Exam — Session 2

Duration: 2 h.
Documents, cell phones, computers, tablets, pocket calculators, etc., are not allowed.
The text contains 4 pages in total, and the 2 exercices are independent from each other.

1 A simple model for a superconductor

Superconductors are materials whose resistivity abruptly vanishes below a critical temperature T_c. We propose a simple model to describe these superconducting properties. We assume that the free electrons of the conductor have a mass m_e, are close in energy to the Fermi level, and have the possibility to associate in pairs to form a bound state known as a *Cooper pair*. These Cooper pairs behave like particles with mass $2m_e$ and spin $s = 1$.

The first two parts of this exercise recall some general properties of the perfect gases of fermions and bosons. The third part describes the superconducting phase.

1.1 Fermion gas: General questions

(a) Which statistical distribution is appropriate to describe the free electron gas of a conductor? Explain your answer.

(b) Recall the expression for the Fermi-Dirac distribution $n_{FD}(\epsilon)$ and give its shape as a function of energy ϵ for different temperatures. Give without demonstration the expression for the energy $\epsilon_{\mathbf{k}}$ of a quantum state with wave vector $\mathbf{k}$?

(c) Consider an electron gas in dimension 3, occupying a volume V at a temperature T. Find the expression for the density of states ρ, as a function of k, then as a function of energy.

(d) Assume that we can place ourselves in the limit $T = 0$. What is the chemical potential in this approximation? Give the relation for calculating the number of electrons in the system, and derive the expression for the Fermi energy E_F as a function of the electron density n_e. In what temperature range is the $T = 0$ approximation correct (give a numerical estimate for a free electron gas with mass $m_e = 9.1 \cdot 10^{-31}$ kg).

1.2 Boson gas: General questions

Consider a perfect gas of N bosons of mass m and spin 1 in contact with a thermostat at a temperature T.

(a) Recall the expression for the Bose-Einstein distribution $n_{BE}(\epsilon)$ and sketch its shape as a function of ϵ for different temperatures. What condition must the chemical potential satisfy?

(b) Sketch qualitatively the curve of the chemical potential as a function of T. The temperature at which the chemical potential cancels out will be denoted T_B. Explain qualitatively what happens for $T < T_B$. One reminds that T_B is defined by the relation

$$\frac{N}{2V} \left(\frac{h^2}{2\pi m k_B T_B} \right)^{3/2} = 2.612 \ .$$

1.3 Superconductivity

Superconductivity is interpreted in a simple model as the possibility for two electrons near the Fermi level to form a bound state called a *Cooper pair*. We denote Δ the binding energy of a pair and assume that the energy of a Cooper pair of wave vector $\mathbf{k}$ is given by

$$E = 2E_{\mathrm{F}} - \Delta + \frac{\hbar^2 k^2}{4m_{\mathrm{e}}}, \qquad (1.1)$$

where E_{F} is the Fermi energy of a gas of N electrons.

So we have the coexistence of a gas of free electrons (1) and a gas of Cooper pairs (2). It is assumed that the free electron gas is composed of N_1 electrons of chemical potential μ_1 at temperature T_1, and that the Cooper pair gas is composed of N_2 pairs of electrons of chemical potential μ_2 at temperature T_2. Interactions between free electrons, between Cooper pairs, and between free electrons and Cooper pairs are all neglected.

(a) Discuss the Cooper pair energy expression (1.1). Why do we have to choose $\Delta > 0$?

(b) Explain why the Cooper pair gas can be treated as a perfect gas of bosons.

(c) Write the relations between T_1, T_2, μ_1 and μ_2 at thermodynamic equilibrium.

(d) Carefully justify that Bose-Einstein condensation for Cooper pairs occurs when $\mu_2 = 2E_{\mathrm{F}} - \Delta$. What is the value of the chemical potential μ_1?

(e) Assuming that the free electrons can be treated as a degenerate Fermi gas, and using the density of state expression given in section 1.1 above (entitled "Fermion gas: General questions"), show that the maximum number of free electrons N_{e} is given by

$$N_{\mathrm{e}} = N \left(1 - \frac{3\Delta}{4E_{\mathrm{F}}} \right).$$

(f) What is the number of Cooper pairs? Deduce that the Bose condensation temperature T_{B} of the Cooper pairs is given by

$$2.612 \left(\frac{4\pi m k_{\mathrm{B}} T_{\mathrm{B}}}{h^2} \right)^{3/2} = \frac{3}{8} \frac{\Delta}{E_{\mathrm{F}}} \frac{N}{V}.$$

2 Ising model and Bethe-Peierls approximation

We consider a d dimensional Ising model consisting of $N \gg 1$ Ising spins $s_i = \pm 1$ at temperature T, arranged at the nodes of a hypercubic lattice. Let us denote $\beta = 1/k_{\mathrm{B}}T$, where k_{B} is the Boltzmann constant. Let h be the external magnetic field (in energy units) and consider only interactions between nearest neighbors. The Hamiltonian of the system can be written as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_{i=1}^{N} s_i, \qquad (2.1)$$

where $J > 0$, and where $\sum_{\langle i,j \rangle}$ denotes a sum over all nearest neighbor pairs of spins (s_i, s_j).

2.1 Mean field approximation

(a) What do the different terms of the Hamiltonian (2.1) correspond to? We note z the number of first neighbors of a site. Express z as a function of the dimension of the space d.

