Physics 5492
Condensed Matter Physics II
Problem Set 1
Due: Tuesday, Jan 20, 2009

1.1 Problem 2, Chapter 17 of A&M, Pg. 351.

1.2 **Koopmans' Theorem.** — Imagine that we have solved the Hartree-Fock equations (Eq. (17.15), pg. 333 in A&M) and obtained the one-electron wave functions ψ_i and the corresponding Hartree-Fock eigenvalues E_i. Let Ψ be the N electron Hartree-Fock ground state of the system, Ψ'_{N-1} be an $N-1$ electron Slater determinant from which the electron in the state ψ_i has been removed, and Ψ'_{N+1} be an $N+1$ electron Slater determinant to which which an electron has been added in the state ψ_j.

(a) Using the expression for the expectation value of the energy (Eq. (17.14), pg. 333 in A&M) show that

$$\langle \Psi'_{N-1} | H | \Psi'_{N-1} \rangle - \langle \Psi | H | \Psi \rangle = -E_i$$

and

$$\langle \Psi'_{N+1} | H | \Psi'_{N+1} \rangle - \langle \Psi | H | \Psi \rangle = E_j$$

(b) What does this result tell you about the interpretation of the Hartree-Fock eigenvalues E_i?

1.3 Problem 3, Chapter 17 of A&M, Pg. 351.

1.4 **Screening and Hartree-Fock.**

(a) Evaluate the integral in Eq. (17.19) (pg. 334 of A&M) and verify the given expression for the exchange contribution to the Hartree-Fock eigenvalues.

(b) Show that if one assumes that Eq. (17.19) can be viewed as an effective one-electron dispersion then the density of states goes to zero at the Fermi surface. Comment on the possible experimental implications of this (and why it cannot be the case!).

(c) Show that if in the exchange term of the Hartree-Fock equations the long-range Coulomb interaction is replaced by the *screened* interaction

$$V_{\text{sc}}(r) = \frac{e^2}{r} \exp -k_0 r$$

then the density of states at the Fermi surface is finite.