MATERIALS PHYSICS II FALL 2007 HOMEWORK PROBLEMS 4

Return to Robert (mailbox Physics 2nd floor) by Tuesday 9.10.2007 at noon.

Comment: working through the weekly problems as team work is completely acceptable and even recommended, as far as each person writes down and returns his/her own solutions! This time I reduced the number of problems and graded them a bit differently according to the expected work load.

1. Estimate the screening length $(k_0^{TF})^{-1}$ for Al, Cu and Na by considering them as free-electron metals, and compare the result to the nearest-neighbour atomic distance in each metal. **(2 points)**

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

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

and show that for a single Slater determinant we have

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

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 $\sum_k F(\mathbf{k}) = V/(2\pi)^3 \int F(\mathbf{k}) d\mathbf{k}$.
(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)**

3. Write an essay, 2 pages on Wigner crystals: You can choose according to your orientation to be "an experimentalist" or "a theorist". If you want to be "an experimentalist", look at the following links as source for material:

http://focus.aps.org/story/v8/st22
http://prola.aps.org/abstract/PRL/v87/i17/e176802

"Theorists" should look at:
http://focus.aps.org/story/v7/st18
http://prola.aps.org/abstract/PRL/v86/i17/p3851_1
http://www.theo-physik.uni-kiel.de/ bonitz/public/e-krist.htm
(**4 points**)