NTNU **Institutt for fysikk**

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Exam in TFY4230 STATISTICAL PHYSICS

Tudnesday 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 $\boldsymbol{S}$ in a magnetic field $\boldsymbol{B}$ has an energy contribution

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

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,

$$g\left(\frac{q}{2m}\right)\boldsymbol{S}\cdot\boldsymbol{B} = g\left(\frac{|q|\hbar}{2m}\right)Bs_z, \tag{2}$$

where $B = |\boldsymbol{B}|$ and $s_z = -s, -s+1, \ldots, s$ is the spin component in the $q\boldsymbol{B}$-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

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

is called the *Bohr magneton*.

a) Write down the partition function for a single electron spin in a magnetic field $\boldsymbol{B}$ in empty space at temperature T. I.e., ignore the translation degrees of freedom and consider only the Hamiltonian (1).

b) 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?

c) 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

d) Write down the partition function Z_N for $N = 10^6$ independent electron spins in a volume $V = 10^{-18}\ \text{m}^3 = 1\ \mu\text{m}^3$. 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

$$M = \frac{1}{\beta V}\,\frac{\partial}{\partial B}\ln Z_N \tag{4}$$

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,

$$\boldsymbol{B}_{\text{ind}} = \mu_0\,\boldsymbol{M}, \tag{5}$$

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

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

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

Problem 2. Numerical computation of second virial coefficient
The Lennard-Jones potential

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

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,

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

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 $x_{\text{min}} \le x \le x_{\text{max}}$.

1. Estimate suitable choices for x_{min} and x_{max}.
2. Estimate the contributions to the integral from the integration ranges $0 \le x \le x_{\text{min}}$ and $x_{\text{max}} \le x < \infty$.

Problem 3. Quantum magnetization

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

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

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

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

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

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

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

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

b) Perform the summations of s_z and n, and the integration over p_z in equation (11).

c) Consider the limit $B \to 0$ 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

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

Calculate this expression to first order in the fugacity $z = \lambda^{-3}\,\mathrm{e}^{\beta\mu}$, 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

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

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

$$\int_0^{\infty} \frac{\mathrm{d}t}{\sqrt{t}}\,\mathrm{e}^{-t} = \sqrt{\pi}. \tag{15}$$