Final Exam- "Thermal Physics 2" (NS-355B)

February 4, 2010
Duration of the exam: 3 hours

1. Use a separate sheet for every exercise.

2. Write your name and initials in all sheets, on the first sheet also your address and your student ID number.

3. Write clearly, unreadable work cannot be corrected.

4. You are NOT allowed to use any kind of books or lecture notes. A list with some useful formulas is given at the end of the exam sheet.

1 Heat capacity of liquid ^{4}He

Liquid ^{4}He, which are bosonic atoms, becomes superfluid below a temperature of 2.17 K. Just as in a crystal, the low energy excitations of liquid ^{4}He are sound waves, whose quanta are the phonons. However, in liquid ^{4}He there is also another type of elementary excitation called the roton, see Figure 1. The dispersion relations for the phonons and rotons are, respectively,

$$\begin{aligned} \epsilon_p &= pc_1, \\ \epsilon_r &= \Delta + \frac{(p-p_0)^2}{2\mu_r}, \end{aligned}$$

where c_1 is the sound velocity, Δ is the energy gap of the rotons, μ_r is the effective mass of the rotons, and $p = \hbar k$ is the momentum of the atoms. As we have seen in crystals, the low energy excitations determine the behaviour of the thermodynamic quantities, such as the specific heat. In this sense liquid ^{4}He can be described as an ideal gas of phonons and an ideal gas of rotons.

(a) **(0.5)** Let us first concentrate on the phonon gas. Calculate the temperature dependence of the free energy of the phonon gas, which is given by the free energy of the ideal Bose gas

$$F = -k_BT\int \ln(1+n)\frac{d^3p}{(2\pi\hbar)^3},$$

where $n = \frac{1}{e^{\beta\epsilon}-1}$ is the Planck distribution. Hint: write it as a dimensionless integral and extract the temperature dependence without solving the integral explicitly. Recall that d^3p is an infinitesimal volume element of a sphere.

(b) **(0.5)** Calculate the temperature dependence of the entropy and specific heat of the phonon gas.

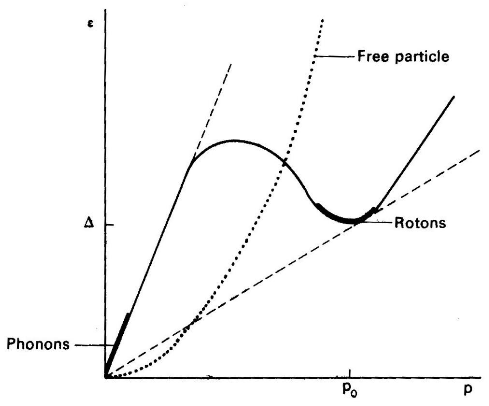

Figure 1: Spectrum of ^{4}He, with energy (vertical axis) versus momentum (horizontal axis), showing the phonon and roton excitations.

(c) **(0.5)** Consider now the roton gas. Argue that if $\Delta \gg k_B T$ the Maxwell-Boltzmann distribution can be used for the rotons instead of the Bose-Einstein distribution function. Furthermore, show that the free energy of the ideal Bose gas reduces to the free energy of a Boltzmann gas

$$F \approx -k_B T \int n_B \frac{d^3p}{(2\pi\hbar)^3},$$

where n_B is the Boltzmann distribution.

(d) **(0.5)** Calculate the temperature dependence of the free energy of the roton gas by approximating the integral assuming that $p_0 \gg \sqrt{\frac{\mu_r}{\beta}}$. Notice that the main contribution from the Gaussian term comes from $p \approx p_0$. Show that

$$F \approx -\frac{4\pi k_B T}{(2\pi\hbar)^3} e^{-\Delta/k_B T} p_0^2 \sqrt{2\pi\mu_r k_B T}.$$

As before, you could then determine the entropy and the specific heat, but you don't need to do it here.

2 Diffusion

Bacteria are injected in the center of a Petri dish, which is a circular transparent dish, used for growing bacteria. The bacteria tend to stay in a layer of the Petri dish which is about 1 mm below the surface. These bacteria swim with a velocity of 20 μm/s. They can however only swim for 1 second, after which they "tumble" for 0.2 second: they make random movements in the same place, during which their spatial orientation changes.

(a) **(0.5)** Assuming that the directions of motion before and after tumbling are completely uncorrelated, determine the effective diffusion coefficient of the bacteria.

(b) **(0.5)** Roughly how long does it take the bacteria, injected in the middle of the Petri dish with a radius $R = 5$ cm, to reach the edge of the Petri dish?

