Unkonventionelle Supraleitung

Serie 3

Verteilung: 15.November Abgabe: 22.November

3.1 Uniform susceptibility of a gas of N interacting electrons in a system with the volume V. Consider the Hamiltonian

$$H_1 = H_{\rm KE} + H_{\rm INT} + H_{\rm Z}^{(A)},$$

with

$$H_{\rm KE} = \sum_{k,s} \xi_k c^\dagger_{k,s} c_{k,s}, \qquad H_{\rm INT} = \int d\mathbf{r} d\mathbf{r}' U \delta^3(\mathbf{r}-\mathbf{r}') \rho_\uparrow(\mathbf{r}) \rho_\downarrow(\mathbf{r}'),$$
$$H_{\rm Z}^{(A)} = -\mu_{\rm B} H \sum_k (n_{k,\uparrow} - n_{k,\downarrow}).$$

Here, H is the uniform magnetic field, $n_{k,s} = c^\dagger_{k,s} c_{k,s}$, $(s = \{\uparrow, \downarrow\})$, and the density operator ρ is given by

$$\rho_s(\mathbf{r}) = \psi^\dagger_s(\mathbf{r}) \psi_s(\mathbf{r}) = \frac{1}{V} \sum_{k,q} e^{i\mathbf{q}\cdot\mathbf{r}} c^\dagger_{k,s} c_{k-q,s} \qquad \text{with} \qquad \psi_s(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k e^{-i\mathbf{k}\cdot\mathbf{r}} c_{k,s}.$$

a) Show that in the molecular-field (mean-field) approximation the energy of the system, $E = \langle H_1 \rangle$, is written in the following form:

$$E = E_0 + \left[D_{\rm F} \cdot \Big(\frac{I\chi}{2\mu_{\rm B}} + \mu_{\rm B} \Big)^2 - \frac{I\chi^2}{4\mu_{\rm B}^2} - \chi \right] H^2, \tag{1}$$

where E_0 is the H-independent contribution to the total energy, $D_{\rm F}$ is the density of states per spin projection at the Fermi level, and $I \equiv U/V$. The magnetization is $M = \chi H$ and $M = \mu_{\rm B}(N_\uparrow - N_\downarrow)$, where $N = N_\uparrow + N_\downarrow$ and $N_s = \sum_k \langle n_{k,s} \rangle$ (the thermal average: $\langle \cdots \rangle$).

b) Show that in this approximation the uniform susceptibility χ is given by

$$\chi = \frac{\chi_{\rm pauli}}{1 - I D_{\rm F}}, \tag{2}$$

where $\chi_{\rm pauli} = 2\mu_{\rm B}^2 D_{\rm F}$ is the Pauli susceptibility.

<u>Hint</u>: Consider the operator $c^\dagger_{k,s} c_{k\pm q.s}$ and its deviation from the thermal average $\langle c^\dagger_{k,s} c_{k\pm q.s} \rangle$. Then, neglect the quadratic term of such deviations in $H_{\rm INT}$. (This is the mean-field approximation.) Set $\langle c^\dagger_{k,s} c_{k\pm q.s} \rangle = 0$ for $\mathbf{q} \neq 0$, because we are interested in a spatially-uniform spin polarization here. If necessary, apply the Taylor expansion to the Fermi distribution function $f(\tilde{\xi}_{k,s}) = \langle n_{k,s} \rangle$ up to the 2nd order with respect to H. Note that $df(\xi)/d\xi = \beta f'(\xi)$, $\beta = 1/k_{\rm B}T$, and at low temperatures $-f'(\xi) \approx \delta(\xi)/\beta$. Neglect a term with the derivative of the density of states at the Fermi level. The magnetization M is obtained from $M = -dE/dH$.

3.2 Non-uniform susceptibility of a gas of N free electrons in a system with the volume V. Consider the Hamiltonian

$$H_2 = H_{\mathrm{KE}} + H_{\mathrm{Z}}^{(B)},$$

where H_{KE} is the same as in Probl. **3.1**. The Zeeman term $H_{\mathrm{Z}}^{(B)}$ due to the non-uniform magnetic field, $\vec{H}(\mathbf{r}) = \vec{H}_q\sqrt{2}\cos(\mathbf{q}\cdot\mathbf{r})$, is given by

$$H_{\mathrm{Z}}^{(B)} = -V\sum_{i=1}^{N}\mu_{\mathrm{B}}\vec{S}(\mathbf{r}_i)\cdot\vec{H}_q\sqrt{2}\cos(\mathbf{q}\cdot\mathbf{r}_i).$$

Here, $\vec{S}(\mathbf{r})$ and $\mathbf{r}_i$ are the spin density operator and the position of the i-th electron, respectively. We define $\vec{S}(\mathbf{r})$ as

$$\vec{S}(\mathbf{r}) = \sum_{s,s'}\psi_s^\dagger(\mathbf{r})\vec{\sigma}_{ss'}\psi_{s'}(\mathbf{r}),$$

where the 2×2 matrices $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices, and $\vec{\sigma}_{ss'}$ means their ss' matrix element.

We assume that the magnetic field is sufficiently small such that $H_{\mathrm{Z}}^{(B)} \ll H_{\mathrm{KE}}$. From now on, we choose $\vec{H}_q = H_q\hat{x}$ in the above $H_{\mathrm{Z}}^{(B)}$ for convenience.

a) Show that the non-uniform susceptibility of the system is given by

$$\chi(\mathbf{q}) = 2\mu_{\mathrm{B}}^2\sum_k\frac{f(\xi_k) - f(\xi_{k+q})}{\xi_{k+q} - \xi_k},$$

where $\chi(\mathbf{q}) = M/H_q = (-dE/dH_q)/H_q$, and $f(\xi_k)$ is the Fermi distribution function. We assume that the electrons are distributed uniformly in the system with the volume V such that $\sum_{i=1}^{N} \to \frac{1}{V}\int_V d\mathbf{r}_i$.

b) Show that for small values of $|\mathbf{q}|$,

$$\chi(\mathbf{q}) \approx 2\mu_{\mathrm{B}}^2 D_{\mathrm{F}}\cdot\left(1 - \frac{|\mathbf{q}|^2}{8k_{\mathrm{F}}^2}\right).$$

Here, we assume $\xi_k = \hbar^2(|\mathbf{k}|^2 - k_{\mathrm{F}}^2)/2m$. D_{F} is the density of states at the Fermi level per spin projection. In this calculation, replace the Fermi distribution function with the step function as an approximation at low temperatures.

<u>Hint</u>: Consider $H_{\mathrm{Z}}^{(B)}$ as a perturbation term, and calculate the energies $\tilde{\xi}_k$ of the single particle states up to the 2nd order correction by the perturbation theory of the quantum mechanics. Here, the unperturbed Hamiltonian H_0 is perturbed by $H_{\mathrm{Z}}^{(B)}$, resulting in $\tilde{H}$:

$$\begin{aligned} H_0 &\equiv H_{\mathrm{KE}} = \sum_{k,s}\xi_k c_{k,s}^\dagger c_{k,s} \\ \rightarrow \qquad \tilde{H} &= \sum_{k,s}\tilde{\xi}_k\tilde{c}_{k,s}^\dagger\tilde{c}_{k,s}. \end{aligned}$$

Then, the energy of the system is

$$E = \langle\tilde{H}\rangle = \sum_{k,s}\tilde{\xi}_k\langle\tilde{c}_{k,s}^\dagger\tilde{c}_{k,s}\rangle = \sum_{k,s}\tilde{\xi}_k f(\tilde{\xi}_k).$$