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Quantum Mechanics 3 Homework 8

1) **Consider the following Hamiltonian for interacting Fermions:**

$$H = \sum_{q,\sigma} \varepsilon(q) a^{+}_{q,\sigma} a_{q,\sigma} + \frac{1}{2V} \sum_{q} V_q \sum_{k,p',\sigma_1,\sigma_2} a^{+}_{k+q,\sigma_1} a^{+}_{p'-q,\sigma_2} a_{p',\sigma_2} a_{k,\sigma_1}$$

a) **Obtain the equation of motion for the operator** $a_{p,\sigma}$**.**

Using $a_{p,\sigma}$

As usual, I have:

$$i\hbar \frac{d}{dt}\left(a_{p,\sigma}\right) = \left[H, a_{p,\sigma}\right]$$

Then, I need the commutator:

$$\left[\sum_{q,\sigma'} \varepsilon(q) a^{+}_{q,\sigma'} a_{q,\sigma'} + \frac{1}{2V} \sum_{q} V_q \sum_{k,p',\sigma_1,\sigma_2} a^{+}_{k+q,\sigma_1} a^{+}_{p'-q,\sigma_2} a_{p',\sigma_2} a_{k,\sigma_1}, a_{p,\sigma}\right]$$

Recall the identity $\left[a_{p,\sigma}, a^{+}_{q,\sigma'}\right] = \delta_{p,q}\delta_{\sigma,\sigma'}$, and since these are Fermions, exchange of any two operators brings a factor of -1.

Then I have:

$$\left[\sum_{q,\sigma'} \varepsilon(q) a^{+}_{q,\sigma'} a_{q,\sigma'}, a_{p,\sigma}\right] = \varepsilon(p) a_{p,\sigma}$$

Note the minus signs appearing from commutation of destruction operators for Fermions!

$$\left[\frac{1}{2V} \sum_{q} V_q \sum_{k,p',\sigma_1,\sigma_2} a^{+}_{k+q,\sigma_1} a^{+}_{p'-q,\sigma_2} a_{p',\sigma_2} a_{k,\sigma_1}, a_{p,\sigma}\right]$$

$$= \frac{1}{2V} \sum_{q} V_q \sum_{k,p',\sigma_1,\sigma_2} \left(-\left[a^{+}_{k+q,\sigma_1}, a_{p,\sigma}\right] a^{+}_{p'-q,\sigma_2} + a^{+}_{k+q,\sigma_1}\left[a^{+}_{p'-q,\sigma_2}, a_{p,\sigma}\right]\right) a_{p',\sigma_2} a_{k,\sigma_1}$$

$$= \frac{1}{2V} \sum_{q} V_q \sum_{k,p',\sigma_1,\sigma_2} \left(\delta_{p,k+q}\delta_{\sigma,\sigma_1} a^{+}_{p'-q,\sigma_2} - a^{+}_{k+q,\sigma_1}\delta_{p,p'-q}\delta_{\sigma,\sigma_2}\right) a_{p',\sigma_2} a_{k,\sigma_1}$$

$$= \frac{1}{2V} \sum_{q} V_q \left(\sum_{p',\sigma_2} a^{+}_{p'-q,\sigma_2} a_{p',\sigma_2} a_{p-q,\sigma} - \sum_{k,\sigma_1} a^{+}_{k+q,\sigma_2} a_{p+q,\sigma} a_{k,\sigma_2}\right)$$

$$use \quad V_q = V_{-q}:$$

$$= \frac{1}{2V}\sum_q V_q \left(\sum_{p',\sigma_2} a^+_{p'+q,\sigma_2} a_{p',\sigma_2} a_{p+q,\sigma} - \sum_{k,\sigma_1} a^+_{k+q,\sigma_2} a_{p+q,\sigma} a_{k,\sigma_2} \right)$$

$$= \frac{1}{2V}\sum_q V_q \left(\sum_{p',\sigma_2} a^+_{p'+q,\sigma_2} a_{p',\sigma_2} a_{p+q,\sigma} + \sum_{k,\sigma_1} a^+_{k+q,\sigma_2} a_{k,\sigma_2} a_{p+q,\sigma} \right)$$

$$dummy - indices:$$

$$= \frac{1}{V}\sum_q V_q \left(\sum_{p',\sigma'} a^+_{p'+q,\sigma'} a_{p',\sigma'} a_{p+q,\sigma} \right)$$