3 Linear Response

The Potts model is a simple generalization of the Ising model to an arbitrary number of states. Here we choose 100 states. The sites of a lattice j carry a variable which takes one of 100 values, say $s_j \in \{1, 2, \dots, 100\}$. The energy is lower when two neighboring sites are in the same state, so the Hamiltonian is:

$$H = -J \sum_{\langle i,j \rangle} \delta(s_i, s_j) - \sum_i \sum_{k=1}^{100} h_k \delta(s_i, k)$$

with $J > 0$, the first sum running over nearest-neighbor pairs of sites, and the second sum running over all sites. Analogous to the magnetization in the Ising model, we now define the 100 quantities $M_k = \sum_i \delta(s_i, k)$, for $k = 1, \dots, 100$.

(a) **(0.5)** Show that the expectation value of these quantities M_k can be written as

$$\langle M_k \rangle = \frac{1}{\beta} \frac{\partial \log(Z)}{\partial h_k},$$

(b) **(0.5)** Show that the fluctuations in M_k are related to the magnetic susceptibilities $\chi_k = \frac{\partial \langle M_k \rangle}{\partial h_k}$ via

$$\chi_k = \beta \left(\langle M_k^2 \rangle - \langle M_k \rangle^2 \right).$$

4 Metamagnetism in $FeCl_2$

Magnets which undergo a first-order phase transition in an increasing magnetic field are called *metamagnets*. There is a variety of metamagnets that exhibit tricritical points. One that has been studied in detail is $FeCl_2$. In this material, Fe^{2+} ions occupy sites on stacks of parallel two-dimensional triangular lattices separated by the chlorine ions. Each Fe^{2+} ion carries an effective spin of $\frac{1}{2}$. The Cl atoms do not carry spin; for this reason we only concentrate on the Fe^{2+} ions. In Figure 2, we show the structure of the Fe planes, and we have left out the Cl atoms for clarity.

The Hamiltonian of the system is

$$H = -\frac{1}{2} \sum_{\vec{j}} \sum_{\vec{j}'} J_{\vec{j},\vec{j}'} S_{\vec{j}} S_{\vec{j}'}, \tag{1}$$

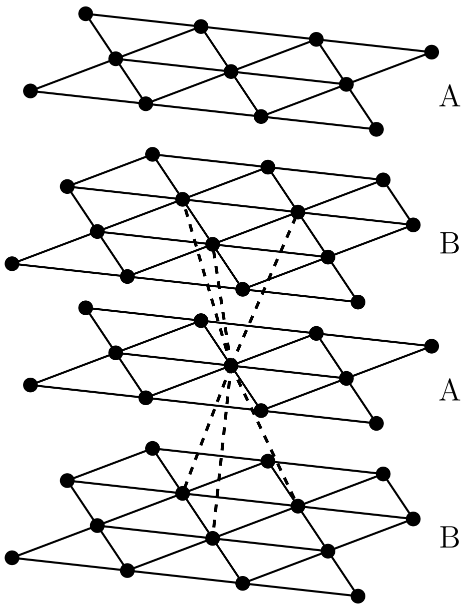

Figure 2: Structure of the Fe ions in the lattice of $FeCl_2$. The Cl atoms are situated between the Fe planes, but have been left out of the figure for the sake of clarity. The in-plane nearest-neighbour bonds are indicated by solid lines. The dashed lines show the bonds of one particular Fe atom towards nearest-neighbour atoms in adjacent planes. On the right, we have indicated the A and B sublattices.

where $S_{\vec{j}}$ is the z-component of the spin at site $\vec{j}$, which can take positive or negative values, $S_{\vec{j}} = \pm 1$ (i.e., it is an Ising variable). The exchange function, which describes the coupling between different sites, is given by

$$J_{\vec{j},\vec{j}'} = \begin{cases} J_1 & \text{if } \vec{j} \text{ and } \vec{j}' \text{ are nearest neighbours in the same plane,} \\ -J_2 & \text{if } \vec{j} \text{ and } \vec{j}' \text{ are nearest neighbours in adjacent planes,} \\ 0 & \text{otherwise.} \end{cases}$$

We assume that $J_1 > 0$ and $J_2 > 0$.

(a) **(0.3)** For zero temperature, describe the orientation of the spins within a single plane. How are the spins in different planes oriented with respect to each other?

The system is well described by a mean-field calculation. We define $m_A = \langle S^A_{\vec{j}} \rangle$ as the average spin per site (magnetisation) of the spins in sublattice A, and m_B as the average spin per site in sublattice B.

