

Exam — Session 1

Duration: 2h.

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 Chemical potential and charge carrier concentration in a homogeneous semiconductor

We consider a two-band semiconductor with an energy gap $E_g = E_c - E_v$ between the conduction (c) and valence (v) band edges. The electrons follow the Fermi–Dirac distribution

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1},$$

with μ the chemical potential, and where $\beta = 1/k_B T$ with k_B the Boltzmann constant and T the temperature. Similarly, holes follow the distribution $1 - f(E)$. The electronic density of states per unit volume in the valence and conduction bands are denoted $g_v(E)$ and $g_c(E)$, respectively.

1.1 Intrinsic semiconductor

We first consider an intrinsic semiconductor with, at zero temperature, a filled valence band and an empty conduction band. The electron concentration in the conduction band and the hole concentration in the valence band are denoted n_0 and p_0 , respectively.

- At finite temperature, express $n_0(T)$ and $p_0(T)$ in terms of an energy integral (do not attempt to calculate explicitly the integral). Express the neutrality condition. What does this imply for the energy location of μ at $T = 0$?
- We now assume that $k_B T \ll E_g$. Provide a sensible approximation for $f(E)$ and show that $n_0(T)$ and $p_0(T)$ can be rewritten in the form

$$\begin{aligned} n_0(T) &\simeq N_c(T) e^{-\beta(E_c - \mu)}, \\ p_0(T) &\simeq N_v(T) e^{-\beta(\mu - E_v)}, \end{aligned}$$

where $N_c(T)$ and $N_v(T)$ are the effective electron and hole densities of states in the conduction and valence bands, respectively.

- Deduce the temperature dependent *intrinsic* chemical potential $\mu_i(T)$ in the case of an undoped semiconductor as well the *intrinsic* electron and hole concentrations $n_i(T)$ and $p_i(T)$, respectively.
- Calculate the product $n_0(T)p_0(T)$ and show that it does not depend on $\mu(T)$.

1.2 Doped semiconductor

We now consider an homogeneously n -doped semiconductor with an impurity band of shallow donors with concentration N_d and energy E_d located slightly below the conduction band edge such that $E_c - E_d = \delta E \ll E_g$. Due to the electrostatic energy cost to accommodate two electrons (with opposite spins) on one impurity level, the probability that the impurity level with energy E_d is occupied by an electron with either spin is given by

$$\tilde{p}(E_d) = \frac{1}{\frac{1}{2} e^{\beta(E_d - \mu)} + 1}.$$

- (a) Express the concentration of electrons $n_0(T)$ in the conduction band at a temperature T and find an equation relating $N_{v,c,d}$, $E_{v,c,d}$ and μ .
- (b) We introduce $T_d = \delta E/k_B$. Find the expressions of $\mu(T)$ and $n_0(T)$ in the three following cases:
- (i) $T \ll T_d$;
 - (ii) $T_d \lesssim T \ll E_g/k_B$;
 - (iii) $T \gg T_d$ and up to $T \sim E_g/k_B$.
- (c) Sketch $\ln(n_0(T))$ as a function of $1/T$.

2 Antiferromagnetic simple cubic crystal with next-nearest neighbor exchange interaction

Let us consider a simple cubic lattice system of volume V , containing N atoms maintained at a temperature T . Each isolated atom has a total angular momentum (in units of \hbar) $\mathbf{J} = \mathbf{S} + \mathbf{L}$, with \mathbf{S} and \mathbf{L} the spin and orbital angular momentum, respectively. The absolute square value of the angular momentum writes $\mathbf{J}^2 = J(J+1)$, where J is the quantum number of the total angular momentum. The magnetic moment of an atom is given by $\boldsymbol{\mu} = -g\mu_B\mathbf{J}$, where g is the Landé factor and μ_B the Bohr magneton. An external magnetic field $\mathbf{B} = B\hat{z}$ is applied in the z direction corresponding to the [001] crystalline direction (and which defines the quantization axis).

In this exercise we consider an antiferromagnetic exchange interaction γ_1 between nearest neighbors on the lattice, as well as a ferromagnetic interaction γ_2 between next-nearest neighbors. The Hamiltonian of the system reads

$$H = \gamma_1 \sum_{\langle i,j \rangle} J_i^z J_j^z - \gamma_2 \sum_{\langle\langle i,j \rangle\rangle} J_i^z J_j^z + g\mu_B B \sum_{i=1}^N J_i^z, \quad (\gamma_1, \gamma_2 > 0) \quad (1)$$

where J_i^z is the z component of the total angular momentum (with $i = 1 \dots, N$ the lattice site index) while $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ represent, respectively, summations over nearest neighbors and next-nearest neighbors.

2.1 Noninteracting case ($\gamma_1 = \gamma_2 = 0$)

We first consider the case where there is no exchange interaction between nearest and next-nearest neighbors, *i.e.*, $\gamma_1 = \gamma_2 = 0$. The Hamiltonian (1) can then be expressed as a sum over N independent terms as $H = \sum_{i=1}^N H_i$, with

$$H_i = g\mu_B B J_i^z.$$

- (a) Specify the possible values J_i^z of the projection of the angular momentum \mathbf{J} of an atom on the z axis.
- (b) Write the (canonical) partition function Z of each atom. Show that it can be expressed as the ratio of two hyperbolic sines. To simplify the notation, you may want to introduce the dimensionless quantity $\alpha = \beta g\mu_B B$, with $\beta = 1/k_B T$.

