



Solution to the exam in TFY4230 STATISTICAL PHYSICS

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This solution consists of 5 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*.

- a) 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).

The canonical partition function

$$Z = \sum_{s_z = \pm 1/2} e^{\beta g \mu_B B s_z} = 2 \cosh \left(\frac{1}{2} g \beta \mu_B B \right). \quad (4)$$

- 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?

$$\begin{aligned} \langle s_z \rangle &= Z^{-1} \sum_{s_z = \pm 1/2} s_z e^{\beta g \mu_B B s_z} = \frac{1}{2 \cosh(\frac{1}{2} g \beta \mu_B B)} \times \sinh \left(\frac{1}{2} g \beta \mu_B B \right) \\ &= \frac{1}{2} \tanh \left(\frac{1}{2} g \beta \mu_B B \right). \end{aligned} \quad (5)$$

Since the electron has a negative charge, $q = -e$, the spin $\langle s_z \rangle$ points in the direction opposite to the magnetic field $\mathbf{B}$. Since $s_z^2 = \frac{1}{4}$ we find

$$\text{Var}(s_z) = \langle s_z^2 \rangle - \langle s_z \rangle^2 = \frac{1}{4} \left[1 - \tanh^2 \left(\frac{1}{2} g \beta \mu_B B \right) \right] = \frac{1}{4 \cosh^2 \left(\frac{1}{2} g \beta \mu_B B \right)}.$$

I.e.

$$\sigma(s_z) = \frac{1}{2 \cosh \left(\frac{1}{2} g \beta \mu_B B \right)}. \quad (6)$$

- 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

We may use the approximation $\tanh x = x + \mathcal{O}(x^3)$ for small x to find $\frac{1}{2}g\beta\mu_B B = \frac{1}{100}$. I.e.,

$$B = \frac{k_B T}{50 g \mu_B} = \frac{1.380\,653 \times 10^{-23} \times 300}{50 \times 2 \times 9.274\,009 \times 10^{-24}} \text{ T} = 4.466\,201 \text{ T}, \quad (7)$$

which is a rather strong field.

- d) Write down the partition function Z_N for $N = 10^6$ independent electron spins in a volume $V = 10^{-18} \text{ m}^3 = 1 \text{ } \mu\text{m}^3$. I.e., ignore interactions between the spins, the translation degrees of freedom, and also the Fermi-Dirac statistics of electrons.

Since all spins are considered independent,

$$Z_N = Z^N = Z^{10^6}, \quad (8)$$

with Z given by equation (4).

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

$$M = \frac{1}{\beta V} \frac{\partial}{\partial B} \ln Z_N \quad (9)$$

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

$$\begin{aligned} M &= \frac{1}{\beta V} \frac{\partial}{\partial B} \ln Z_N = \frac{N}{\beta V} \frac{\partial}{\partial B} \ln \cosh \left(\frac{1}{2} g \beta \mu_B B \right) = \frac{N}{V} \frac{1}{2} g \mu_B \tanh \left(\frac{1}{2} g \beta \mu_B B \right) \\ &= \frac{10^6}{10^{-18}} \times 9.274\,009 \times 10^{-24} \times \frac{1}{50} \frac{\text{J}}{\text{T m}^3} = 0.185\,480 \frac{\text{J}}{\text{T m}^3} \end{aligned} \quad (10)$$

- f) How large are the relative fluctuations in the magnetization in this case?

The microscopic magnetization is the random quantity

$$\mathcal{M}_z = \frac{1}{V} \frac{1}{2} g Q \mu_B \sum_i s_z^{(i)}, \quad (11)$$

where Q is the particle charge in units of the positron charge, and $s_z^{(i)}$ is the spin of particle i in the direction of $\mathbf{B}$. We have

$$M = \langle \mathcal{M}_z \rangle = \frac{1}{V} \frac{1}{2} g Q \mu_B N \langle s_z \rangle,$$

and

$$\langle \mathcal{M}_z^2 \rangle = \left(\frac{1}{V} \frac{1}{2} g Q \mu_B \right)^2 \left\langle \sum_{i,j} s_z^{(i)} s_z^{(j)} \right\rangle = \langle \mathcal{M}_z \rangle^2 + \left(\frac{1}{V} \frac{1}{2} g Q \mu_B \right)^2 \sum_i \left[\langle s_z^{(i)2} \rangle - \langle s_z^{(i)} \rangle^2 \right].$$

