

HOME WORK #7

(due date: Wed., 5 December 2007)

Consider a degenerate Fermion system with a ground state $|\Phi_o\rangle$ given by

$$|\Phi_o\rangle = \prod_{\alpha\sigma}^{occ} c_{\alpha\sigma}^+ |0\rangle = \prod_{\alpha\sigma} \theta(\epsilon_F - \epsilon_\alpha) c_{\alpha\sigma}^+ |0\rangle$$

where the basis function $\{\phi_\alpha\}$ is defined by the single particle Schrodinger equation

$$h_o |\phi_\alpha\rangle = \epsilon_\alpha |\phi_\alpha\rangle.$$

Now consider another basis set of $\{\phi_i\}$ such that ϕ_i is not an eigenstate of h_o , and $\{\phi_\alpha\}$ and $\{\phi_i\}$ are related by the unitary matrix U:

$$|\phi_\alpha\rangle = \sum_i |\phi_i\rangle \langle \phi_i | \phi_\alpha \rangle = \sum_i |\phi_i\rangle U_{i\alpha}.$$

1. Express the expectation value P_{ij}^σ defined by

$$P_{ij}^\sigma = \langle \Phi_o | c_{i\sigma}^+ c_{j\sigma} | \Phi_o \rangle$$

in terms of the unitary matrix U.

2. Show that

$$\langle \Phi_o | c_{i\sigma}^+ c_{k\sigma'}^+ c_{l\sigma'} c_{j\sigma} | \Phi_o \rangle = P_{ij}^\sigma P_{kl}^{\sigma'} - \delta_{\sigma\sigma'} P_{il}^\sigma P_{kj}^\sigma.$$

3. We can represent the one-particle operator $F_1 = \sum_a f_1(\mathbf{r}_a)$ in the second quantization form by

$$\hat{F}_1 = \sum_{ij} \langle i | f_1 | j \rangle c_i^+ c_j$$

where

$$\langle i | f_1 | j \rangle = \int \phi_i^*(\mathbf{r}_a) f_1(\mathbf{r}_a) \phi_j(\mathbf{r}_a) d\mathbf{r}_a.$$

Similarly, the two particle operator $F_2 = \sum_{a \neq b} f_2(\mathbf{r}_a, \mathbf{r}_b)$ can be represented by

$$\hat{F}_2 = \sum_{ijklm} \langle ij | f_2 | lm \rangle c_i^+ c_j^+ c_m c_l$$

where

$$\langle ij | f_2 | lm \rangle = \int \phi_i^*(\mathbf{r}_a) \phi_j^*(\mathbf{r}_b) f_2(\mathbf{r}_a, \mathbf{r}_b) \phi_l(\mathbf{r}_a) \phi_m(\mathbf{r}_b) d\mathbf{r}_a d\mathbf{r}_b.$$

Considering a free electron system with hamiltonian $h_o = -(1/2)\nabla^2$ with $\phi_{\alpha=k}(\mathbf{r}) = (1/\sqrt{V}) \exp(i\mathbf{k} \cdot \mathbf{r})$, show that the number density operator $\rho(\mathbf{r}) = \sum_a \delta(\mathbf{r} - \mathbf{r}_a)$ can be written by

$$\hat{\rho}(\mathbf{r}) = \sum_{k,q,\sigma} e^{-i\mathbf{q} \cdot \mathbf{r}} c_{k\sigma}^+ c_{k-q\sigma}.$$

Also, calculate the expectation value of the number density

$$\rho(\mathbf{r}) = \langle \Phi_o | \hat{\rho}(\mathbf{r}) | \Phi_o \rangle$$

where

$$|\Phi_o\rangle = \prod_{k\sigma} \theta(k_F - |\mathbf{k}|) c_{k\sigma}^+ |0\rangle.$$

4. Repeat the exercise #3 above for the two particle density operator,

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{a \neq b} \delta(\mathbf{r} - \mathbf{r}_a) \delta(\mathbf{r}' - \mathbf{r}_b).$$