PROBLEM SET #4

"Magnetism of electron gas — II"

due on 5/3/2021

Physics–172 / Applied Physics–272

Introduction to Solid State Physics

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Comment. *Note that since these lecture notes are part of a manuscript, much of the language used here follows that of a book, with reference to chapters, sections, etc. In addition, some material in the notes may be more advanced, or will not directly be related to discussions in class. Please view these parts as stimulating extensions, where you are welcome to contact us about questions and relevant references.*

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

Problem 4.1 (Classical diamagnetism — **2 points**)**.** Ampére's classical calculation of a magnetic moment from a charge $-|e|$ particle circling in orbit is

$$\mathbf{m} = -\frac{|e|}{2c}[\mathbf{r} \times \mathbf{v}]. \tag{4.1.1}$$

The single–particle classical Hamiltonian of a free electron in magnetic field is:

$$\mathcal{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{|e|}{2c}[\mathbf{r} \times \mathbf{H}]\right)^2$$

Using Hamilton's equations of motion, show the equivalence of Ampére's calculation of $\mathbf{m}$ to the expected result of

$$\mathbf{m} = -\frac{\partial E}{\partial \mathbf{H}},$$

where E is the energy of the particle. Identify the velocity and relate it to the canonical momentum of a charged particle in magnetic field.

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. Such loop creates a magnetic moment (4.1.1), which points in the direction opposite of the magnetic field.

Problem 4.2 (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 $\mathbf{H} = H\hat{z}$ (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. (**1 point**) 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 to apply it).

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

3. (**1 point**) You have previously calculated paramagnetic contribution to the magnetic susceptibility of a metal (**problem 3.2**). Of course, in a real solid you always have both $\chi = \chi_{\text{dia}} + \chi_{\text{para}}$. Compare the two.

$$\frac{\chi_{\text{dia}}}{\chi_{\text{para}}} = ?$$

Remark. In **problem 1.4** 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.

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

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.

Problem 4.3 (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 $m = m(T, H \to +0)$ 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–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 (a.k.a. real version of saddle point approximation).

   (d) Find critical temperature T_c and net magnetisation $m = m(T, H \to +0)$ (draw a rough plot). Which order transition is this?

Problem 4.4 (Screened potential — **6 points**). Find physical solutions (i.e. vanishing at infinity) of the following problems. These problems could be tackled by Fourier transform method. Alternatively, you can guess the answer and check that it satisfies the equation.

1. (**1 point**) Poisson equation in $D = 3$ dimensions

$$-\nabla^2\phi(\mathbf{r}) = 4\pi\delta(\mathbf{r}). \qquad \mathbf{r} = (x, y, z).$$

   Hint. Integral form of a delta function.

$$\delta(\mathbf{r}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}}.$$

2. (**1 point**) Poisson equation in $D = 2$ dimensions

$$-(\partial_x^2 + \partial_y^2)\phi(\boldsymbol{\rho}) = 4\pi\delta(\boldsymbol{\rho}), \qquad \boldsymbol{\rho} = (x, y).$$

   This problem requires introduction of a regularization of some sort.

3. (**1 point**) Screened Poisson equation in $D = 3$ dimensions

$$(-\nabla^2 + \lambda^{-2})\phi(\mathbf{r}) = 4\pi\delta(\mathbf{r}).$$

4. (**1 point**) Screened Poisson equation in $D = 2$ dimensions.

$$(-\nabla_{x,y}^2 + \lambda^{-2})\phi(\boldsymbol{\rho}) = 4\pi\delta(\boldsymbol{\rho}), \qquad \boldsymbol{\rho} = (x, y).$$

   Exact answer could be expressed through Macdonald function of zeroth order $K_0(z)$, however, we only ask you to find asymptotic behavior of $\phi(\rho)$ at $\rho \ll \lambda$ and $\rho \gg \lambda$.

5. (**2 points**) Three–dimensional Poisson equation screened in two–dimensional plane.

$$(-\nabla^2 + 2\lambda^{-1}\delta(z))\phi(\boldsymbol{\rho}, z) = 4\pi\delta(\boldsymbol{\rho})\delta(z), \qquad \boldsymbol{\rho} = (x, y). \tag{4.4.1}$$

   Exact answer for $\phi(\boldsymbol{\rho}, z = 0)$ could be expressed through Neumann $N_0(z)$ and Struve functions $H_0(z)$, however, we only ask you to find asymptotic behavior of $\phi(\rho, z = 0)$ at $\rho \ll \lambda$ and $\rho \gg \lambda$. Can you predict what it is going to be like without calculation?

   Remark. To understand where equation (4.4.1) comes from, you can imagine that you have a point charge, which lies within a plane of screening media, but half–space above and below it is empty. Another system where such problem appears is a description of vortex in a thin superconductor.