problem set #3 "Magnetism of electron gas" due on 4/25/2021

Physics–172 / Applied Physics–272 Introduction to Solid State Physics Spring quarter, 2022

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Remark. For brevity, we set Boltzmann constant $k_B = 1$ to unity in this problem set.

Problem 3.1 (Pauli paramagnetism $-$ 3 points). Let's consider electron gas that interacts with magnetic field via Zeeman mechanism only (orbital field could be considered separately)

$$
\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} - m_z H, \qquad \hat{m}_z = -2\mu_B \hat{s}_z = -\mu_B \hat{\sigma}_z, \quad \mu_B = \frac{|e|\hbar}{2mc}.
$$

Compute magnetic susceptibility in the $T \ll E_F$ limit and small enough magnetic field (what it should be compared to for $D = 2$? for $D = 3$?). For the sake of exercise, we ask you to do the calculation using canonical ensemble free energy $F = \Omega + \mu N$.

$$
\mathbf{m} = -\frac{1}{V} \left(\frac{\partial F}{\partial \mathbf{H}} \right)_{N,V,T}
$$

.

Remark. In the next problem we are going to calculate the diamagnetic contribution to the magnetic susceptibility of electron gas. Its meaning is simple. In the presence of magnetic field moving electrons experience Lorenz force that makes them go in a closed loop.

$$
\mathbf{F}_L = q \left[\frac{\mathbf{v}}{c} \times \mathbf{H} \right] = m_e v^2 / r \qquad r = m_e v c / qH
$$

Such loop creates a magnetic moment, which points in the direction opposite to the magnetic field.

$$
\mathbf{m} = \frac{q}{2c} [\mathbf{r} \times \mathbf{v}] = -\frac{m_e v^2}{2c} \frac{\mathbf{H}}{H}
$$

Problem 3.2 (Landau diamagnetism $-$ 3 points). Using steps outlined below, calculate diamagnetic contribution to the magnetic susceptibility of the electron gas in metals at low fields and temperatures $T \ll \epsilon_F$ (what magnetic field should be compared to?).

1. (1 point) Hamiltonian of an electron in a metal in the presence of magnetic field $H = H\hat{z}$ (without Zeeman term) reads

$$
\hat{\mathcal{H}} = \frac{1}{2m^*} \left(\hat{p} + \frac{|e|}{c} \mathbf{A} \right)^2
$$

Write down the energies ε_{n,p_z} of such system (ignore spin), don't forget the degeneracies g_{n,p_z} . You don't need to solve the Schrodinger equation, but if you do, we suggest you use Landau gauge. Pay attention to the fact that m^* is the *effective mass* of electron.

2. (2 points) Grand canonical free energy for fermions is as usual

$$
\Omega = -2T \sum_{p_z = -\infty}^{\infty} \sum_{n=0}^{\infty} g_{n, p_z} \ln \left[1 + \exp \frac{\mu - \varepsilon_{n, p_z}}{T} \right].
$$

Factor of 2 comes from spin. Calculate magnetic moment and from it the susceptibility according to

$$
\mathbf{m} = -\left(\frac{\partial \Omega}{\partial \mathbf{H}}\right)_{\mu, V, T}
$$

To simplify the calculation, we ignore dependence of chemical potential on temperature since we are only interested in the leading term in T/ϵ_F expansion.

You most probably want to use Euler-Maclaurin formula (write down the condition on magnetic field that allows you to apply it).

$$
\sum_{n=0}^{\infty} F\left(n + \frac{1}{2}\right) = \int_0^{\infty} F(x) dx + \frac{F'(0)}{24} + \dots
$$

Remark. In problem set $\#1$ we have learned about quantum mechanism that holds atoms in a lattice – *exchange interaction*. It so happens that the very same mechanism is responsible for the existence of magnets. In a Hydrogen molecule there is an energy difference between state that corresponds to a total spin of two electron being $S = 0$ or $S = 1$. That allows to write down effective Hamiltonian in terms of spins of the electrons.

$$
\hat{\mathcal{H}} = -\sum_{i,j} J_{i,j} \hat{\textbf{S}}_i \cdot \hat{\textbf{S}}_j
$$

Constant *J* is called exchange integral, it is proportional to the difference $E_a - E_s$. In the next problem we will solve the simplest variation of such problem — Cluster Ising model — and discover the mechanism of [ferromagnetism.](https://en.wikipedia.org/wiki/Ferromagnetism)

Problem 3.3 (Ferromagnetism -4 points). Consider a system of N Ising spins $s_i = \pm$ that have all–to–all ferromagnetic $(J > 0)$ interaction.

$$
E = -\frac{J}{2N} \sum_{i \neq j} s_i s_j - H \sum_{i=1}^{N} s_i,
$$

Here *J* is the exhange interaction constant and *H* is the external magnetic field ($\mu_B = 1$). Such system exhibits ferromagnetic transition: at the temperature below Curie temperature $T < T_c$ all spins have the same value, while for $T > T_c$ there is no net magnetization. To demonstrate that, we ask you to calculate average spin value at finite temperature T in the limit $N \to \infty$.

$$
m \equiv \frac{1}{N} \sum_{i=1}^{N} \langle s_i \rangle = \langle s_1 \rangle, \qquad \langle s_1 \rangle = \frac{1}{Z} \sum_{\{s_i\}} s_1 \exp\left[-\frac{E}{T}\right].
$$

We ask you to do it in two different ways.

- 1. (1 point) Find average spin $m = m(T, H \rightarrow +0)$ within mean-field approximation (you assume that all spins except one are already equal to their average value m and solve effective problem for the last spin, condition of self-consistency defines the value of m).
- 2. (3 points) Calculate free energy $F = F(T, H)$ exactly (in thermodynamic limit $N \to \infty$)

$$
F = -T \lim_{N \to \infty} \ln Z, \qquad Z(T, H) = \sum_{\{s_i\}} \exp \left[-\frac{E(\{s_i\}, H)}{T} \right]
$$

and determine the magnetization as function of temperature and external field.

$$
m = -\frac{1}{N} \left(\frac{\partial F}{\partial H} \right)_{N,T}
$$

Here are detailed steps that should help you to solve it.

- (a) Rewrite the energy in terms of total spin $S = \sum_{i=1}^{n} s_i$ and decouple S^2 using [Hubbard–](https://en.wikipedia.org/wiki/Hubbard\T2A\textendash Stratonovich_transformation) [Stratonovich transformation.](https://en.wikipedia.org/wiki/Hubbard\T2A\textendash Stratonovich_transformation)
- (b) Transform exponent of the sum of spins to the product of the exponents. You should end up with the following expression.

$$
Z = \sqrt{\frac{NJ}{2\pi T}} \int_{-\infty}^{\infty} \exp\left[-N\frac{J\mu^2}{2T} + N\ln\left(2\cosh\frac{H+J\mu}{T}\right)\right] d\mu.
$$

- (c) Compute integral over effective magnetization μ (dummy variable you have introduced during Hubbard–Stratonovich) in the $N \to \infty$ limit using [Laplace method](https://en.wikipedia.org/wiki/Laplace%27s_method) (a.k.a. real version of [saddle point approximation\)](https://physics.stackexchange.com/questions/14639/how-is-the-saddle-point-approximation-used-in-physics).
- (d) Find critical temperature T_c and net magnetisation $m = m(T, H \to +0)$ (draw a rough plot). Which order transition is this?