So I have:

$$i\hbar \frac{d}{dt}\left(a_{p,\sigma}\right) = \varepsilon(p) a_{p,\sigma} + \frac{1}{V}\sum_q V_q \left(\sum_{p',\sigma'} a^+_{p'+q,\sigma'} a_{p',\sigma'} a_{p+q,\sigma} \right)$$

Now I use the Hartree-Fock-like approximation to linearize the term with three operators:

$$\left\langle GS \middle| a^+_{p'+q,\sigma'} a_{p',\sigma'} a_{p+q,\sigma} \middle| GS \right\rangle \equiv \left\langle GS \middle| a^+_{p'+q,\sigma'} a_{p',\sigma'} \middle| GS \right\rangle a_{p+q,\sigma} - \left\langle GS \middle| a^+_{p'+q,\sigma'} a_{p+q,\sigma} \middle| GS \right\rangle a_{p',\sigma'}$$

Above, $\left|GS\right\rangle$ is the ground state.

Then, $\left\langle GS \middle| a^+_{p'+q,\sigma'} a_{p',\sigma'} \middle| GS \right\rangle = n_{p',\sigma'} \delta_{q,0}$, the direct term.

Further, $\left\langle GS \middle| a^+_{p'+q,\sigma'} a_{p+q,\sigma} \middle| GS \right\rangle = n_{p+q,\sigma} \delta_{p,p'} \delta_{\sigma,\sigma'}$, the exchange term.

In this problem, no assumption about V_q is made explicit, so that the direct term might remain. For an electron gas, however, in the Jellium model this term vanishes since the neutralizing background removes the $q = 0$ states.

This substitution leaves me with:

$$i\hbar \frac{d}{dt}\left(a_{p,\sigma}\right) = \varepsilon(p) a_{p,\sigma} - \frac{1}{V}\sum_q V_q n_{p+q,\sigma} a_{p,\sigma}$$

Since in this case the ground state is the Fermi sphere, I can write in terms of the Fermi momentum k_F:

$$i\hbar \frac{d}{dt}\left(a_{p,\sigma}\right) = \varepsilon(p) a_{p,\sigma} - \left[\frac{1}{V}\int \frac{d^3k}{(2\pi)^3} V\left(\vec{k} - \vec{p}\right)\theta\left(k_F - k\right) \right] a_{p,\sigma}$$

Just as in the notes.

b) Obtain the equation of motion for $a^{+}_{p+k,\sigma}a_{p,\sigma}$ and write it in terms of $\rho_q = \sum_{p,\sigma} a^{+}_{p+q,\sigma}a_{p,\sigma}$.

Again,

$$i\hbar\frac{d}{dt}\left(a^{+}_{p+k,\sigma}a_{p,\sigma}\right)=\left[H, a^{+}_{p+k,\sigma}a_{p,\sigma}\right].$$

Above, the Hamiltonian was defined in part (a).

Remembering that commuting operators brings a -1 factor since these are Fermions,

$$\left[\sum_{q,\sigma'}\varepsilon(q)a^{+}_{q,\sigma'}a_{q,\sigma'}, a^{+}_{p+k,\sigma}a_{p,\sigma}\right]=\varepsilon(p+k)\delta_{q,p+k}a^{+}_{q,\sigma'}a_{p,\sigma}+\varepsilon(p)\delta_{q,p}a_{q,\sigma}a^{+}_{p+k,\sigma}$$
$$=\left[\varepsilon(p+k)-\varepsilon(p)\right]a^{+}_{p+k,\sigma}a_{p,\sigma}$$