I.e.,

$$\text{Var}(\mathcal{M}_z) \equiv \langle \mathcal{M}_z^2 \rangle - \langle \mathcal{M}_z \rangle^2 = \left(\frac{1}{V} \frac{1}{2} g Q \mu_B \right)^2 N \text{Var}(s_z).$$

A good measure of the relative fluctuations is

$$\frac{\sigma(\mathcal{M}_z)}{\langle \mathcal{M}_z \rangle} = \frac{\sqrt{\text{Var}(\mathcal{M}_z)}}{\langle \mathcal{M}_z \rangle} = \frac{1}{\sqrt{N}} \frac{\sqrt{\text{Var}(s_z)}}{\langle s_z \rangle} = \frac{1}{\sqrt{N}} \frac{1}{\sinh \frac{1}{2} g \beta \mu_B B} = \frac{1}{1000} \times 100 = 0.1. \quad (12)$$

- g)** The magnetization of the system will give rise to an induced magnetic field,

$$\mathbf{B}_{\text{ind}} = \mu_0 \mathbf{M}, \quad (13)$$

where $|\mathbf{M}| = M$ of equation (9).

1. What is the ratio $|\mathbf{B}_{\text{ind}}|/|\mathbf{B}|$ in this case?

From the previous results we find

$$|\mathbf{B}_{\text{ind}}|/|\mathbf{B}| = 4\pi \times 10^{-7} \times \frac{0.185\,480}{4.466\,201} = 5.2 \times 10^{-8}. \quad (14)$$

2. Does $\mathbf{B}_{\text{ind}}$ point in the direction of $\mathbf{B}$, or opposite to it?

It is implicit from equation (9) that B is defined to point in the direction of $\mathbf{B}$ (which is the case), but this can be deduced from equation (2). Since derivation with respect to B gives a positive result it must be that $\mathbf{B}_{\text{ind}}$ points in the direction of $\mathbf{B}$.

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?

The partition function is the same for electrons and positrons. Hence $\mathbf{B}_{\text{ind}}$ will point in the direction of $\mathbf{B}$ for positrons also.

Comment: For a particle with negative charge Q the average spin $\langle s_z \rangle$ will point opposite to $\mathbf{B}$. But since the contribution to magnetization is proportional to $Q \langle s_z \rangle$ the sign of Q does not matter.

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

$$V_{\text{LJ}}(\mathbf{r}) = \frac{a}{r^{12}} - \frac{b}{r^6}, \quad r = |\mathbf{r}|, \quad (15)$$

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,

$$B_2(T) = \frac{1}{2} \int d^3r \left[1 - e^{-\beta V_{\text{LJ}}(\mathbf{r})} \right], 0 \quad (16)$$

for a set of temperatures T .

- a)** What are the physical dimensions of $B_2(T)$, and the parameters a and b ?

B_2 has dimension m^3 , a must have dimension J m^{12} , and b must have dimension J m^6 .

- 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 $x = r/r_0$.

A natural unit of energy is

$$E_0 = b^2/a, \quad (17)$$

corresponding to a natural unit of temperature

$$T_0 = E_0/k_B. \quad (18)$$

A natural unit of length is

$$r_0 = (a/b)^{1/6}. \quad (19)$$

With $x = r/r_0$ and $\tau = T/T_0$ the virial coefficient becomes

$$b_2(\tau) \equiv \frac{1}{2\pi r_0^3} B_2(\tau T_0) = \int_0^\infty x^2 dx \left[1 - e^{(x^{-6} - x^{-12})/\tau} \right]. \quad (20)$$

It may be convenient to introduce another integration variable, $y = x^{-6}$, to obtain the equivalent form

$$b_2(\tau) = \frac{1}{6} \int_0^\infty \frac{dy}{y^{3/2}} \left[1 - e^{(y - y^2)/\tau} \right]. \quad (21)$$

- c) Depending on the quality of your numerical integration routine you may have to restrict the integration range to $x_{\min} \leq x \leq x_{\max}$.

