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## 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 one another.*

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### 1 The $p$ - $n$ junction at equilibrium

#### 1.1 The mass action law

We consider a three-dimensional homogeneous two-band, direct gap semiconductor, with an energy gap  $E_g = E_c - E_v$  between the conduction (c) and valence (v) band edges. The electron concentration in the conduction band and the hole concentration in the valence band at a temperature  $T$  are denoted  $n_0(T)$  and  $p_0(T)$ , respectively. In this section, we study thermally assisted generation and recombination of electrons and holes in the semiconductor.

- We assume that the electron (or hole) generation rate writes  $\mathcal{A} \exp(-E_g/k_B T)$ , where  $k_B$  is the Boltzmann constant. Comment on this expression. What is the unit of the constant  $\mathcal{A}$ ?
- We assume that the electron-hole pair recombination rate writes  $\mathcal{B} n_0(T) p_0(T)$ . Comment on this expression. What is the unit of the constant  $\mathcal{B}$ ?
- Write the expression of  $\dot{n}_0(T) \equiv dn_0(T)/dt$ , *i.e.*, the kinetic equation for the electron concentration. In the steady state, give a simple expression of the product  $n_0(T) p_0(T)$  in terms of the constants of the problem introduced above.
- Express the product  $n_0(T) p_0(T)$  in the case of an intrinsic (*i.e.*, undoped) semiconductor and give the expression of the intrinsic charge carrier concentration  $n_i(T)$ .

#### 1.2 Doped semiconductors

For now, starting from the same intrinsic material, we separately consider a  $p$ -doped (hole doped) and an  $n$ -doped (electron doped) bulk semiconductor, where  $p$ -doping (resp.  $n$ -doping) arises from an impurity band, with acceptor (resp. donor concentration) denoted  $N_a$  (resp.  $N_d$ ), situated at energies  $\delta E_a \ll E_g$  (resp.  $\delta E_d \ll E_g$ ) above the valence band maximum (resp. below the conduction band minimum).

- Take silicon (Si) as an example of a semiconducting material. How can one obtain  $p$ -doped Si and  $n$ -doped Si, respectively?
- In the following, we shall consider the *saturation regime*, *i.e.*, all acceptors and donors are ionized in the  $p$ -doped and  $n$ -doped region, respectively, but thermal generation of charge carriers across the semiconductor bandgap remains negligible. Define the temperature range that corresponds to the saturation regime.
- Express the charge neutrality condition in the  $n$ -doped and  $p$ -doped cases. Knowing that the *intrinsic* charge concentration at room temperature (300 K) is typically  $n_i \sim 10^{16} \text{ m}^{-3}$  and that  $N_{a,d} \sim 10^{22} \text{ m}^{-3}$ , give a numerical estimate of  $n_0$  in the  $p$ -doped region and of  $p_0$  in the  $n$ -doped region, respectively, at room temperature.
- Define the “majority carriers” and “minority carriers” in the  $p$ -doped and  $n$ -doped regions, respectively.
- Draw the energy diagram of the  $p$ -doped semiconductor (top of the valence band, bottom of the conduction band, impurity band) and separately that of the  $n$ -doped semiconductor. Indicate qualitatively the position of the chemical potential  $\mu_p$  in the  $p$ -doped case, and  $\mu_n$  in the  $n$ -doped case, respectively.

### 1.3 Energy diagram and electrostatics of the $p$ - $n$ junction

The two energy diagrams drawn in Question 1.2(e) can be viewed as a  $p$ - $n$  junction before contacting the  $p$ -doped and  $n$ -doped regions. We now explicitly consider the abrupt junction formed when the  $p$ -doped and  $n$ -doped semiconductors are contacted. For simplicity, we assume a one-dimensional problem along the  $\hat{x}$  axis, with the junction at  $x = 0$ , and translational invariance in the  $(\hat{y}, \hat{z})$  plane.

- (a) Draw the energy diagram of the  $p$ - $n$  junction along the  $\hat{x}$  axis. Indicate the chemical potential of the junction and give the expression of the built-in electrostatic potential  $\phi_i$  as a function of  $\mu_p$  and  $\mu_n$ .
- (b) Explain how a *depletion region* (also known as *depletion layer*) forms near  $x = 0$  when the  $p$ - $n$  junction is formed.
- (c) Express and represent graphically the charge carrier density  $\rho(x)$  in and out of the depletion region and justify why this region is also called a *space-charge* region.  
Hint: You may consider that the space-charge region spans from  $x = -d_p$  to  $x = 0$  on the  $p$  side of the junction and from  $x = 0$  to  $x = d_n$  on the  $n$  side of the junction (with  $d_{p,n} > 0$ ).
- (d) We introduce the electrostatic potential  $\phi(x)$ , which obeys Poisson's equation

$$\frac{d^2\phi(x)}{dx^2} + \frac{\rho(x)}{\epsilon} = 0, \quad (1.1)$$

where  $\epsilon = \epsilon_0\epsilon_r$ , with  $\epsilon_0$  the vacuum permittivity and  $\epsilon_r$  the dielectric constant of the bulk semiconductor. We assume that  $\phi(x)$  is constant outside of the depletion layer, *i.e.*, for  $x \leq -d_p$  and  $x \geq d_n$ . The corresponding electric field  $\mathcal{E}(x)$  is thus vanishing outside the depletion layer. Solve Eq. (1.1) and express  $\phi(x)$  and  $\mathcal{E}(x)$ .

