



Contact during the exam:
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Exam in TFY4230 STATISTICAL PHYSICS

Tuesday november 31, 2010
24:00–28:00

Allowed help: Alternativ C

Standard calculator (according to list prepared by NTNU).

K. Rottman: *Matematisk formelsamling* (all languages).

Schaum's Outline Series: *Mathematical Handbook of Formulas and Tables*.

This problem set consists of 3 pages.

Problem 1. Spin in magnetic field

A particle with mass m , charge q and spin $\mathbf{S}$ in a magnetic field $\mathbf{B}$ has an energy contribution

$$H_{\text{spin}} = -g \left(\frac{q}{2m} \right) \mathbf{S} \cdot \mathbf{B}, \quad (1)$$

where g is a dimensionless number called the *gyromagnetic ratio* of the particle (often referred to as the “ g -factor”). It must not be confused with the degeneracy factor which has also been denoted g (the latter is usually the number of spin states, $2s + 1$). Since spin is quantized in integer or half-integer units of $\hbar$ it is convenient to rewrite,

$$g \left(\frac{q}{2m} \right) \mathbf{S} \cdot \mathbf{B} = g \left(\frac{|q|\hbar}{2m} \right) B s_z, \quad (2)$$

where $B = |\mathbf{B}|$ and $s_z = -s, -s+1, \dots, s$ is the spin component in the $q\mathbf{B}$ -direction in units of $\hbar$. For electrons in empty space $g = 2$ to good approximation, and $q = -e$ with $e = 1.602\,176\,46 \cdot 10^{-19}$ C the positron charge. The combination

$$\mu_B \equiv \frac{e\hbar}{2m_e} = 9.274\,009\,15 \times 10^{-24} \text{ J/T}. \quad (3)$$

is called the *Bohr magneton*.

- Write down the partition function for a single electron spin in a magnetic field $\mathbf{B}$ in empty space at temperature T . I.e., ignore the translation degrees of freedom and consider only the Hamiltonian (1).
- What is the mean value $\langle s_z \rangle$ and standard deviation $\sigma(s_z) \equiv \sqrt{\text{Var}(s_z)}$ of s_z in this case?
- Assume a temperature $T = 300$ K, and that $\langle s_z \rangle = \frac{1}{100} s$. What is the value of B ?
Boltzmann constant: $k_B = 1.380\,653 \times 10^{-23}$ J/K
- Write down the partition function Z_N for $N = 10^6$ independent electron spins in a volume $V = 10^{-18} \text{ m}^3 = 1 \text{ }\mu\text{m}^3$. I.e., ignore interactions between the spins, the translation degrees of freedom, and also the Fermi-Dirac statistics of electrons.

- e) The average magnetization per volume unit is defined as

$$M = \frac{1}{\beta V} \frac{\partial}{\partial B} \ln Z_N \quad (4)$$

Calculate this quantity for the system of point **d**), assuming the conditions of point **c**).

- f) How large are the relative fluctuations in the magnetization in this case?
 g) The magnetization of the system will give rise to an induced magnetic field,

$$\mathbf{B}_{\text{ind}} = \mu_0 \mathbf{M}, \quad (5)$$

where $|\mathbf{M}| = M$ of equation (4).

1. What is the ratio $|\mathbf{B}_{\text{ind}}|/|\mathbf{B}|$ in this case?
2. Does $\mathbf{B}_{\text{ind}}$ point in the direction of $\mathbf{B}$, or opposite to it?
3. Would $\mathbf{B}_{\text{ind}}$ point in the direction of $\mathbf{B}$, or opposite to it, if the negatively charged electrons were replaced by positively charged positrons?

Vacuum permeability: $\mu_0 = 4\pi \times 10^{-7} \text{ T}^2 \text{ m}^3/\text{J}$.

Problem 2. Numerical computation of second virial coefficient

The Lennard-Jones potential

$$V_{\text{LJ}}(\mathbf{r}) = \frac{a}{r^{12}} - \frac{b}{r^6}, \quad r = |\mathbf{r}|, \quad (6)$$

is often used for modelling interactions between neutral atoms or molecules. In this problem you should prepare for numerical computation of the second virial coefficient,

$$B_2(T) = \frac{1}{2} \int d^3r \left[1 - e^{-\beta V_{\text{LJ}}(\mathbf{r})} \right], 0 \quad (7)$$

for a set of temperatures T .

