Physics 240A: Homework Problem Set 6

Due 12/5/07.

1. Density and Density Operator in Many Body Theory. 30 points.
The density operator $\hat{n}(r)$ in an N-particle system, and the from of many body wave-function in the Hartree approximation, are given by

$$\hat{n}(r) = \sum_j^N \delta(\vec{r} - \vec{r}_j). \quad \Psi(\{\vec{r}_j\}) = \Pi_j^N \phi_j(\vec{r}_j).$$

Show that the density of the system is $n(\vec{r}) = \sum_j^N |\phi_j(\vec{r}_j)|^2$. Here ϕ_j are just some collection of one-particle (wave)functions.

2. Electron Gas Energy in Hartree-Fock Theory. 30 points.
(i) Evaluate the energy of the homogeneous electron gas from the expression given in Eq. (9.48). Note that the sum over ℓ in this expression is the sum over (occupied) states, we normally use the label k for this, and after changing to an integral the variable will be $\vec{k}$.
(ii) Express both the kinetic energy and the potential energy in (i) in terms of k_F. Find the value of the density (in electrons/Å^3) where they are equal.
(iii) As the density increases and the electrons are squeezed closer together, does the kinetic or potential energy dominate? Interpret your answer.

See page 2.

3. Thomas-Fermi Screening. 40 points.
Thomas-Fermi 'theory' give Eq. 9.76, which is

$$An^{2/3}(r) + U(r) + \int dr' \frac{e^2 n(r)}{|r - r'|} - Bn^{1/3}(r) = \mu,$$

where you'll substitute in the constants A and B toward the end of the problem. Suppose this holds for a constant (jellium) density $n_\circ$, and then for an 'impurity' potential $U(r) = -e^2/r$ centered at the origin. Suppose U can be treated as small, so it gives rise to a new density $n_\circ + \delta n(r)$ where the change in density is small. Substitute these into the Thoms-Fermi equation and expand to first order in $\delta n(r)$, and use Fourier transformation $\delta n(r) = \sum_q \delta n_q exp(iq \cdot r)$ to solve for $\delta n(r)$. Show that it has the form

$$\delta n(r) \sim e^{-r/\xi}/r$$

and determine the expression for the "screening length" ξ. How is it affected by the exchange term (which Thomas and Fermi originally did not include)? Note that although this is a three-dimensional problem and the r and q are really vectors, it is a spherically symmetric problem so the final expression is for $r \equiv |\vec{r}|$.