(b) We neglect in this question the interactions between the spins. Calculate the partition function and the free energy of the system. Deduce the mean magnetization $m = \langle s \rangle$ per site. Plot m as a function of h.

(c) Spin interactions are now taken into account. Show that the effective field seen by a spin in the mean-field approximation is $h_{\text{eff}} = h + h_m$, where $h_m = zJm$ is called the molecular field. Briefly justify this name. Show that the mean magnetization $m = \langle s \rangle$ per site is the solution of a self-consistent equation, which will be explicitly written.

(d) Assume a vanishing external magnetic field ($h = 0$). Show that there is a paramagnetic-ferromagnetic phase transition for a critical temperature T_c, whose value will be given in terms of the various parameters of the problem. What does the approximation predict for the case $d = 1$? For the case $d = 2$?

2.2 Bethe-Peierls approximation

To improve the results of the mean-field approximation, Bethe and Peierls proposed a somewhat more sophisticated approach in 1935. Consider a subsystem $\mathcal{C}$ of the spin lattice, consisting of a spin denoted s_0 and its ring of nearest neighbors denoted s_i with $i = 1, \ldots, z$. We note n_+ the number of spins in this ring that are in the state $s_i = +1$ and n_- the number of spins in the $s_i = -1$ state.

The Hamiltonian of the system is described as follows:

- On the one side, the interactions between the spin s_0 and its nearest are described exactly.

- On the other side, the interactions between the spins s_i ($i = 1, \ldots, z$) and the rest of the system, are described as in the mean field, by a molecular field h_m, which we do not know a priori.

(a) Give a simple relationship between n_+, n_- and z.

(b) Show that the energy $\mathcal{H}_\mathcal{C}$ of the subsystem $\mathcal{C}$ can be expressed as $-\beta \mathcal{H}_\mathcal{C}(n_+, n_-, s_0) = (H + H_m + K s_0)(n_+ - n_-) + H s_0$, where we have defined the dimensionless quantities $K = \beta J, H = \beta h$ and $H_m = \beta h_m$.

(c) We define the joint probability $P(s_0 = s, n_+ = n)$ which allows to keep in the probability reference to both $s_0 = s$ and $n_+ = n$. Calculate the partition function $Z_\mathcal{C}$ from $\mathcal{C}$ and show that we have

$$P(s_0 = s, n_+ = n) = \frac{z!}{n!(z-n)!} \frac{1}{Z_\mathcal{C}} e^{(H+H_m+Ks)(2n-z)+Hs}. \tag{2.2}$$

(d) Show that $\langle s_0 \rangle = \sum_{n=0}^{z} [P(s_0 = +1, n_+ = n) - P(s_0 = -1, n_+ = n)]$.

(e) Now we want to express the average magnetization at a site in terms of the joint probabilities $P(s_0 = s, n_+ = n)$. We define the quantity $\mathcal{S}$ as $\mathcal{S} = \sum_{i=1}^{z} s_i$.

   (i) Show that $\langle \mathcal{S} \rangle = z \langle s_0 \rangle$. Justify carefully.

   (ii) Express $\mathcal{S}$ as a function of n_+ and z. Derive an expression for the mean of $\mathcal{S}$ ($\langle \mathcal{S} \rangle$) as a function of $P(s_0 = s, n_+ = n)$ (do not attempt to compute the discrete sum that appears in the result).

   (iii) Deduce from the two previous relations the equation

$$z \sum_{n=0}^{z} P(s_0 = 1, n_+ = n) = \sum_{n=0}^{z} n \left[P(s_0 = +1, n_+ = n) + P(s_0 = -1, n_+ = n) \right]. \tag{2.3}$$

(f) Using the equation (2.3) and the expression for the joint probabilities (2.2), show that the molecular field H_m must satisfy the relation

$$\frac{H_m}{z-1} = \frac{1}{2} \ln \left(\frac{\cosh(H_m + H + K)}{\cosh(H_m + H - K)} \right).$$

(g) It is now assumed that the external magnetic field is zero ($H = 0$). Graphically discuss the solutions of the self-consistent equation for the molecular field h_m. In particular, show that there is a phase transition for a critical temperature T_c, given by

$$\frac{k_B T_c}{J} = \frac{2}{\ln\left(\frac{d}{d-1}\right)}.$$

(h) Recall that the exact resolution of the Ising model in dimension $d = 2$ gives $k_B T_c/J = 2/\ln\left(1 + \sqrt{2}\right)$. Numerical methods calculate exact values for $k_B T_c/J$ given in Table 1. Fill in the table and discuss the obtained results.

Table 1: Values of $k_B T_c/J$ as a function of d for a hypercubic lattice.

d	Exact value	Mean-Field prediction	Bethe-Peierls prediction
1			
2			
3	4,54545		
4	20/3		

Mathematical Formulæ

- $\tanh x \simeq x - x^3/3$ for $x \ll 1$

- $\tanh^{-1} x = \frac{1}{2} \ln\left(\frac{1+x}{1-x}\right)$.

- $\sum_{n=0}^{N} \frac{N!}{n!(N-n)!} x^n y^{N-n} = (x+y)^N$

- $\sum_{n=0}^{N} \frac{N!}{n!(N-n)!} n x^n y^{N-n} = Nx (x+y)^{N-1}$