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Problem Set 6

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M1-S2 2021—2022

Exercise 1 : Electrodynamics in a material

a) Are Maxwell's equations valid inside a material ?

b) Describe the effect of the material by writing the source terms $\rho = \rho_m + \rho_{\text{ind}}$ and $\vec{j} = \vec{j}_m + \vec{j}_{\text{ind}}$ as sums of macroscopic and induced contributions. Define the polarization $\vec{P}$ of the material such that $\vec{\nabla} \cdot \vec{P} = -\rho_{\text{ind}}$ and show that the displacement $\vec{D} = \epsilon_0 \vec{E} + \vec{P}$ depends only on ρ_m.

$$\begin{aligned} \vec{\nabla} \cdot \vec{D} &= \vec{\nabla}(\epsilon_0 \vec{E} + \vec{P}) \\ &= \rho - \rho_{\text{ind}} \end{aligned}$$

Using $\rho = \rho_m + \rho_{\text{ind}}$, we get

$$\vec{\nabla} \cdot \vec{D} = \rho_m$$

c) Define the magnetization $\vec{M}$ such that $\vec{\nabla} \times \vec{M} = \vec{j}_{\text{ind}} - \partial \vec{P}/\partial t$, and introduce the magnetic field $\vec{H}$ through $\vec{B} = \mu_0(\vec{H} + \vec{M})$. Derive an equation for $\vec{H}$ in terms of the macroscopic sources.

$$\begin{aligned} \vec{\nabla} \times \vec{H} &= \vec{\nabla} \times \left(\frac{\vec{B}}{\mu_0} - \vec{M} \right) \\ &= \vec{j} + \epsilon_0 \frac{\partial \vec{E}}{\partial t} - \vec{j}_{\text{ind}} + \frac{\partial \vec{P}}{\partial t} \\ &= \vec{j}_m + \frac{\partial}{\partial t} \vec{D} \end{aligned}$$

And so we get,

$$\vec{\nabla} \times \vec{H} = \vec{j}_{\text{ind}} + \frac{\partial \vec{D}}{\partial t}$$

d) The magnetic susceptibility χ_m is defined through $\vec{M} = \chi_m \vec{H}$. Determine the relation between χ_m and the relative permeability μ_r that is defined through $\vec{B} = \mu_0 \mu_r \vec{H}$.

$$\vec{B} = \mu_0 \mu_0 \vec{H} = \mu_0(\vec{H} + \vec{M}) = \mu_0(\vec{H} + \chi_m \vec{H})$$

So by identification,

$$\mu_r = 1 + \chi_m$$

e) In CGS units, $\epsilon_0 = \mu_0 = 1$, and Maxwell's equations read

$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho \qquad \vec{\nabla} \cdot \vec{B} = 0 \qquad \vec{\nabla} \times \vec{E} = -\frac{1}{c}\partial\vec{B}/\partial t \qquad \vec{\nabla} \times \vec{B} = \frac{1}{c}(4\pi\vec{j} + \partial\vec{E}/\partial t).$$

Define $\vec{D}$ and $\vec{H}$ through $\vec{D} = \vec{E} + 4\pi\vec{P}$ and $\vec{B} = \vec{H} + 4\pi\vec{M}$. Repeat the steps above with appropriate definitions of $\vec{P}$ and $\vec{M}$, and find the relation between the magnetic susceptibility and the relative permeability μ_r. Determine how the magnetic susceptibility (a dimensionless quantity!) changes when going from SI to CGS units.

b)

$$\begin{aligned}\vec{\nabla} \cdot \vec{D} &= \vec{\nabla} \cdot \vec{E} + 4\pi\vec{\nabla} \cdot \vec{P} \\ &= 4\pi\rho + 4\pi\vec{\nabla} \cdot \vec{P} \\ &= 4\pi\rho_m + 4\pi(\vec{\nabla} \cdot \vec{P}) + 4\pi\rho_{\text{ind}}\end{aligned}$$

So we get,

$$\vec{\nabla} \cdot \vec{P} = -\rho_{\text{ind}}$$

c)

$$\begin{aligned}\vec{\nabla} \times \vec{H} &= \vec{\nabla} \times (\vec{B} - 4\pi\vec{M}) \\ &= \frac{1}{c}\left(4\pi(\vec{j}_m + \vec{j}_{\text{ind}}) + \frac{\partial\vec{E}}{\partial t}\right) - 4\pi\vec{\nabla} \times \vec{M} \\ &= \frac{4\pi}{c}(\vec{j}_m + \vec{j}_{\text{ind}}) + \frac{\partial}{\partial t}\left(\frac{\vec{D} - 4\pi\vec{P}}{c}\right) - 4\pi\vec{\nabla} \times \vec{M} \\ &= \frac{4\pi}{c}\vec{j}_m + \frac{1}{c}\frac{\partial\vec{D}}{\partial t} + \frac{4\pi}{c}\vec{j}_{\text{ind}} - \frac{4\pi}{c}\frac{\partial\vec{P}}{\partial t} - 4\pi\vec{\nabla} \times \vec{M}\end{aligned}$$

