Exam — Session 1

Duration: 2 h
Documents, cell phones, and calculators are not allowed
The text contains 4 pages in total

1 The Blume–Capel model [∼14 points]

The Blume–Capel model describes a magnetic material with some nonmagnetic vacancies. Let us consider a lattice [we denote by $N(\gg 1)$ the number of lattice sites and by z the number of nearest neighbors] of spins S_i that can take the values -1, 0 and $+1$. A spin 0 corresponds to a vacancy (nonmagnetic impurity or empty site) and spins $+1$ or -1 correspond to the two different orientations of the magnetic species. We assume that the Hamiltonian of the system in presence of an homogeneous magnetic field h is given by

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_i S_j + \Delta \sum_{i=1}^{N} S_i^2 - h\sum_{i=1}^{N} S_i \tag{1.1}$$

where $J > 0$ is the exchange interaction and where Δ is a constant that can be either negative or positive. In the Hamiltonian above, $\langle i,j\rangle$ denotes a summation over nearest neighbors.

1.1 General discussion

(a) Justify that $-\Delta$ is the energy of creation of a vacancy. In which case ($\Delta > 0$ or $\Delta < 0$) is it favorable to create a vacancy?

(b) At $T = 0$ and $h = 0$, calculate the energy of the system in the three different states $\langle S_i\rangle = +1$, $\langle S_i\rangle = -1$, and $\langle S_i\rangle = 0$. Which state is selected at $T = 0$?

(c) Which limit of Δ corresponds to the usual two-state Ising model? How would you call the $\Delta = 0$ model?

1.2 Mean-field approximation

We now aim at performing a mean-field approximation (MFA). We write $S_i = m + \delta S_i$, where $m = \langle S_i\rangle$ is the average magnetization.

(a) Define the spin-spin correlation function C_{ij}. What is the value of C_{ij} in the MFA?

(b) Show that within the MFA, it is possible to write the Hamiltonian (1.1) as

$$\mathcal{H} \simeq \frac{1}{2}NzJm^2 - (h + zJm)\sum_{i=1}^{N} S_i + \Delta\sum_{i=1}^{N} S_i^2.$$

(c) Calculate the free energy F within the MFA.

(d) Demonstrate that the average value $m = \langle S_i\rangle$ is given by the expression

$$m = -\frac{1}{N}\frac{\partial F}{\partial h}.$$

Deduce that, within the MFA, the magnetization obeys the self-consistent equation (SCE)

$$m = \frac{2\sinh\left(\beta[h + zJm]\right)}{\exp\left(\beta\Delta\right) + 2\cosh\left(\beta[h + zJm]\right)}.$$

From now on, we consider the case of vanishing magnetic field, $h = 0$.

(e) In the case $\Delta \to -\infty$, discuss the solutions of the SCE.

(f) In the general case, show that $m = 0$ is a solution of the SCE.

(g) We now aim at discussing graphically the solutions of the SCE. We define $t = k_{\mathrm{B}}T/zJ$ and $\delta = \Delta/zJ$.

(i) Express the SCE in term of the function

$$f(m) = \frac{2\sinh(m/t)}{\exp(\delta/t) + 2\cosh(m/t)}.$$

(ii) What is the value of $f(0)$?

(iii) What are the limits of $f(m)$ when $m \to \pm\infty$?

(iv) Calculate

$$\left.\frac{\mathrm{d}f}{\mathrm{d}m}\right|_{m=0}$$

and discuss graphically the number of solutions to the SCE. Show that there is a critical reduced temperature t_{c} defined by the equation

$$t_{\mathrm{c}} = \frac{2}{2 + \exp(\delta/t_{\mathrm{c}})}.$$

(v) In figure 1 (colored lines) is plotted the function $g(t,\delta) = 2/[2 + \exp(\delta/t)]$ as a function of t for different values δ_i of δ. Which δ_i's are positive and which of them are negative? Sort by ascending order the δ_i's.

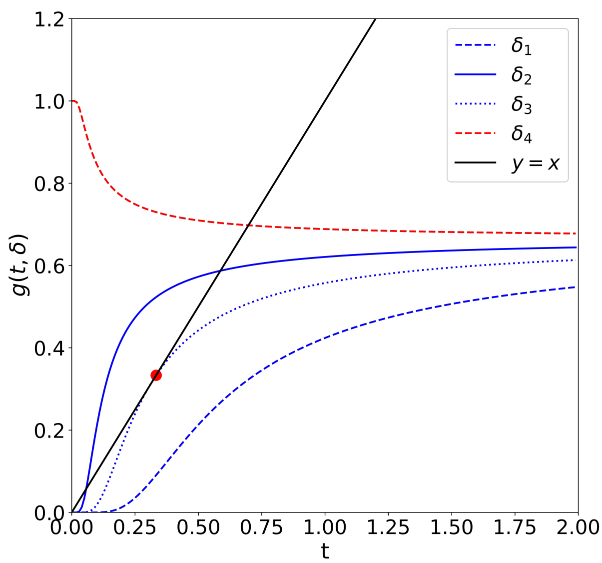

Figure 1: Colored lines: Plot of $g(t,\delta) = 2/[2 + \exp(\delta/t)]$ as a function of t for different values δ_i of δ. Black solid line: t.