Further,

$$\left[\frac{1}{2V}\sum_{q}V_q\sum_{k,p',\sigma_1,\sigma_2}a^{+}_{k+q,\sigma_1}a^{+}_{p'-q,\sigma_2}a_{p',\sigma_2}a_{k,\sigma_1}, a^{+}_{p+k,\sigma}a_{p,\sigma}\right]$$
$$=\frac{1}{2V}\sum_{q}V_q\left\{\left[a^{+}_{p+k,\sigma}a_{p+q,\sigma}-a^{+}_{p+k-q,\sigma}a_{p,\sigma}\right]\rho_k+\rho_k\left[a^{+}_{p+k,\sigma}a_{p+q,\sigma}-a^{+}_{p+k-q,\sigma}a_{p,\sigma}\right]\right\}$$

Now using the Random Phase Approximation, an analog of Hartree-Fock, I have:

$$a^{+}_{p+k,\sigma}a_{p+q,\sigma}\rightarrow\left\langle FS\left|a^{+}_{p+k,\sigma}a_{p+q,\sigma}\right|FS\right\rangle=n_{p+k}\delta_{k,q}$$

and

$$a^{+}_{p+k-q,\sigma}a_{p,\sigma}\rightarrow\left\langle FS\left|a^{+}_{p+k-q,\sigma}a_{p,\sigma}\right|FS\right\rangle=n_{p}\delta_{k,q}$$

This leaves me with:

$$i\hbar\frac{d}{dt}\left(a^{+}_{p+k,\sigma}a_{p,\sigma}\right)=\left[\varepsilon(p+k)-\varepsilon(p)\right]a^{+}_{p+k,\sigma}a_{p,\sigma}-\frac{1}{V}\left(n_{p+k}-n_p\right)\rho_k$$

Just as in the notes.

2) For Fermi operators $\psi(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{k,\sigma} a_{k,\sigma} e^{i\vec{k}\cdot\vec{x}}$, compute the pair correlation function $\langle FS | \psi^{+}(\vec{x}) \psi^{+}(\vec{y}) \psi(\vec{y}) \psi(\vec{x}) | FS \rangle$ with $|FS\rangle$ the ground state of the free Fermi gas for N fermions. Plot your result as a function or $R = |\vec{x} - \vec{y}|$ and explain the behavior near $R = 0$.

First, let me write:

$$\begin{aligned} &\left\langle FS \left| a^{+}_{k_1,\sigma_1} a^{+}_{k_2,\sigma_2} a_{k_2',\sigma_2'} a_{k_1',\sigma_1'} \right| FS \right\rangle \\ &= \left(\delta_{k_1,k_1'} \delta_{k_2,k_2'} \delta_{\sigma_1,\sigma_1'} \delta_{\sigma_2,\sigma_2'} - \delta_{k_1,k_2'} \delta_{k_2,k_1'} \delta_{\sigma_1,\sigma_2'} \delta_{\sigma_2,\sigma_1'} \right) n_{k_1} n_{k_2} \end{aligned}$$

Then:

$$\langle FS | \psi^{+}(\vec{x}) \psi^{+}(\vec{y}) \psi(\vec{y}) \psi(\vec{x}) | FS \rangle = \frac{1}{V^2} \sum_{p_q, p_2, \sigma_1, \sigma_2} n_{p_1} n_{p_2} \left(1 - e^{i\vec{p}_1\cdot(\vec{x}-\vec{y})} e^{-i\vec{p}_2\cdot(\vec{x}-\vec{y})} \right)$$

Take:

$$\frac{1}{V} \sum_{p} \rightarrow \int \frac{d^3 p}{(2\pi)^3}$$

$$\sum_{p} e^{-i\vec{p}_2\cdot\vec{x}} n_2 \rightarrow \sum_{p} e^{i\vec{p}_2\cdot\vec{x}} n_2$$

since in the second case the sign is irrelevant, I have:

