Physics 556 Spring 2004
Problem Set 2, Due Friday May 14

1. **Exchange Hole in Hartree-Fock Theory**

   (a) Let $p_{\sigma\sigma'}(\vec{x},\vec{y})$ be the probability to find one electron at $\vec{r}=\vec{x}$ with spin σ and another electron at $\vec{r}=\vec{y}$ with spin σ'. Consider a system consisting of two electrons in a 3d box of side L; one electron is in a plane-wave state with wavevector $\vec{k}_1$ and the other with wavevector $\vec{k}_2$. Show that in single Slater determinant approximation,

$$p_{\sigma\sigma'}(\vec{x},\vec{y}) = \frac{1}{L^6} g_{\sigma\sigma'}(\vec{x},\vec{y})$$

   and that

$$g_{\sigma\sigma'}(\vec{x},\vec{y}) = 1 - \cos[(\vec{k}_1 - \vec{k}_2)\cdot(\vec{y}-\vec{x})]\delta(\sigma,\sigma').$$

   (b) Now consider a filled Fermi sea with Fermi wavevector k_F. The Hartree-Fock ground state is a single Slater determinant, which is also written as

$$|\mathrm{HF}>= \prod_{k\sigma}^{\epsilon_k<\epsilon_F} c^\dagger_{k\sigma}|\mathrm{vac}> .$$

   Show that the average correlation of pairs is

$$< g_{\sigma\sigma'}(\vec{x},\vec{y}) >= 1 - F^2(k_F r)\delta(\sigma,\sigma')$$

   where $r = |\vec{y}-\vec{x}|$ and

$$F(x) = 3\frac{\sin x - x\cos x}{x^3}.$$

   Make a sketch of $g_{\uparrow\uparrow}(r)$.

2. **Wigner's divergence in Rayleigh-Schrödinger Perturbation Theory**

   Consider the Rayleigh-Schrödinger perturbation expression for the ground state energy of the electron gas,

$$E_0 = \sum_{k\sigma}\frac{\hbar^2k^2}{2m}f_k + <\mathrm{HF}|\mathcal{H}_1|\mathrm{HF}> + \sum_n \frac{|<\mathrm{HF}|\mathcal{H}_1|n>|^2}{\epsilon_0-\epsilon_n} + \ldots$$

   where $|n>$ is an excited state such as

$$c^\dagger_1 c^\dagger_2 c_3 c_4|\mathrm{HF}>$$

   and ϵ_n is the corresponding eigenvalue of the kinetic energy,

$$\mathcal{H}_0|n>= \epsilon_n|n> .$$

   (a) Show that

$$<\mathrm{HF}|\mathcal{H}_1|\mathrm{HF}>= -\frac{1}{2}\sum_{kk'\sigma} f_{k\sigma}f_{k'\sigma}\frac{4\pi e^2}{|\vec{k}-\vec{k}'|^2}.$$

   (Note that this expression is just one half the sum over occupied states of the exchange contribution to the Hartree-Fock single-particle eigenvalue.) You may use the second-quantized form (Doniach and Sondheimer eq. (6.1.3)) of the Hamiltonian operators.

   (b) Show that the second-order contribution to E_0 diverges logarithmically as $\int dq/q$ where $q = |\vec{k}-\vec{k}'|$. It is permitted to use $f_k(1-f_{k+q}) \approx \vec{q}\cdot\vec{v}_k(-\partial f/\partial\epsilon_k)$ to extract the small q behavior.