(vi) Plot the curve $g(t,\delta)$ for the value of δ corresponding to the Ising model and give the corresponding t_{c}.

(vii) Using your previous discussion and question 1.1(b), sketch the general behavior of t_{c} as a function of δ.

2 Pauli paramagnetism of a two-dimensional electron gas [∼6 points]

In this exercice, we wish to understand one of the magnetic properties of a noninteracting electron gas: the Pauli paramagnetism which is due to the alignment of the electronic magnetic moments with the applied magnetic field. The one-electron Hamiltonian describing this phenomenon is given by

$$H = \frac{\mathbf{p}^2}{2m} - \mu_z B. \tag{2.1}$$

Here, $\mathbf{p}$ is the electron momentum, m its mass, $\mu_z = qS_z/m$ its magnetic moment, which is related to its spin S_z through the gyromagnetic factor $\gamma = q/m$, where $q = -e$ (with $e = 1.6 \times 10^{-19}\,\mathrm{C}$ the elementary charge). In what follows, we consider a homogeneous magnetic field B parallel to the z axis, and we assume that electrons are confined to a two-dimensional rectangular surface with area $\mathcal{A} = L_x L_y$, where L_x and L_y are the lateral dimensions of the electron gas in the x and y directions, respectively.

We recall that electrons are spin $1/2$ particles, so that they obey the Fermi–Dirac statistics. The average occupancy of an energy state ϵ is then given by

$$f(\epsilon) = \frac{1}{\mathrm{e}^{\beta(\epsilon-\mu)} + 1}, \tag{2.2}$$

where $\beta = 1/k_\mathrm{B}T$, with T the temperature of the gas, and where $\mu = \mu(T)$ is the chemical potential.

2.1 Warm up

(a) Plot the Fermi–Dirac distribution (2.2) for both $T = 0$ and $T \neq 0$.

(b) How is defined the Fermi energy ϵ_F in terms of μ?

(c) In absence of magnetic field, the Hamiltonian (2.1) reduces to

$$H = \frac{\mathbf{p}^2}{2m}. \tag{2.3}$$

Using periodic boundary conditions, one can easily show that the spectrum corresponding to the Hamiltonian (2.3) is given by $\epsilon_\mathbf{k} = \hbar^2|\mathbf{k}|^2/2m$, where the wavevector $\mathbf{k} = (k_x, k_y)$ is quantized according to $k_x = 2\pi n_x/L_x$ and $k_y = 2\pi n_y/L_y$, with n_x and n_y integer numbers. Show that the corresponding density of states (including the spin degeneracy) is energy independent and is given in the thermodynamic limit by

$$\rho_0 = \frac{m\mathcal{A}}{\pi\hbar^2}. \tag{2.4}$$

(d) Still in absence of a magnetic field, show that $\epsilon_\mathrm{F} = N/\rho_0$, where N is the total number of electrons in the two-dimensional gas.

2.2 Pauli paramagnetism

The energy spectrum corresponding to the Hamiltonian (2.1) is spin dependent, and given by

$$\epsilon_\mathbf{k}^\pm = \frac{\hbar^2|\mathbf{k}|^2}{2m_*} \mp \epsilon_B,$$

where $+$ ($-$) corresponds to a spin up (down) electron. Here, $\epsilon_B = \mu_\mathrm{B} B$, with $\mu_\mathrm{B} = \hbar q/2m$ the Bohr magneton.

(a) Show that the density of states of the two spin species is energy dependent and given by

$$\rho_\pm(\epsilon) = \frac{1}{2}\rho_0\,\theta(\epsilon \pm \epsilon_B),$$

where $\theta(x)$ is the Heaviside step function.

(b) Let us first assume that both the temperature T and the chemical potential μ are fixed. Show that the average number of spin up and spin down electrons, denoted by $N_\pm$, is given by

$$N_\pm = \frac{\rho_0}{2\beta} \ln\left(1 + \mathrm{e}^{\beta[\pm\epsilon_B + \mu]}\right).$$

(c) Let us now consider that the total number of electrons $N = N_+ + N_-$ is fixed. Deduce from the preceding question a quadratic equation for the fugacity $z = \mathrm{e}^{\beta\mu}$. Give the resulting expression of the chemical potential as a function of ϵ_F and ϵ_B. In particular, analyze the low temperature ($\beta\epsilon_\mathrm{F} \gg 1$) and low magnetic field ($\beta\epsilon_B \ll 1$) limits.

(d) The magnetization of the electron gas is given by $M = \mu_\mathrm{B}(N_+ - N_-)/\mathcal{A}$, and the corresponding susceptibility is defined as

$$\chi_\mathrm{P} = \lim_{B\to 0} \frac{\partial M}{\partial B}.$$

Calculate the Pauli susceptibility χ_P as a function of ρ_0, $\mathcal{A}$, and μ_B in the degenerate limit $\beta\epsilon_\mathrm{F} \gg 1$.