \cdots c_{N-1} (\delta_{i,N} - c_i^\dagger c_N)(\delta_{j,N} - c_N^\dagger c_j) c_{N-1}^\dagger \cdots c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&= \delta_{i,N}\delta_{j,N} \underbrace{\langle F^{(N-1)}|F^{(N-1)}\rangle}_{1} - \delta_{i,N} \underbrace{\langle F^{(N-1)}|c_N^\dagger c_j|F^{(N-1)}\rangle}_{0} \\
&\qquad - \delta_{j,N} \underbrace{\langle F^{(N-1)}|c_i^\dagger c_N|F^{(N-1)}\rangle}_{0} + \langle F^{(N-1)}|c_i^\dagger c_N c_N^\dagger c_j|F^{(N-1)}\rangle \\
&= \delta_{i,N}\delta_{j,N} + \langle F^{(N-1)}|c_i^\dagger (1 - \underbrace{c_N^\dagger c_N}_{0}) c_j|F^{(N-1)}\rangle \\
&= \delta_{i,N}\delta_{j,N} + \sum_{n=1}^{N-1} \delta_{i,n}\delta_{j,n} \\
&= \sum_{n=1}^{N} \delta_{i,n}\delta_{j,n}
\end{aligned}$$

(g) Compute the expectation value of an arbitrary biquadratic operator string. You should find that

$$\langle F^{(N)}|c_i^\dagger c_j^\dagger c_k c_l|F^{(N)}\rangle = (\delta_{i,l}\delta_{j,k} - \delta_{i,k}\delta_{j,l})(1 - \delta_{i,j})(1 - \delta_{k,l})\langle \hat{n}_i\rangle\langle \hat{n}_j\rangle.$$

(h) The ground state of the three-fermion system is $|F^{(3)}\rangle = c_3^\dagger c_2^\dagger c_1^\dagger|\text{vac}\rangle$. Show that it has energy

$$\sum_m \varepsilon_m \langle F^{(3)}|c_m^\dagger c_m|F^{(3)}\rangle = \varepsilon_1 + \varepsilon_2 + \varepsilon_3.$$

Hint: have a look at what you proved in question 1(f).

(i) Recall that in single-particle quantum mechanics, the wave function $\Psi(x) = \langle x|\Psi\rangle$ is just the position representation of the state $|\Psi\rangle$. With this in mind, compute the real-space, many-body wave function corresponding to the state $|F^{(3)}\rangle$. First, build a state with three fermions in definite positions, $|x_1, x_2, x_3\rangle = \hat{\psi}^\dagger(x_3)\hat{\psi}^\dagger(x_2)\hat{\psi}^\dagger(x_1)|\text{vac}\rangle$. Then take its overlap with the ket of interest:

$$\Psi(x_1, x_2, x_3) = \langle x_1, x_2, x_3|F^{(3)}\rangle = \langle \text{vac}|\hat{\psi}(x_1)\hat{\psi}(x_2)\hat{\psi}(x_3) c_3^\dagger c_2^\dagger c_1^\dagger|\text{vac}\rangle.$$

Hint: use the field operator expansion and remember what you did in question 1(g).

$$\begin{aligned}
\Psi(x_1, x_2, x_3) &= \langle \text{vac}|\hat{\psi}(x_1)\hat{\psi}(x_2)\hat{\psi}(x_3)c_3^\dagger c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&= \langle \text{vac}|\Big(\sum_{l=1}^{\infty}\phi_l(x_1)c_l\Big)\Big(\sum_{m=1}^{\infty}\phi_m(x_2)c_m\Big)\Big(\sum_{n=1}^{\infty}\phi_n(x_3)c_n\Big)c_3^\dagger c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&= \sum_{l,m,n}\phi_l(x_1)\phi_m(x_2)\phi_n(x_3)\langle \text{vac}|c_l c_m c_n c_3^\dagger c_2^\dagger c_1^\dagger|\text{vac}\rangle \\
&= \sum_{l,m,n}\phi_l(x_1)\phi_m(x_2)\phi_n(x_3)\sum_P(-1)^P\delta_{P1,l}\delta_{P2,m}\delta_{P3,n} \\
&= \sum_P(-1)^P\phi_{P1}(x_1)\phi_{P2}(x_2)\phi_{P3}(x_3) \\
&= \phi_1(x_1)\phi_2(x_2)\phi_3(x_3) - \phi_2(x_1)\phi_1(x_2)\phi_3(x_3) + \phi_2(x_1)\phi_3(x_2)\phi_1(x_3) \\
&\quad - \phi_1(x_1)\phi_3(x_2)\phi_2(x_3) + \phi_3(x_1)\phi_1(x_2)\phi_2(x_3) - \phi_3(x_1)\phi_2(x_2)\phi_1(x_3)
\end{aligned}$$