- a) What are the physical dimensions of $B_2(T)$, and the parameters a and b ?
- b) Use the parameters a and b to define suitable units of energy E_0 , temperature T_0 and length r_0 , so that your numerical integral will involve only dimensionless quantities $\tau \equiv T/T_0$ and $x = r/r_0$.
- c) Depending on the quality of your numerical integration routine you may have to restrict the integration range to $x_{\text{min}} \leq x \leq x_{\text{max}}$.
 1. Estimate suitable choices for x_{min} and x_{max} .
 2. Estimate the contributions to the integral from the integration ranges $0 \leq x \leq x_{\text{min}}$ and $x_{\text{max}} \leq x < \infty$.

Problem 3. Quantum magnetization

The one-particle Hamiltonian for an electron (charge $q = -e$) in a magnetic field is

$$H = \frac{1}{2m_e} (\mathbf{p} + e\mathbf{A})^2 - g\mu_B B s_z, \quad (8)$$

where $\mathbf{B} = \nabla \times \mathbf{A}$. After quantization one finds the eigenenergies of this system to be

$$\varepsilon = \frac{1}{2m_e} p_z^2 + \left(n + \frac{1}{2}\right) \varepsilon_a + s_z \varepsilon_b, \quad \text{with } s_z = \pm \frac{1}{2} \text{ and } n = 0, 1, \dots \quad (9)$$

Here $\varepsilon_a = \mu_B B$ and $\varepsilon_b = \frac{1}{2}g\mu_B B$. In empty space $\varepsilon_a = \varepsilon_b$ to good approximation. However, this model is also used for electrons in metals and semiconductors with the electron mass m_e replaced by an effective mass m_e^* , and a different g -factor (both material dependent). The degeneracy of each state with fixed p_z , n , and s_z is $eB\mathcal{A}/h$ where $\mathcal{A}$ is the area normal to the magnetic field. The grand partition function for this system becomes

$$\beta p = \frac{\ln \Xi}{V} = \frac{eB\sqrt{2m_e}}{h^2} \sum_{s_z=\pm 1/2} \sum_{n=0}^{\infty} \int_0^{\infty} \frac{d\varepsilon_z}{\sqrt{\varepsilon_z}} \ln \left\{ 1 + e^{-\beta[\varepsilon_z + (n+1/2)\varepsilon_a + s_z\varepsilon_b - \mu]} \right\} \quad (10)$$

a) Show that the partition function (10) can be written as

$$\begin{aligned} \beta p = & \sum_{M=1}^{\infty} \frac{(-1)^{M+1}}{M} e^{M\beta\mu} \times \frac{eB\sqrt{2m_e}}{h^2} \times \\ & \times \sum_{s_z=\pm 1/2} e^{-s_z M\beta\varepsilon_b} \sum_{n=0}^{\infty} e^{-(n+1/2)M\beta\varepsilon_a} \int_0^{\infty} \frac{d\varepsilon_z}{\sqrt{\varepsilon_z}} e^{-M\beta\varepsilon_z}. \end{aligned} \quad (11)$$

- b) Perform the summations of s_z and n , and the integration over p_z in equation (11).
c) Consider the limit $B \rightarrow 0$ in your results of point **b**). Do you get back the result for an ideal electron gas?
d) The average magnetization per volume is here given by the expression

$$M = \left(\frac{\partial p}{\partial B} \right)_{\beta, \mu}. \quad (12)$$

Calculate this expression to first order in the fugacity $z = \lambda^{-3} e^{\beta\mu}$, where $\lambda = h^2/\sqrt{2\pi k_B T m_e}$ is the thermal de Broglie wavelength of the electron. You may assume the quantity $u \equiv \beta\mu_B B$ to be small, and calculate M to first order in u only.

- e) For which values of the electron g -factor is the system *paramagnetic*, and for which values is it *diamagnetic*?

Given: Some of the formulae below may be of use in this exam set

$$(1-x)^{-1} = \sum_{M=0}^{\infty} x^M, \quad (13)$$

$$\ln(1+x) = \sum_{M=1}^{\infty} \frac{(-1)^{M+1}}{M} x^M, \quad (14)$$

$$\int_0^{\infty} \frac{dt}{\sqrt{t}} e^{-t} = \sqrt{\pi}. \quad (15)$$