- (e) Plot  $\phi(x)$  and  $\mathcal{E}(x)$ .
- (f) Considering the continuity of  $\phi(x)$  and  $\mathcal{E}(x)$  at  $x = 0$ , express  $d_p$  and  $d_n$  as a function of  $N_a$ ,  $N_d$ ,  $\epsilon$ ,  $\phi_i$  and  $e$ , with  $e$  the elementary charge. Comment on these expressions. Show that  $w = d_p + d_n$ , the width of the depletion layer, writes

$$w = \sqrt{\frac{N_a + N_d}{N_a N_d} \frac{2\epsilon\phi_i}{e}}.$$

- (g) We give  $e = 1.6 \times 10^{-19}$  C,  $\phi_i = 1$  V,  $\epsilon_0 = 8.85 \times 10^{-12}$  Fm<sup>-1</sup>,  $\epsilon_r = 10$ , and  $N_a = N_d = 10^{22}$  m<sup>-3</sup>. Give an estimate of  $w$  and give an order of magnitude for the built-in electric field  $\mathcal{E}$  across the junction.

## 2 Antiferromagnetic simple cubic crystal

Let us consider a simple cubic lattice crystal of volume  $V$ , containing  $N$  atoms maintained at a temperature  $T$ . Each isolated atom has a spin angular momentum (in units of  $\hbar$ )  $\mathbf{S}$ . The magnetic moment of an atom, which comprise a single unpaired electron, is given by  $\boldsymbol{\mu} = -g\mu_B\mathbf{S}$ , where  $g = 2$  is the Landé factor and  $\mu_B$  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  $J < 0$  between nearest neighbors on the lattice. The Hamiltonian of the system reads

$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z + 2\mu_B B \sum_{i=1}^N S_i^z, \quad (2.1)$$

where  $S_i^z = \pm 1/2$  is the  $z$  component of the spin angular momentum (with  $i = 1, \dots, N$  the lattice site index) while  $\langle i, j \rangle$  represents a summation over nearest neighbors.

### 2.1 Noninteracting case ( $J = 0$ )

We first consider the case where there is no exchange interaction between nearest neighbors, *i.e.*,  $J = 0$ . The Hamiltonian (2.1) can then be expressed as a sum over  $N$  independent terms as  $H = \sum_{i=1}^N H_i$ , with

$$H_i = 2\mu_B B S_i^z.$$

- Calculate the (canonical) partition function  $Z$  of each atom.
- 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

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

- 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.

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

$$\langle M^z \rangle = M_s \tanh(\beta \mu_B B), \quad (2.2)$$

with  $\beta = 1/k_B T$  and where the saturation magnetization

$$M_s = n \mu_B. \quad (2.3)$$

- Sketch the magnetization (2.2) as a function of  $\mu_B B/k_B T$  and comment on your result. Is the system paramagnetic, diamagnetic, ferromagnetic, or antiferromagnetic?
- The zero-field magnetic susceptibility is defined as

$$\chi = \mu_0 \left. \frac{\partial \langle M^z \rangle}{\partial B} \right|_{B=0},$$

where  $\mu_0$  is the vacuum magnetic permeability. Show that the susceptibility follows the Curie law  $\chi = C/T$ . Give the expression of the constant  $C$  in terms of  $\mu_0$ ,  $\mu_B$ ,  $k_B$ , and  $n$ .

## 2.2 Interacting case ( $J < 0$ )

We now consider the full Hamiltonian of Eq. (2.1) including an antiferromagnetic exchange interaction between nearest neighbors, *i.e.*,  $J < 0$ .

- (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  $+1/2$  or  $-1/2$  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  $S_i^A$  is given by

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

where

$$\lambda = \frac{3|J|}{n\mu_B^2}.$$

Justify carefully the above expression of  $\lambda$ . Within the same approximation, what is the effective magnetic field  $B_{\text{eff}}^B$  seen by a spin  $S_i^B$  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

$$\langle M^A \rangle = \frac{M_s}{2} \tanh(\beta\mu_B [B - \lambda \langle M^B \rangle]), \quad (2.4a)$$

$$\langle M^B \rangle = \frac{M_s}{2} \tanh(\beta\mu_B [B - \lambda \langle M^A \rangle]), \quad (2.4b)$$

where  $M_s$  is defined in Eq. (2.3).

- (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 (2.4) simplify to

$$m = \tanh\left(\frac{3\beta|J|}{2}m\right), \quad (2.5)$$

with  $m = 2M/M_s$ .

- (e) Solve Eq. (2.5) graphically and discuss its solutions. In particular, show that there is a antiferromagnetic/paramagnetic phase transition at the Néel temperature  $T_N$ . Give the expression of  $T_N$  as a function of  $|J|$ . Sketch  $|m|$  as a function of  $T/T_N$ . Where is the antiferromagnetic phase? The paramagnetic one?
- (f) 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  $T$ .
- (g) We now consider a finite applied magnetic field. Using Eqs. (2.4), determine the zero-field magnetic susceptibility for  $T \gtrsim T_N$  and show that it can be expressed as

$$\chi = \frac{C}{T + T_N},$$

where  $C$  is the constant determined at Question 2.1(g). Sketch  $\chi$  as a function of  $T$ .

- (h) If the exchange interaction were ferromagnetic, what would be the behavior of the magnetic susceptibility in the vicinity of the critical temperature (no detailed justification needed)?