MATERIALS PHYSICS II FALL 2006 HOMEWORK PROBLEMS 5

Return to Michael by Wednesday 18.10.2006 at noon

1. Calculate the pair-correlation function $g(r) = g_{\uparrow\uparrow}(r) + g_{\uparrow\downarrow}(r)$ for jellium.
(a) Start from definition

$$g_{\sigma_1\sigma_2}(\mathbf{r}_1, \mathbf{r}_2) = \frac{N(N-1)}{n(\mathbf{r}_1)n(\mathbf{r}_2)} \sum_{\sigma_3\ldots\sigma_N} \int \cdots \int |\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N)|^2 \, d\mathbf{r}_3 \ldots d\mathbf{r}_N \qquad (1)$$

and show that for a single Slater determinant we have

$$\begin{aligned} g_{\sigma_1\sigma_2}(\mathbf{r}_1, \mathbf{r}_2) &= \frac{1}{n(\mathbf{r}_1)n(\mathbf{r}_2)} \sum_{i,j} \{ |\psi_i(\mathbf{r}_1\sigma_1)|^2 |\psi_j(\mathbf{r}_2\sigma_2)|^2 - \psi_i^*(\mathbf{r}_1\sigma_1)\psi_j^*(\mathbf{r}_2\sigma_2)\psi_j(\mathbf{r}_1\sigma_1)\psi_i(\mathbf{r}_2\sigma_2) \\ &- \psi_j^*(\mathbf{r}_1\sigma_1)\psi_i^*(\mathbf{r}_2\sigma_2)\psi_i(\mathbf{r}_1\sigma_1)\psi_j(\mathbf{r}_2\sigma_2) + |\psi_j(\mathbf{r}_1\sigma_1)|^2 |\psi_i(\mathbf{r}_2\sigma_2)|^2 \}. \end{aligned} \qquad (2)$$

Alternatively you can just verify this result in case of $N = 3$.
(b) In the jellium the single-electron states are $\psi_j(\mathbf{r}\sigma) = \exp(i\mathbf{k}_j \cdot \mathbf{r})/\sqrt{V}\chi_{s_i}(\sigma)$ and for the spinor $\chi_{s_i}(\sigma)$ we have $\chi^*_{s_i}(\sigma)\chi_{s_j}(\sigma) = \delta_{s_i s_j}$. Furthermore the density n of the jellium is constant N/V. Put this information into eq. (2) and show that

$$\begin{aligned} g_{\uparrow\downarrow}(\mathbf{r}_1, r_2) &= \frac{1}{2} \\ g_{\uparrow\uparrow}(\mathbf{r}_1, \mathbf{r}_2) &= \frac{1}{2}[1 - \phi(\mathbf{r}_1 - \mathbf{r}_2)^2], \end{aligned}$$

where

$$\phi(\mathbf{r}) = \frac{3}{(rk_F)^3}[\sin(rk_F) - (rk_F)\cos(rk_F)] = \frac{3}{rk_F} j_1(rk_F)$$

Use handy formula $\sum_{\mathbf{k}} F(\mathbf{k}) = V/(2\pi)^3 \int F(\mathbf{k}) d\mathbf{k}$.
(c) Define exchange hole density $n_x(\mathbf{r}) = N/V(g(\mathbf{r}) - 1)$ and show that it satisfies the sum rule

$$\int n_x(\mathbf{r}) d\mathbf{r} = -1$$

and that the Coulomb interaction energy between an electron and $n_x(\mathbf{r})$,

$$\int \frac{e^2 n_x(\mathbf{r})}{r} d\mathbf{r},$$

yields the exchange energy of the jellium.
Hints: $\int_0^\infty j_1(x)^2 dx = \pi/6$ and $\int_0^\infty j_1(x)^2/x dx = 1/8$ **(4 points)**

2. (a) Derive the result for the thermal conductivity coefficient: $\kappa_T = \frac{1}{3} c_V \tau v_F^2$. Make a one-dimensional model which has a thermal gradient dT/dx. Consider electrons at point x. The energy of electrons depends on the position through T: $\varepsilon = \varepsilon(T(x))$. What is the contribution to

the thermal current density J_Q at x by electrons arriving from "left (cooler)" or "right (hotter)" regions? Expand J_Q about the point x, recognize the term consisting of the electronic heat capacity per unit volume (c_V) and generalize the equation to 3D, which will give you the desired result.
(b) Conversely, a temperature gradient in a long, thin metal bar will induce an electric field that is directed opposed to the temperature gradient (*Seebeck effect*). That is, $\mathbf{E} = Q \bigtriangledown T$. By a similar consideration of a 1D model and generalization to 3D, derive the *thermopower constant* $Q = -c_V/3ne$. (**3 points**)

3. Show that near the band minimum ($\mathbf{k}$=0) the Hartree-Fock one-electron energy

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} - \frac{2e^2}{\pi} F(x)$$

where $x = k/k_F$ and

$$F(x) = \frac{1}{4x}\left[(1-x^2)ln\left|\frac{1+x}{1-x}\right| + 2x\right]$$

is parabolic in k:

$$\varepsilon(k) \approx \frac{\hbar^2 k^2}{2m^*},$$

where

$$\frac{m^*}{m} = \frac{1}{1+0.22(r_s/a_0)}.$$

(**3 points**)