1. Estimate suitable choices for $x_{\min}$ and $x_{\max}$.

For small x (large y) the exponential becomes neglectible small. A safe lower limit is f.i. to choose $x_{\min}$ where the exponential is equal to 10^{-16} . I.e., so that

$$\begin{aligned} \left(y_{\max} - \frac{1}{2}\right)^2 &= \frac{1}{4} + 16\tau \ln 10, \\ y_{\max} &= \frac{1}{2} \left(1 + \sqrt{1 + 64\tau \ln 10}\right), \\ x_{\min} &= \left[\frac{1}{2} \left(1 + \sqrt{1 + 64\tau \ln 10}\right)\right]^{-1/6}. \end{aligned} \quad (22)$$

For large x (small y) we may expand the exponential in a power series of its argument, and integrate term by term. A simple choice is to take $x_{\max}$ so large that only the x^{-6} -term in the expansion is important. I.e., so that the next order term,

$$\left|\left(\frac{1}{\tau} - \frac{1}{2\tau^2}\right)\right| \int_{x_{\max}}^{\infty} x^2 dx \frac{1}{x^{12}} = \left|\left(\frac{1}{\tau} - \frac{1}{2\tau^2}\right)\right| \frac{1}{9x_{\max}^9} \leq 10^{-16}, \quad (23)$$

which can be solved for $x_{\max}$ (with use of the equal sign).

2. Estimate the contributions to the integral from the integration ranges $0 \leq x \leq x_{\min}$ and $x_{\max} \leq x < \infty$.

The contribution from the interval $0 < x \leq x_{\min}$ becomes $\frac{1}{3}x_{\min}^3 = \frac{1}{3}y_{\max}^{-1/2}$.

The contribution from the interval $x_{\max} \leq x < \infty$ becomes $-\frac{1}{3\tau}x_{\max}^{-3} = -\frac{1}{3\tau}y_{\min}^{1/2}$.

Remark: The Python numerical integration routine `scipy.integrate.quad` is able to handle the integral (21) without introduction of $y_{\min}$ and $y_{\max}$, but it complains about slow convergence when τ becomes small.

Problem 3. Quantum magnetization

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

$$H = \frac{1}{2m_e} (\mathbf{p} + e\mathbf{A})^2 - g\mu_B B s_z, \quad (24)$$

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

$$\varepsilon = \frac{1}{2m_e} p_z^2 + \left(n + \frac{1}{2}\right) \varepsilon_a + s_z \varepsilon_b, \quad \text{with } s_z = \pm \frac{1}{2} \text{ and } n = 0, 1, \dots \quad (25)$$

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 eBA/h where $\mathcal{A}$ is the area normal to the magnetic field. The grand partition function for this system becomes

$$\beta p = \frac{\ln \Xi}{V} = \frac{eB\sqrt{2m_e}}{h^2} \sum_{s_z = \pm 1/2} \sum_{n=0}^{\infty} \int_0^{\infty} \frac{d\varepsilon_z}{\sqrt{\varepsilon_z}} \ln \left\{ 1 + e^{-\beta[\varepsilon_z + (n+1/2)\varepsilon_a + s_z\varepsilon_b - \mu]} \right\} \quad (26)$$

- a) Show that the partition function (26) can be written as

$$\begin{aligned} \beta p &= \sum_{L=1}^{\infty} \frac{(-1)^{L+1}}{L} e^{L\beta\mu} \times \frac{eB\sqrt{2m_e}}{h^2} \times \\ &\times \sum_{s_z = \pm 1/2} e^{-s_z L\beta\varepsilon_b} \sum_{n=0}^{\infty} e^{-(n+1/2)L\beta\varepsilon_a} \int_0^{\infty} \frac{d\varepsilon_z}{\sqrt{\varepsilon_z}} e^{-L\beta\varepsilon_z}. \end{aligned} \quad (27)$$

We expand the logarithm in a series, using the formula

$$\ln(1+x) = \sum_{L=1}^{\infty} \frac{(-1)^{L+1}}{L} x^L, \quad (28)$$

with $x = e^{-\beta[\varepsilon_z + (n+1/2)\varepsilon_a + s_z\varepsilon_b - \mu]}$.