So we get,

$$\vec{\nabla} \times \vec{M} = \frac{1}{c}\vec{j}_{\text{ind}} - \frac{1}{c}\frac{\partial\vec{P}}{\partial t}$$

d)

$$\vec{B} = \mu\vec{H} = \vec{H} + 4\pi\vec{M}$$

Meaning,

$$\mu = 1 + 4\pi\chi_m$$

$$\chi_{\text{SI}} = 4\pi\chi_{\text{CGS}}$$

Exercise 2 : Hund's rules

Consider an atom with many electrons i in states characterized by the orbital angular momentum $\vec{l}_i$ and the spin $\vec{s}_i$ in units of $\hbar$. We define the total orbital angular momentum $\vec{L} = \sum \vec{l}_i$, the total spin $\vec{S} = \sum \vec{s}_i$, and the total angular momentum $\vec{J} = \vec{L} + \vec{S}$. According to Hund's rules, for the case of a partially filled shell, the lowest energy values are found in the following way :

1. Maximize $S = |\vec{S}|$, respecting the Pauli exclusion principle.
2. Maximize $L = |\vec{L}|$, respecting the Pauli exclusion principle and rule (1).
3. $\vec{J} = |\vec{J}| = L + S$ when the shell is more than half filled and $J = |L - S|$ when the shell is less than half filled.

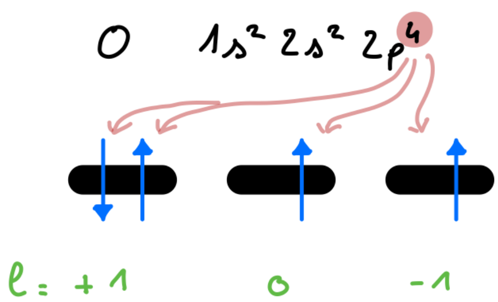
The notation of the resulting configuration is $^{(2S+1)}L_J$, where the orbital angular momentum is usually given by a letter following the convention

L	0	1	2	3	4	5	6
symbol	S	P	D	F	G	H	I

Explain why filled shells are irrelevant and apply Hund's rules to determine the ground state angular momenta for the following cases :

It is irrelevant because of Pauli's exclusion principle, the total spin of the filled shells is zero and same for the orbital angular momentum, it will always be zero because of the totally filled shells.

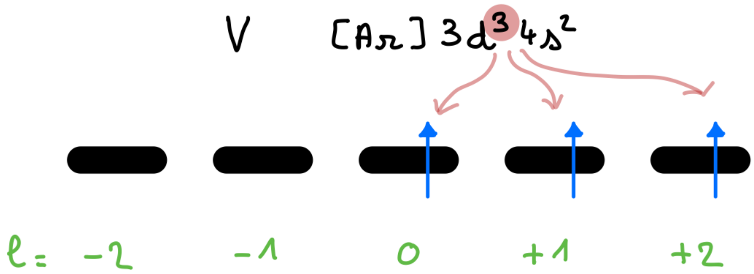
a) O in the configuration $1s^2 2s^2 2p^4$



Total spin is $S = 1$, thus $L = -1 - 0 + 2 = 1$ and thus $J = 2$,

$$^3P_2$$

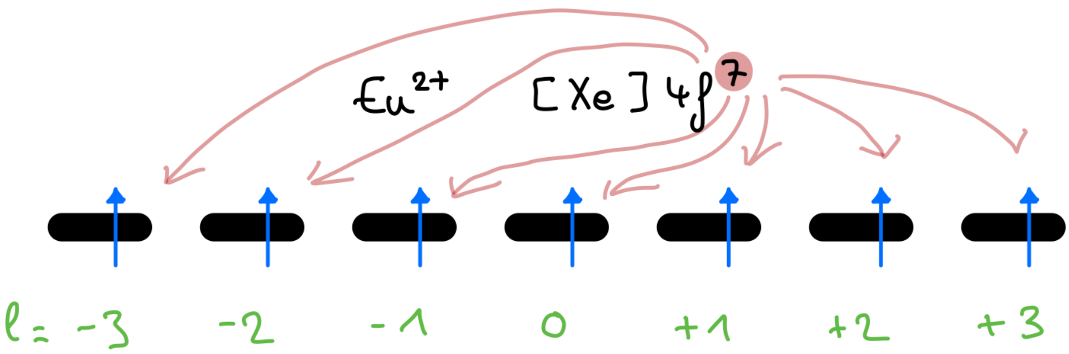
b) V in the configuration $[Ar]3d^3 4s^2$



