**NTNU**

**Institutt for fysikk**

**Fakultet for fysikk, informatikk og matematikk**

# Solution to the exam in TFY4230 STATISTICAL PHYSICS

Tudnesday november 31, 2010

This solution consists of 5 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).

The canonical partition function

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

**b)** What is the mean value $\langle s_z\rangle$ and standard deviation $\sigma(s_z) \equiv \sqrt{\mathrm{Var}(s_z)}$ of $s_z$ in this case?

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

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

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

I.e.

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

**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.,

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

which is a rather strong field.

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

$$Z_N = Z^N = Z^{10^6}, \tag{8}$$

with $Z$ given by equation (4).

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

$$M = \frac{1}{\beta V} \frac{\partial}{\partial B} \ln Z_N \tag{9}$$

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

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

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

The microscopic magnetization is the random quantity

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

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 $\boldsymbol{B}$. We have

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

and

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

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

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

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

$$\boldsymbol{B}_{\text{ind}} = \mu_0 \boldsymbol{M}, \tag{13}$$

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

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

   From the previous results we find

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

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

   It is implicit from equation (9) that $B$ is defined to point in the direction of $\boldsymbol{B}$ (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 $\boldsymbol{B}_{\text{ind}}$ points in the direction of $\boldsymbol{B}$.

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?

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

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

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

## Problem 2. Numerical computation of second virial coefficient

The Lennard-Jones potential

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

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,

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

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 $\mathrm{m}^3$, $a$ must have dimension $\mathrm{J\,m}^{12}$, and $b$ must have dimension $\mathrm{J\,m}^6$.

**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

$$E_0 = b^2/a, \tag{17}$$

corresponding to a natural unit of temperature

$$T_0 = E_0/k_B. \tag{18}$$

A natural unit of length is

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

With $x = r/r0$ and $\tau = T/T_0$ the virial coefficient becomes

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

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

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

**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 $x_{\text{min}}$ and $x_{\text{max}}$.

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

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

   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 $x_{\text{max}}$ so large that only the $x^{-6}$-term in the expansion is important. I.e., so that the next order term,

$$\left|\left(\frac{1}{\tau} - \frac{1}{2\tau^2}\right)\right| \int_{x_{\text{max}}}^{\infty} x^2\,\mathrm{d}x\,\frac{1}{x^{12}} = \left|\left(\frac{1}{\tau} - \frac{1}{2\tau^2}\right)\right| \frac{1}{9\,x_{\text{max}}^9} \le 10^{-16}, \tag{23}$$

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

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

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

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

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

## Problem 3. Quantum magnetization

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

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

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

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

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

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

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

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

We expand the logarithm in a series, using the formula

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

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

**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 $(L\beta)^{-1/2}\,\Gamma\left(\frac{1}{2}\right) = (\pi k_B T/L)^{1/2}$.

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

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

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

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

Since $\varepsilon_a$ and $\varepsilon_b$ is proportional to $B$ they will also go to 0 as $B\to 0$. In this limit the factor from $s_z$-summation, $2\cosh(L\beta\varepsilon_b/2)\to 2$, which is the correct degeneracy factor for a spin-$\frac{1}{2}$ particle. Since further the factor from $n$-summation, $(L\beta\varepsilon_a/2)\,[\sinh(L\beta\varepsilon_a/2)]^{-1}\to 1$, 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

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

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.

To first order

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

which gives

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

**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. $g > 1.633\ldots$) and diamagnetic for $g^2 < \frac{8}{3}$.

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

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

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

$$\int_0^{\infty}\frac{\mathrm{d}t}{\sqrt{t}}\,\mathrm{e}^{-t} = \sqrt{\pi}. \tag{34}$$