$$\begin{aligned} &\langle FS | \psi^{+}(\vec{x}) \psi^{+}(\vec{y}) \psi(\vec{y}) \psi(\vec{x}) | FS \rangle = \frac{1}{V^2} \sum_{p_q, p_2, \sigma_1, \sigma_2} n_{p_1} n_{p_2} \left(1 - e^{i\vec{p}_1\cdot(\vec{x}-\vec{y})} e^{-i\vec{p}_2\cdot(\vec{x}-\vec{y})} \right) \\ &= 4\left(\left[\int \frac{d^3 p_1}{(2\pi)^3} n_{p_1} \right] \left[\int \frac{d^3 p_2}{(2\pi)^3} n_{p_2} \right] - \left[\int \frac{d^3 p_1}{(2\pi)^3} n_{p_1} e^{i\vec{p}_1\cdot(\vec{x}-\vec{y})} \right] \left[\int \frac{d^3 p_2}{(2\pi)^3} n_{p_2} e^{-i\vec{p}_2\cdot(\vec{x}-\vec{y})} \right] \right) \end{aligned}$$

Recall that within the Fermi sphere, I have $n_p = \theta(p_F - p)$.

$$\int \frac{d^3 p}{(2\pi)^3} n_p = \frac{1}{(2\pi)^3} \left(\frac{4}{3} \pi p_F^3 \right) = \frac{p_F^3}{6\pi^2}$$

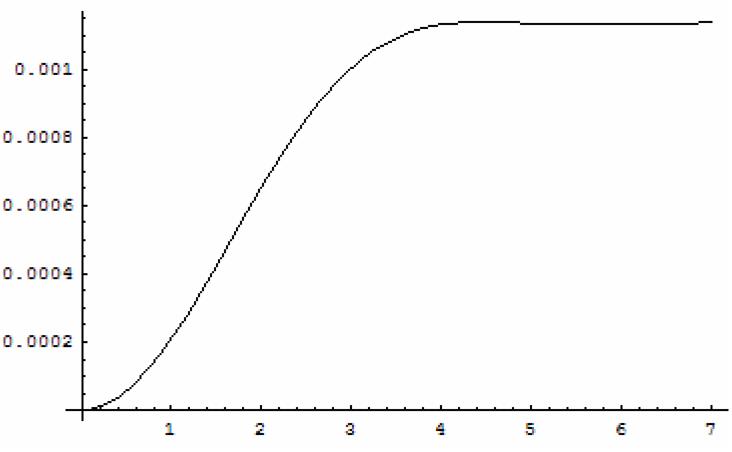
Next,

$$\int \frac{d^3 p}{(2\pi)^3} n_p e^{i\vec{p}\cdot(\vec{x}-\vec{y})} = \frac{1}{(2\pi)^2}\int p^2 d\cos\theta dp n_p e^{ipR\cos\theta} = \frac{1}{2\pi^2}\int \frac{pdp}{R}\sin(pR) n_p$$
$$= \frac{(-p_F R\cos(p_F R) + \sin(p_F R))}{R^3\pi^2}$$

This yields:

$$\langle FS|\psi^+(\vec{x})\psi^+(\vec{y})\psi(\vec{y})\psi(\vec{x})|FS\rangle = 4\left(\left[\frac{p_F^3}{6\pi^2}\right]^2 - \left[\frac{(-p_F R\cos(p_F R) + \sin(p_F R))}{R^3\pi^2}\right]^2\right)$$

For a sample value of p_F,



Thus, I see that near $R = 0$, the "Fermi Hole" comes from the repulsion due to the statistical interaction, e.g. the Pauli Exclusion Principle.

Just as in the notes.

3) **A simple model of neutral (neutron) nuclear matter describes N neutrons in interaction with a repulsive local pair potential** $V(\vec{x}-\vec{y}) = V_0\delta^3(\vec{x}-\vec{y})$, $V_0 > 0$ **in this model there is no "neutralizing background" therefore the direct term contributes.**

a) **Obtain the first order (in** V_0**) energy shift of the ground state (both direct and exchange now contribute). Show that it can be written as** $\Delta E_0^{(1)} = \sum_{k,\sigma} n_{k,\sigma}\sum(k,\sigma)$**. Obtain** $\sum(k,\sigma)$ **and give the total energy of the ground state up to first order in** V_0 **as a function of** $n = \frac{N}{V}$**.**

First, take $V_q = \int d^3x e^{i\vec{q}\cdot\vec{x}} V_0 \delta^3(\vec{x}) = V_0$

