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Theoretical Solid-State Physics, Herbstsemester 2012

Blatt 3

Abgabe: 11. Oktober, 12:00H (Treppenhaus 4. Stock)
Tutor: Samuel Aldana Zi.: 4.13

(1) **Spin-polarized electron gas** (4 Points)
Consider a polarized electron gas with N_+ spin-up and N_- spin-down electrons.

(a) Through a convenient generalization of the results derived for the unpolarized Fermi gas, find the ground-state energy (E) of the system to first order in the interaction potential. Express this energy as a function of the total electron number $N \equiv N_+ + N_-$ and the polarization $\xi \equiv (N_+ - N_-)/N$.

(b) Show that the ferromagnetic state ($\xi = 1$) has a lower energy than the unmagnetized state ($\xi = 0$) if the condition

$$r_s > \frac{2\pi}{5}\left(\frac{9\pi}{4}\right)^{1/3}\left(2^{1/3}+1\right) \approx 5.45$$

is satisfied.

(2) **Second-order contribution to the ground-state energy of an electron gas from Rayleigh-Schrödinger perturbation theory** (6 Points)

(a) Show that the second-order contribution to the ground-state energy (per particle) of an electron gas can be expressed as

$$\frac{E^{(2)}}{N} = \frac{e^2}{2a_0}(\epsilon_2^d + \epsilon_2^{ex}) \, ,$$

where

$$\epsilon_2^d = -\frac{3}{8\pi^5}\int \frac{d^3\mathbf{q}}{\mathbf{q}^4}\int_{|\mathbf{k}+\mathbf{q}|>1} d^3\mathbf{k}\int_{|\mathbf{p}+\mathbf{q}|>1} d^3\mathbf{p}\,\frac{\theta(1-|\mathbf{k}|)\theta(1-|\mathbf{p}|)}{\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{k}+\mathbf{p})} \, ,$$

$$\epsilon_2^{ex} = \frac{3}{16\pi^5}\int \frac{d^3\mathbf{q}}{\mathbf{q}^2}\int_{|\mathbf{k}+\mathbf{q}|>1} d^3\mathbf{k}\int_{|\mathbf{p}+\mathbf{q}|>1} d^3\mathbf{p}\,\frac{\theta(1-|\mathbf{k}|)\theta(1-|\mathbf{p}|)}{(\mathbf{q}+\mathbf{k}+\mathbf{p})^2[\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{k}+\mathbf{p})]} \, ,$$

are the contributions stemming from the direct and exchange processes, respectively. Here, $\theta(x)$ is the Heaviside function, and all the integration momenta on the right-hand-sides are expressed in units of the Fermi momentum k_F.

Please turn over!

Hint: Recall that the second-order change of the energy in ordinary (Rayleigh-Schrödinger) perturbation theory for the Hamiltonian $H = H_0 + V$ (V is the perturbation) is

$$E^{(2)} = \sum_{n>0} \frac{|\langle 0|V|n\rangle|^2}{E_0 - E_n} .$$

Here $|0\rangle$ is the ground state of H_0, E_0 is the corresponding ground-state energy, while $|n\rangle$ are the excited states with energies E_n.

(b) We now want to show that the term ϵ_2^d is actually divergent. Consider the function

$$F(|\mathbf{q}|) = \int_{|\mathbf{k}+\mathbf{q}|>1} d^3\mathbf{k} \int_{|\mathbf{p}+\mathbf{q}|>1} d^3\mathbf{p}\, \frac{\theta(1-|\mathbf{k}|)\theta(1-|\mathbf{p}|)}{\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{k}+\mathbf{p})} .$$

Show that

$$F(|\mathbf{q}|) \sim \left(\frac{4\pi}{3}\right)^2 |\mathbf{q}|^{-2} \quad \text{as} \quad |\mathbf{q}| \to \infty$$

and that

$$F(|\mathbf{q}|) \sim \frac{2}{3}(2\pi)^2(1-\ln 2)|\mathbf{q}| \quad \text{as} \quad |\mathbf{q}| \to 0 .$$

Using these results, show that ϵ_2^d diverges logarithmically because of the contributions at small momentum transfer $\mathbf{q}$.