Total spin is $S = 3/2$ and $L = 2 + 1 = 3$ and so $J = 3/2$,

$$^4\mathrm{F}_{3/2}$$

c) Eu^{2+} in the configuration $[\mathrm{Xe}]4f^7$



The total spin $S = 7/2$, thus $L = 0$ and so $J = 7/2$,

$$^8\mathrm{S}_{7/2}$$

Exercise 3 : Paramagnetic Curie susceptibility (classical treatment)

In this exercise we calculate the contribution of localized magnetic moments to the magnetic susceptibility χ. We consider that the magnetic moments are fixed at the lattice sites of the crystal and take them as distinguishable and independent.

a) To check the validity of the assumption of independence of magnetic moments, one can compare the potential energy (Zeeman energy) $E_Z = -\vec{\mu} \cdot \vec{B}$ of a magnetic moment $\vec{\mu}$ (with $|\vec{\mu}| = \mu_B$) in a magnetic field $\vec{B} = B\vec{e}_z$ to the dipole interaction energy

$$E_{\text{dip}} = \frac{\mu_0}{4\pi} \left[\frac{\vec{\mu}_i \vec{\mu}_j}{r^3} - \frac{3(\vec{\mu}_i \vec{r})(\vec{\mu}_j \vec{r})}{r^5} \right] \sim \frac{\mu_0 \mu_B^2}{4\pi r^3}$$

between two magnetic moments i and j, where $\vec{r} = \vec{r}_i - \vec{r}_j$. Estimate the order of magnitude of these energies in eV when r is the typical distance between atoms in a solid and for a magnetic field $B = 1$ T. Compare the Zeeman energy to the energy of thermal fluctuations at room temperature.
Values : $\mu_0 = 4\pi \times 10^{-7}$ Tm/A, $\mu_B = 9.27 \times 10^{-24}$ J/T, $1eV = 1.6 \times 10^{-19}$ J.

$$E_Z(B = 1 \text{ T}) \simeq 6 \times 10^{-5} \text{ eV} = 9 \times 10^{-24} \text{ J}$$

$$E_{\text{dip}}(r = 3 \text{ Å}) \simeq 4 \times 10^{-25} \text{ J}$$

At room temperature, $k_B T \simeq 25$ meV, thus $\gg E_Z$.

b) We now treat the magnetic moment classically and allow for arbitrary orientation of $\vec{\mu}$ with respect to the magnetic field $\vec{B}$. Express the Zeeman energy E_Z in terms of the absolute values of those vectors and the angle θ between them.

$$E_Z = -\vec{\mu} \cdot \vec{B} = -||\vec{\mu}|| ||\vec{B}|| \cos\theta = -\mu B \cos\theta$$

c) The probability density for a given orientation of the magnetic moment $\vec{\mu}$ in an external magnetic field is determined by the energy through

$$P(\vec{\mu}) = \frac{1}{Z} e^{-E_Z(\theta)/k_B T}$$

where Z is the partition sum given by the integral over all orientations

$$Z = \int \mathrm{d}\Omega e^{-E_Z(\theta)/k_B T}.$$

Calculate Z.

$$
\begin{aligned}
Z &= \int \mathrm{d}\Omega e^{-E_Z(\theta)/k_B T} \\
&= \int_0^{2\pi} \int_0^{\pi} e^{-E_Z(\theta)/k_B T} \sin(\theta)\mathrm{d}\theta\mathrm{d}\varphi \\
&= 2\pi \int_0^{\pi} e^{\mu B \cos\theta/k_B T} \sin(\theta)\mathrm{d}\theta \\
&= 2\pi \left[-k_B T \frac{e^{\mu B \cos\theta}}{\mu B} \right]_0^{\pi} \\
&= -\frac{4\pi k_B T}{\mu B} \sinh\left(\frac{\mu B}{k_B T} \right)
\end{aligned}
$$

d) The mean magnetization $\langle \vec{M} \rangle$ of a material that contains a density $n = N/V$ of those magnetic moments, under the influence of an external magnetic field, is proportional to the average magnetic moment $\langle \vec{\mu} \rangle$. Show that the magnetization component $\langle M_z \rangle$ parallel to the external field $\vec{B}$ at temperature T is given by $\langle M_z \rangle = n\mu_B L(\mu_B B/k_B T)$, where L is the Langevin function

$$
L(x) = \coth(x) - \frac{1}{x}.
$$

$$
\langle \vec{M} \rangle = n \langle \vec{\mu} \rangle \qquad\qquad \langle M_z \rangle = n \langle \mu_z \rangle
$$