For free neutrons, $H_0 = \sum_{p,\sigma} \varepsilon(p) a^+_{p,\sigma} a_{p,\sigma}$, and in this case the interaction Hamiltonian is

$$H_I = \frac{1}{2V}\sum_q V_q \sum_{k,p',\sigma_1,\sigma_2} a^+_{k+q,\sigma_1} a^+_{p'-q,\sigma_2} a_{p',\sigma_2} a_{k,\sigma_1} = \frac{V_0}{2V}\sum_q \sum_{k,p',\sigma_1,\sigma_2} a^+_{k+q,\sigma_1} a^+_{p'-q,\sigma_2} a_{p',\sigma_2} a_{k,\sigma_1}$$

Now I need:

$$\Delta E_0^{(1)} = \langle GS | \frac{V_0}{2V} \sum_q \sum_{k,p',\sigma_1,\sigma_2} a^+_{k+q,\sigma_1} a^+_{p'-q,\sigma_2} a_{p',\sigma_2} a_{k,\sigma_1} | GS \rangle$$

$$= \frac{V_0}{2V}\sum_q \langle GS | \sum_{k,p',\sigma_1,\sigma_2} a^+_{k+q,\sigma_1} a^+_{p'-q,\sigma_2} a_{p',\sigma_2} a_{k,\sigma_1} | GS \rangle$$

Taking a result from problem (2), then, I'm left with;

$$\Delta E_0^{(1)} = \langle GS | \frac{V_0}{2V} \sum_q \sum_{k,p',\sigma_1,\sigma_2} a^+_{k+q,\sigma_1} a^+_{p'-q,\sigma_2} a_{p',\sigma_2} a_{k,\sigma_1} | GS \rangle$$

$$= \frac{V_0}{2V}\sum_q \sum_{k,p',\sigma_1,\sigma_2} \left(\delta_{k+q,k}\delta_{p'-q,p'} - \delta_{k+q,p'}\delta_{p'-q,k}\delta_{\sigma_1,\sigma_2}\right) n_k n_{p'}$$

$$= \frac{V_0}{2V}\sum_q \sum_{k,p',\sigma_1,\sigma_2} \left(\delta_{k+q,k}\delta_{p'-q,p'} - \delta_{k+q,p'}\delta_{p'-q,k}\delta_{\sigma_1,\sigma_2}\right) n_k n_{p'}$$

$$= \frac{V_0}{2V} \sum_{q,k,p',\sigma_1,\sigma_2} \left[\delta_{q,0} - \delta_{p',k+q}\delta_{\sigma_1,\sigma_2}\right] n_k n_{p'}$$

$$= \frac{V_0}{V}\sum_{k,\sigma} n_k \sum_{q,p'} \left[2\delta_{q,0} - \sum_k \delta_{p',k+q}\right] n_{p'} = \frac{V_0}{V}\sum_{k,\sigma} n_k \left[2\sum_p n_p - \sum_q n_{k+q}\right]$$

$$\therefore \sum(k,\sigma) \equiv \frac{V_0}{V}\sum_q \left[2n_q - n_{k+q}\right]$$

Now take:

$$\sum_k \rightarrow V \int \frac{d^3k}{(2\pi)^3} \quad \frac{1}{V}\sum_q \rightarrow \int \frac{d^3q}{(2\pi)^3}$$

Further, inside the Fermi sphere I have: $n_k = \theta\left(k_F - |\vec{k}|\right)$

$$\Delta E_0^{(1)} = VV_0 \int \frac{d^3k}{(2\pi)^3} n_k \int \frac{d^3q}{(2\pi)^3} (2n_q - n_{k+q})$$

$$= 2VV_0 \int \frac{d^3k}{(2\pi)^3} n_k \int \frac{d^3q}{(2\pi)^3} n_q - VV_0 \int \frac{d^3k}{(2\pi)^3} n_k \int \frac{d^3q}{(2\pi)^3} n_{k+q}$$

$$= \frac{VV_0}{(2\pi)^6} \left(\frac{4}{3} \pi k_F^3 \right)^2$$

b) **Using the result for the equation of motion obtained in problem 1 for the operator $a_{p,\sigma}$, use the Hartree-Fock approximation to linearize the equation of motion. Again, both direct and exchange contribute. Show that in the Hartree-Fock approximation $i \frac{da_{p,\sigma}}{dt} = [\varepsilon(p) + \sum(p,\sigma)] a_{p,\sigma}$ where $\sum(p,\sigma)$ the "self energy" the same as obtained in part (a).**

