8.511 Theory of Solids I **Problem Set 8** **Due November 16, 2004**

1. (a) Solve the Hartree-Fock equations for an electron gas in a uniform positive background charge with density n. Calculate the Hartree-Fock eigenvalues and the ground state energy.

   (b) Show that within the local density functional approximation, the ground state energy of an electron gas in an external potential $v(\mathbf{r})$ is given by

$$E = \sum_{i=1}^{N} \varepsilon_i - \frac{e^2}{2} \int\int \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}d\mathbf{r}' + \int n(\mathbf{r})[\varepsilon_{xc}(n(\mathbf{r})) - \mu_{xc}(n(\mathbf{r}))]d\mathbf{r}$$

   where ε_i are the solution of the equation

$$\left[-\frac{\hbar^2\nabla^2}{2m} + v(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(n(\mathbf{r}))\right] \varphi_i = \varepsilon_i \varphi_i$$

   and

$$\mu_{xc} = \frac{d(n\varepsilon_{xc}(n))}{dn}.$$

   (c) Now specialize to the case of an electron gas in a uniform background charge. Suppose $\varepsilon_{xc}(n)$ is approximated by the exchange energy found in part (a). Solve for the eigenvalues ε_i. Are they the same as the Hartree-Fock eigenvalues? Compare the Fermi velocity and the "bandwidth" (defined as the energy difference between ε_i at k_F and $k = 0$) as predicted by the present approximation and the Hartree-Fock approximation. Use part (b) to compute the ground state energy within this approximation. Does the result agree with the Hartree-Fock answer? [Note that in order to obtain a finite answer, it is necessary to include the Coulomb interaction between the positive background charges.]

2. Read Marder Appendix C and learn about second quantization.