$$
\begin{aligned}
\langle \mu_z \rangle &= \int_0^{2\pi} \int_0^{\pi} \frac{e^{-E_Z(\theta)/k_B T}}{Z} \mu_z(\theta) \sin(\theta)\mathrm{d}\theta\mathrm{d}\varphi \\
&= \frac{2\pi}{Z} \int_0^{\pi} e^{\mu B \cos(\theta)/k_B T} \mu \cos(\theta) \sin(\theta)\mathrm{d}\theta \\
&= \frac{2\pi\mu}{Z} \left(\left[-k_B T \cos\theta \frac{e^{\mu B \cos\theta/k_B T}}{\mu B} \right]_0^{\pi} + \int_0^{\pi} \frac{e^{\mu B \cos(\theta)/k_B T}}{\mu B} k_B T(-\sin(\theta))\mathrm{d}\theta \right) \\
&= \frac{2\pi\mu}{Z} \left(k_B T \frac{e^{-\mu B/k_B T}}{\mu B} + k_B T \frac{e^{\mu B/k_B T}}{\mu B} \right) - \frac{\mu k_B T}{\mu B} \\
&= \mu \left(\coth\left(\frac{\mu B}{k_B T} \right) - \frac{k_B T}{\mu B} \right) \\
&= \mu L \left(\frac{\mu B}{k_B T} \right)
\end{aligned}
$$

e) Discuss the dependence of the magnetization in the limits of low field/high temperature $\mu_B B/k_B T \ll 1$ and strong field/low temperature $\mu_B B/k_B T \gg 1$. Sketch $\langle M_z \rangle$ as a function of $x = \mu_B B/k_B T$.

$$
\begin{aligned}
\coth(x) &= \frac{e^x + e^{-x}}{e^x - e^{-x}} \\
&\approx \frac{1 + x + \frac{x^2}{2} + 1 - x + \frac{x^2}{2}}{1 + x - 1 + x + \frac{x^3}{6} + \frac{x^3}{6}} \\
&= \frac{2 + x^2}{2x + \frac{x^3}{3}} \\
&= \frac{1}{x}\left(\frac{2 + x^2}{2 + \frac{x^2}{3}}\right) \\
&= \frac{1}{2x}(2 + x)\left(\frac{1}{1 + \frac{x^2}{6}}\right) \\
&= \frac{1}{2x}(2 + x^2)\left(1 - \frac{x^2}{6}\right) \\
&= \frac{1}{x} + \frac{x}{3}
\end{aligned}
$$

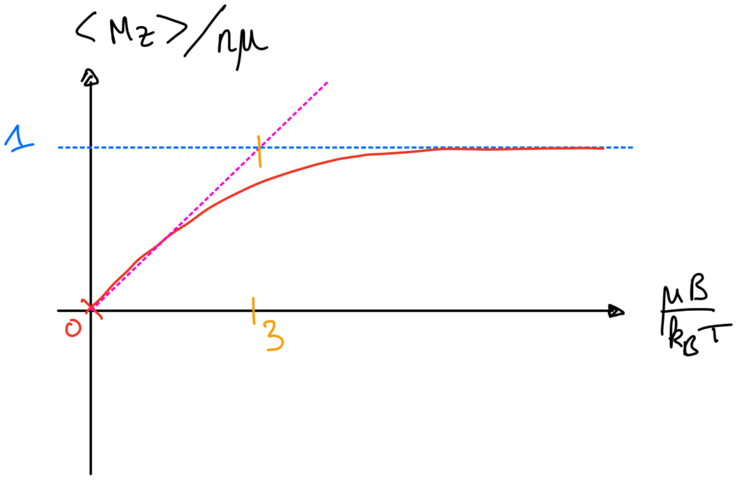
- $\mu_B B/k_B T \ll 1$

$$\langle M_z \rangle \approx n\mu \frac{\mu B}{k_B T}$$

- $\mu_B B/k_B T \gg 1$

$$\langle M_z \rangle \approx n\mu$$

It is the saturation magnetisation (the maximum you can get)



f) The magnetic susceptibility is defined (when $\langle M_z \rangle \ll H$) by

$$\chi = \frac{\partial \langle M_z \rangle}{\partial H}\bigg|_{H=0} \approx \mu_0 \frac{\partial \langle M_z \rangle}{\partial B}\bigg|_{B=0}$$

Calculate the magnetic susceptibility using the low field limit and show that it is always paramagnetic and follows the Curie law $\chi = C/T$.

$$\langle M_z \rangle \approx n\mu \frac{\mu B}{k_B T} = \chi H$$

Thus,

$$\chi_c = \frac{n\mu^2}{3k_B T}$$