Hint: Note that

$$\sum_{k=0}^n q^k = \frac{1 - q^{n+1}}{1 - q}, \quad (q \neq 1).$$

- (c) The free energy (per atom) is defined as $F = -k_B T \ln Z$. Show that the mean value of the magnetic moment of each atom is given by

$$\langle \mu^z \rangle = -\frac{\partial F}{\partial B}.$$

- (d) Show that the average magnetization in z direction $\langle M^z \rangle$, defined as the mean total magnetic moment per unit volume, is linked to $\langle \mu^z \rangle$ by the relationship

$$\langle M^z \rangle = n \langle \mu^z \rangle,$$

with $n = N/V$ the density of atoms in the crystal.

- (e) Deduce from the preceding questions that the average magnetization can be expressed as

$$\langle M^z \rangle = M_s B_J(\beta g \mu_B J B) \quad (2)$$

where the saturation magnetization

$$M_s = n g \mu_B J. \quad (3)$$

Here,

$$B_J(x) = \frac{2J+1}{2J} \coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J} \coth\left(\frac{1}{2J}x\right) \quad (4)$$

denotes the Brillouin function, which has for small argument $x \ll 1$ the Taylor expansion

$$B_J(x) = \frac{J+1}{3J}x + \mathcal{O}(x^3).$$

- (f) Justify why M_s is called the *saturation* magnetization?
- (g) For a given, arbitrary value of J , sketch the magnetization (2) as a function of $g\mu_B J B/k_B T$ and comment on your result. Is the system paramagnetic, diamagnetic, ferromagnetic, or antiferromagnetic?

2.2 Interacting case ($\gamma_1 > 0, \gamma_2 > 0$)

We now consider the full Hamiltonian of Eq. (1) including antiferromagnetic (ferromagnetic) exchange interaction between nearest (next-nearest) neighbors, *i.e.*, $\gamma_1 > 0$ and $\gamma_2 > 0$.

- (a) Let us consider for this question that $T = 0$ and $B = 0$. Justify that the system splits into two sublattices A and B , such that the angular momenta take the value $+J$ or $-J$ depending on the sublattice to which they belong. These states are called *Néel states*. How many Néel states are there?
- (b) Let us call $\langle M^A \rangle$ ($\langle M^B \rangle$) the average magnetization of the A (B) sublattice in the z direction (from now on, we omit for simplicity the z superscript). By writing down the energy E_i^A of one lattice site i belonging to the A sublattice and within the mean (molecular) field approximation due to Pierre Weiss, argue that the effective magnetic field seen by the spin J_i^A is given by

$$B_{\text{eff}}^A = B - \lambda_1 \langle M^B \rangle + \lambda_2 \langle M^A \rangle,$$

with

$$\lambda_1 = \frac{12\gamma_1}{n(g\mu_B)^2}, \quad \lambda_2 = \frac{16\gamma_2}{n(g\mu_B)^2}.$$

Within the same approximation, what is the effective magnetic field B_{eff}^B seen by a spin J_i^B belonging to the B sublattice?

- (c) Deduce from the preceding questions that $\langle M^A \rangle$ and $\langle M^B \rangle$ obey the set of coupled self-consistent equations

$$\langle M^A \rangle = \frac{M_s}{2} B_J(\beta g \mu_B J [B - \lambda_1 \langle M^B \rangle + \lambda_2 \langle M^A \rangle]), \quad (5a)$$

$$\langle M^B \rangle = \frac{M_s}{2} B_J(\beta g \mu_B J [B - \lambda_1 \langle M^A \rangle + \lambda_2 \langle M^B \rangle]), \quad (5b)$$

where M_s and B_J are defined in Eqs. (3) and (4), respectively.

- (d) Argue that for vanishing applied magnetic field ($B = 0$), $\langle M^A \rangle = -\langle M^B \rangle \equiv M$, so that the self-consistent equations (5) simplify to

$$m = B_J(\beta J^2 [6\gamma_1 + 8\gamma_2] m), \quad (6)$$

with $m = 2M/M_s$.

- (e) Solve Eq. (6) graphically and discuss its solutions. In particular, show that there is a antiferromagnetic/paramagnetic phase transition at a critical temperature T_c . Give the expression of T_c as a function of J , γ_1 , and γ_2 . Sketch $|m|$ as a function of T/T_c . Where is the antiferromagnetic phase? The paramagnetic one?
- (f) If one neglects the ferromagnetic interaction between next-nearest neighbors [*i.e.*, $\gamma_2 = 0$ in the Hamiltonian (1)], the result for the critical temperature T_c from the previous question is given by

$$T_c(\gamma_2 = 0) = \frac{2J(J+1)\gamma_1}{k_B}.$$

Your result from the previous question should indicate a *larger* critical temperature. Using physical arguments, justify why is that the case.

- (g) Still for $B = 0$, sketch the total magnetization $M_{\text{tot}} = \langle M^A \rangle + \langle M^B \rangle$ and the staggered magnetization $M_{\text{sta}} = \langle M^A \rangle - \langle M^B \rangle$ as a function of T .
- (h) We now consider a finite applied magnetic field. Using Eqs. (5), determine the zero-field magnetic susceptibility

$$\chi = \mu_0 \left. \frac{\partial M_{\text{tot}}}{\partial B} \right|_{B=0}$$

for $T \gtrsim T_c$ and show that it can be expressed as

$$\chi = \frac{C}{T + \theta}, \quad (7)$$

with

$$\theta = \frac{6\gamma_1 - 8\gamma_2}{6\gamma_1 + 8\gamma_2} T_c, \quad (8)$$

where C is a constant. What is the expression of C as a function of the parameters of the problem?

- (i) Using physical arguments, discuss why in general, the quantity θ from Eq. (8) is positive. Sketch then for $\theta > 0$ the magnetic susceptibility (7) as a function of temperature.