Materials physics II — Fall 2004 — Problems 3

Return by tue 28.9. by 2 pm.

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

(a) Start from definition

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

and show that for a single Slater determinant we have

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

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

(c) Define exchange hole density $n_x(\mathbf{r}) = N/V(g(\mathbf{r}) - 1)$ and show that it satisfies the sum rule

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

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

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

yields the exchange energy of the jellium.
Hints: $\int_0^\infty j_1(x)^2 \mathrm{d}x = \pi/6$ and $\int_0^\infty j_1(x)^2/x \mathrm{d}x = 1/8$ **(3 points)**

2. Calculate Fourier transformation $\mathcal{F}[\phi_s(\mathbf{r})]$ of the screened Coulomb potential (Yukawa potential) $\phi_s(\mathbf{r}) = -e\exp(-k_0 r)/r, \quad k_0 > 0$:

$$\mathcal{F}[\phi_s(\mathbf{r})] := \tilde{\phi}_s(\mathbf{k}) = \int e^{-i\mathbf{k}\cdot\mathbf{r}} \phi_s(\mathbf{r}) \, \mathrm{d}\mathbf{r}.$$

What is the Fourier transformation of the bare (unscreened) Coulomb potential $\phi(\mathbf{r})$?
Check your result by solving the Poisson's equation of a point charge,

$$\nabla^2 \phi(\mathbf{r}) = 4\pi e \delta(\mathbf{r}),$$

with Fourier transformation. Recall that $\mathcal{F}[\nabla^2 \phi(\mathbf{r})] = -k^2 \tilde{\phi}(\mathbf{k})$. **(1 point)**

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

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

where

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

(2 points)