FYST530 Quantum Mechanics II Spring 2012

Problem set 12 Return before **15 on Wednesday 18.4.** to the box labeled FYST530

1. (a) Show that the Fock space 1-particle operator, $F^{(1)} = \sum_{\mu,\nu} \langle\mu|\hat{f}|\nu\rangle a_\mu^\dagger a_\nu$, acts as

$$F^{(1)}|1_{\nu_1}1_{\nu_2}\cdots 1_{\nu_N}\rangle = \sum_\mu \sum_{i=1}^N \langle\mu|\hat{f}|\nu_i\rangle |1_{\nu_1}1_{\nu_2}\cdots 0_{\nu_i}1_\mu \cdots 1_{\nu_N}\rangle.$$

in a system of N fermions.

(b) Taking the ansatz

$$F^{(2)} = K \sum_{\mu\mu'\nu\nu'} \langle\mu\mu'|\hat{g}|\nu\nu'\rangle a_\mu^\dagger a_{\mu'}^\dagger a_\nu a_{\nu'}$$

for the Fock space 2-particle operator, and requiring that

$$F^{(2)}|1_{\nu_1}1_{\nu_2}\rangle = \sum_{\mu_1\mu_2} \langle\mu_1\mu_2|\hat{g}|\nu_1\nu_2\rangle |1_{\mu_1}1_{\mu_2}\rangle,$$

show that $K = -\frac{1}{2}$.

2. The fermionic pair distribution function $g_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}')$ for the ground state $|F\rangle$ of the Fermi gas is defined as

$$\left(\frac{n}{2}\right)^2 g_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') \equiv \langle F|\Psi^\dagger(\mathbf{x},\sigma)\Psi^\dagger(\mathbf{x}',\sigma')\Psi(\mathbf{x}',\sigma')\Psi(\mathbf{x},\sigma)|F\rangle,$$

where $\Psi(\mathbf{x},\sigma)$s are fermionic field operators. Show that

(a) If $\sigma \neq \sigma'$, then

$$g_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') = 1.$$

(b) If $\sigma = \sigma'$, then

$$g_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') = 1 - \left[G_\sigma(\mathbf{x}-\mathbf{x}')\right]^2,$$

where $G_\sigma(\mathbf{x}-\mathbf{x}')$ is the single-particle correlator

$$G_\sigma(\mathbf{x}-\mathbf{x}') \equiv \frac{2}{n}\langle F|\Psi^\dagger(\mathbf{x},\sigma)\Psi(\mathbf{x}',\sigma)|F\rangle.$$

3. Consider a system of N identical <u>bosons</u>, spin-0, enclosed to a box with volume V, in the state

$$|\phi\rangle = |n_{\mathbf{p}_0}\, n_{\mathbf{p}_1}\, n_{\mathbf{p}_2}, ...\rangle \qquad n_{\mathbf{p}_i} = 0, 1, 2, 3, ...$$

(a) Show that

$$\langle\phi|\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x})|\phi\rangle = \frac{N}{V} \equiv n.$$

(b) Show that the pair distribution function is ($\mathbf{k} \equiv \mathbf{p}/\hbar$)

$$\begin{aligned} n^2 g(\mathbf{x}-\mathbf{x}') &\equiv \langle\phi|\Psi^\dagger(\mathbf{x})\Psi^\dagger(\mathbf{x}')\Psi(\mathbf{x}')\Psi(\mathbf{x})|\phi\rangle \\ &= n^2 + \left|\frac{1}{V}\sum_k e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} n_\mathbf{k}\right|^2 - \frac{1}{V^2}\sum_k n_\mathbf{k}(n_\mathbf{k}+1). \end{aligned}$$

(c) Consider two examples of $g(\mathbf{x}-\mathbf{x}')$:

(i) Suppose all the bosons occupy the same state, $n_{\mathbf{p}_0} = N$. Show that

$$n^2 g(\mathbf{x}-\mathbf{x}') = \frac{N(N-1)}{V^2}.$$

(ii) Suppose the particles are distributed over many momentum values with Gaussian distribution

$$n_{\mathbf{p}} = \frac{(2\pi)^3 n}{(\sqrt{\pi}\Delta)^3} e^{-(\mathbf{k}-\mathbf{k}_0)^2/\Delta^2}.$$

Show that if the density of particles n, and the width Δ of the momentum distribution are held fixed, then, in the limit of large volume V, the pair distribution function is given by

$$n^2 g(\mathbf{x}-\mathbf{x}') = n^2 \left(1 + e^{-\frac{\Delta^2}{2}(\mathbf{x}-\mathbf{x}')^2}\right).$$

Sketch the behaviour of $g(\mathbf{x}-\mathbf{x}')$ as a function of $(\mathbf{x}-\mathbf{x}')$. Can you see the bosonic nature of the particles showing up in $g(\mathbf{x}-\mathbf{x}')$?

4. Suppose the Hamilton operator for system of N fermions (in a box with volume V) is of the form

$$H = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + \sum_{i<j} V_2(\mathbf{x}_i - \mathbf{x}_j),$$

which is invariant in translations. Show that in this case the plane-waves

$$\varphi_{\mathbf{k},s}(\mathbf{x},\sigma) = \frac{1}{\sqrt{V}} e^{i\mathbf{x}\cdot\mathbf{k}} \delta_{\sigma s}$$

are solutions for the Hartree-Fock equations. Compute the single-particle energies in terms of Fouries components $V_{\mathbf{q}}$ of V_2:

$$V_2(\mathbf{x}) = \sum_{q} e^{i\mathbf{q}\cdot\mathbf{k}} V_{\mathbf{q}}.$$

Compute also the total energy in terms of spins and momenta of the occupied states.