- b) Perform the summations of s_z and n , and the integration over p_z in equation (27).

The summation over s_z gives a factor $2 \cosh(L\beta\varepsilon_b/2)$.

The summation over n gives a factor $[2 \sinh(L\beta\varepsilon_a/2)]^{-1}$.

The integration over p_z gives a factor $(L\beta)^{-1/2} \Gamma(\frac{1}{2}) = (\pi k_B T/L)^{1/2}$.

Since $\varepsilon_a = \frac{e\hbar B}{2m_e}$ we may write

$$\frac{eB}{2 \sinh(L\beta\varepsilon_a/2)} = \frac{2\pi m_e k_B T}{Lh} \frac{(L\beta\varepsilon_a)}{\sinh(L\beta\varepsilon_a/2)}$$

to obtain

$$\beta p = \frac{1}{\lambda^3} \sum_{L=1}^{\infty} \frac{(-1)^{L+1}}{L^{5/2}} e^{L\beta\mu} \times 2 \cosh(L\beta\varepsilon_b/2) \times \frac{(L\beta\varepsilon_a/2)}{\sinh(L\beta\varepsilon_a/2)}, \quad (29)$$

where $\lambda = h/\sqrt{2\pi m_e k_B T}$ is the thermal de Broglie wavelength.

- c) Consider the limit $B \rightarrow 0$ in your results of point b). Do you get back the result for an ideal electron gas?

Since ε_a and ε_b is proportional to B they will also go to 0 as $B \rightarrow 0$. In this limit the factor from s_z -summation, $2 \cosh(L\beta\varepsilon_b/2) \rightarrow 2$, which is the correct degeneracy factor for a spin- $\frac{1}{2}$ particle. Since further the factor from n -summation, $(L\beta\varepsilon_a/2) [\sinh(L\beta\varepsilon_a/2)]^{-1} \rightarrow 1$, we get back the correct fugacity expansion for an ideal non-relativistic spin- $\frac{1}{2}$ Fermi gas.

- d) The average magnetization per volume is here given by the expression

$$M = \left(\frac{\partial p}{\partial B} \right)_{\beta, \mu}. \quad (30)$$

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.

To first order

$$\begin{aligned} \beta p = \rho &= \frac{1}{\lambda^3} e^{\beta\mu} \times 2 \cosh(g\beta\mu_B B/4) \times \frac{(\beta\mu_B B/2)}{\sinh(\beta\mu_B B/2)} \\ &\approx \frac{2}{\lambda^3} e^{\beta\mu} \left\{ 1 + \left(\frac{g^2}{8} - \frac{1}{3} \right) (\beta\mu_B B/2)^2 + \dots \right\}, \end{aligned}$$

which gives

$$\begin{aligned} M &= \frac{1}{\beta} \frac{\partial}{\partial B} \beta p = \frac{2}{\lambda^3} e^{\beta\mu} \times \left(\frac{g^2}{8} - \frac{1}{3} \right) \frac{1}{2} \beta \mu_B^2 B \\ &= \frac{1}{2} \beta \rho \left(\frac{g^2}{8} - \frac{1}{3} \right) \mu_B^2 B. \end{aligned} \quad (31)$$

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

We see from equation (31) that the system is paramagnetic for $g^2 > \frac{8}{3}$ (i.e. $g > 1.633\dots$) and diamagnetic for $g^2 < \frac{8}{3}$.

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

$$(1-x)^{-1} = \sum_{L=0}^{\infty} x^L, \quad (32)$$

$$\ln(1+x) = \sum_{L=1}^{\infty} \frac{(-1)^{L+1}}{L} x^L, \quad (33)$$

$$\int_0^{\infty} \frac{dt}{\sqrt{t}} e^{-t} = \sqrt{\pi}. \quad (34)$$