In problem 1a, I never assumed that the result was for electrons, so the derivation is exactly the same. Substituting from part (a) here, then, I need only take the Hartree-Fock simplified state.

$$i\hbar \frac{d}{dt}(a_{p,\sigma}) = \varepsilon(p) a_{p,\sigma} - \sum(p,\sigma) a_{p,\sigma}$$

$$i\hbar \frac{d}{dt}(a_{p,\sigma}) = \frac{\hbar^2}{2m} a_{p,\sigma} - \frac{V_0}{2V} \sum_q [n_q - n_{k+q}] a_{p,\sigma}$$

c) **Obtain the single particle dispersion relation.**

Combining the free neutron energy with the energy shift, then, I have:

$$\varepsilon(p) = \frac{\hbar^2 p^2}{2m} + \Delta E^{(1)} = \frac{\hbar^2 p^2}{2m} + \frac{VV_0}{(2\pi)^6} \left(\frac{4}{3} \pi k_F^3 \right)^2$$

So I see that the shift manifests itself as a zero-point energy.

4)

a) **In the Jellium model obtain the exchange contribution (not direct) for $\sum(p,\sigma)$, carry out the integrals and give the final form for $\sum(p,\sigma)$.**

In the Jellium model,

$$\sum_{ex}(p,\sigma) = -\frac{1}{2V}\sum_{q\neq 0} V_q n_{p+q,\sigma}$$

$$= -\int \frac{d^3k}{(2\pi)^3}\frac{4\pi e^2}{\left|\vec{k}-\vec{p}\right|^2}\theta(k_F - k)$$

$$= -\frac{4\pi e^2}{(2\pi)^3}\int_0^{k_F} k^2 dk \int_{-1}^{1} d\cos\theta \frac{1}{k^2 + p^2 - 2pk\cos\theta} = -e^2\frac{p_F}{\pi}\left(1 + \frac{p_F^2 - p^2}{2pp_F}\ln\left|\frac{p_F + p}{p_F - p}\right|\right)$$

Just as in the notes.

b) The effective mass of a fermionic excitation is defined as $m^* = p_F\left[\left.\frac{\partial\varepsilon(p)}{\partial p}\right|_{p_F}\right]^{-1}$ **where** $\varepsilon(p)$ **is the dispersion relation including the interaction corrections. Show that for the Jellium model** m^* **diverges logarithmically. This is an artifact of the Hartree-Fock approximation.**

Ignore the zero-order energy term $\varepsilon(p) = \sqrt{m^2c^4 + p^2c^2}$, as this will not cause any issues.

$$\frac{\partial\sum_{ex}(p,\sigma)}{\partial p} = \frac{e^2}{2p_F p^2}\left(-2p_F p + \left(p_F^2 + p^2\right)\ln\left|\frac{p_F + p}{p_F - p}\right|\right)$$

$$= \frac{e^2}{2p_F p^2}\left(-2p_F p + \left(p_F^2 + p^2\right)\left(\ln|p_F + p| - \ln|p_F - p|\right)\right)$$

The highest-order diverging term as $p_F \to p$ is then

$$\left.\frac{\partial\sum_{ex}(p,\sigma)}{\partial p}\right|_{p\to p_F} \propto -\frac{e^2}{2p_F}\ln|p_F - p|$$

a logarithmic singularity, as expected.

However, the power in $m^* = p_F\left[\left.\frac{\partial\varepsilon(p)}{\partial p}\right|_{p_F}\right]^{-1}$ indicates then that $m^* \to 0$, so it is in fact $\left(m^*\right)^{-1}$ that diverges.