2. Consider a collection of interacting fermions (again, spinless for simplicity). In second quantized form, the Hamiltonian is

$$\hat{H} = \int dx\,\hat{\psi}^\dagger(x)T(x)\hat{\psi}(x) + \frac{1}{2}\int dx\int dy\,\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)V(x,y)\hat{\psi}(y)\hat{\psi}(x).$$

Suppose that the one-body term has eigenfunctions $\phi_m(x)$ that satisfy $T\phi_m = \varepsilon_m\phi_m$. Proceed by expressing the field operators as an expansion in these one-body modes:

$$\hat{\psi}(x) = \sum_{m=1}^{\infty}\phi_m(x)c_m \quad\text{and}\quad \hat{\psi}^\dagger(x) = \sum_{m=1}^{\infty}\phi_m^*(x)c_m^\dagger.$$

(a) Show that the Hamiltonian can be written as

$$\hat{H} = \sum_m \varepsilon_m c_m^\dagger c_m + \sum_{j,k,l,m} V_{j,k,l,m}c_j^\dagger c_k^\dagger c_l c_m,$$

in terms of a two-body matrix element

$$V_{j,k,l,m} = \frac{1}{2}\int dx\int dy\,\phi_j^*(x)\phi_k^*(y)V(x,y)\phi_l(y)\phi_m(x).$$

Substitute for $\hat{\psi}$. Make use of the fact that $\int\phi_n^* T\phi_m = \varepsilon_m\delta_{m,n}$ and the definition of $V_{j,k,l,m}$.

(b) If the interactions are sufficiently weak, we may be able to treat their effect as a perturbation on the noninteracting system, which has a ground state $|F^{(N)}\rangle$. Show that the first-order energy shift is

$$\Delta E = \sum_{i,j,k,l} V_{i,j,k,l}\,\langle F^{(N)}|c_i^\dagger c_j^\dagger c_k c_l|F^{(N)}\rangle = \sum_{1\le i<j\le N} 2(V_{i,j,j,i} - V_{i,j,i,j}).$$

From the result in 1(g),

$$\begin{aligned}
\Delta E &= \sum_{i,j,k,l} V_{i,j,k,l} \, \langle F^{(N)} | c_i^\dagger c_j^\dagger c_k c_l | F^{(N)} \rangle \\
&= \sum_{i,j,k,l} V_{i,j,k,l} \, (\delta_{i,l}\delta_{j,k} - \delta_{i,k}\delta_{j,l})(1-\delta_{i,j})(1-\delta_{k,l})\langle \hat{n}_i \rangle \langle \hat{n}_j \rangle \\
&= \sum_{i \neq j} (V_{i,j,j,i} - V_{i,j,i,j}) \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle \\
&= \sum_{i \neq j} (V_{i,j,j,i} - V_{i,j,i,j}) \theta(i \leq N)\theta(j \leq N) \\
&= \sum_{1 \leq i < j \leq N} 2(V_{i,j,j,i} - V_{i,j,i,j})
\end{aligned}$$

(c) Suppose that the fermions interact via a repulsive contact potential $V(x, y) = U a_0 \delta(x - y)$, where U and a_0 are positive constants with units of energy and length. Compute the first-order energy shift for this case. Explain why the answer you get is a direct consequence of the fermions being spinless.

In that case, $V_{i,j,j,i} = V_{i,j,i,j}$, and thus $\Delta E = 0$.