(b) **(0.5)** Show that in this mean-field approximation, the energy per site is

$$u \equiv U/N = \tfrac{1}{2} z_2 J_2 m_A m_B - \tfrac{1}{4} z_1 J_1 (m_A^2 + m_B^2),$$

where z_1 is the number of nearest neighbours within one plane and z_2 is the number of nearest neighbours in adjacent planes. Justify why you get the prefactor $\frac{1}{2}$ for the first term and $\frac{1}{4}$ for the second term.

(c) **(0.8)** Now, we want to derive the entropy of the system. The entropy per site is given by $S/N = s(m_\mathrm{A}) + s(m_\mathrm{B})$, where $s(m_\mathrm{A})$ and $s(m_\mathrm{B})$ are the *entropies of mixing*. In order to determine the function s, let us limit ourselves to $s(m_\mathrm{A})$ (i.e., we restrict ourselves to the sublattice A). Compute the number of spins up $N_\mathrm{A}^\uparrow$ in terms of the magnetisation m_A and of the total number of spins N_A, and use that the total entropy is given by the logarithm of the number of configurations with a given $N_\mathrm{A}^\uparrow$,

$$S_\mathrm{A} = k_\mathrm{B} \log \binom{N_\mathrm{A}}{N_\mathrm{A}^\uparrow}$$

to derive that

$$\begin{aligned} s(m_\mathrm{A}) &= S_\mathrm{A}/N_\mathrm{A} \\ &= k_\mathrm{B}\left[\log 2 - \tfrac{1}{2}(1+m_\mathrm{A})\log(1+m_\mathrm{A}) - \tfrac{1}{2}(1-m_\mathrm{A})\log(1-m_\mathrm{A})\right]. \end{aligned}$$

(d) **(0.2)** Using the results of (b) and (c), write down the free energy per particle $f(m_\mathrm{A}, m_\mathrm{B})$.

Now, if one defines the average magnetisation m and the staggered magnetisation m_s via

$$m = \tfrac{1}{2}(m_\mathrm{A} + m_\mathrm{B}), \qquad m_\mathrm{s} = \tfrac{1}{2}(m_\mathrm{A} - m_\mathrm{B}),$$

and one expands f to sixth order in m_s with coefficients depending on m (don't do this expansion yourself), one finds that

$$f_0(m, m_s) = c_0(m) + \tfrac{1}{2}c_2(m)m_\mathrm{s}^2 + \tfrac{1}{4}c_4(m)m_\mathrm{s}^4 + \tfrac{1}{6}c_6(m)m_\mathrm{s}^6, \tag{2}$$

where

$$\begin{aligned} c_0(m) &= \tfrac{1}{2}\alpha_m m^2 - T\,s(m), && \text{with } \alpha_m = z_2 J_2 - z_1 J_1, \\ c_2(m) &= \frac{k_\mathrm{B}T}{1-m^2} - \alpha_N, && \text{with } \alpha_N = z_1 J_1 + z_2 J_2, \\ c_4(m) &= \frac{k_\mathrm{B}T(1+3m^2)}{3(1-m^2)^3}, \\ c_6(m) &> 0. \end{aligned}$$

(e) **(0.4)** Do you recognise expression (2) for the free energy as something known? How is it called? What can you describe with it? Discuss the region of validity of the expansion.

(f) **(0.5)** There is a second-order phase transition between the paramagnetic (no spin order) phase and the antiferromagnetic phase. Using equation (2), determine the expression for the temperature $T(m)$ where the transition takes place.

(g) **(0.5)** Can you also have a first order phase transition in this case? Justify your answer.

Now, we apply a magnetic field in the z-direction. Therefore, the Hamiltonian gets an extra contribution from the magnetic field, and becomes

$$H = -\frac{1}{2}\sum_{\vec{j}}\sum_{\vec{j}'} J_{\vec{j},\vec{j}'} S_{\vec{j}} S_{\vec{j}'} - h\sum_{\vec{j}} S_{\vec{j}}, \tag{3}$$

where h measures the strength of the magnetic field.

(h) **(0.3)** What should happen with the spin configuration when the magnetic field is very strong?

(i) **(0.7)** Argue that the free energy per particle $f(m, m_\mathrm{s})$ gets an extra contribution $-hm$ compared to f_0 of equation (2). Explain that in order to find the minima of the free energy for fixed m_s, we have to find the solutions of $h = \frac{\partial f_0}{\partial m}$ (where f_0 is the free energy without magnetic field). Under the assumption that we fix $m_\mathrm{s} = 0$, derive that m satisfies the transcendental equation

$$m = \tanh\left(\frac{h - \alpha_m m}{k_\mathrm{B} T}\right). \tag{4}$$

Hint: $\log\frac{1+x}{1-x} = 2\,\mathrm{arctanh}\,x$.

We now incorporate the staggered magnetisation, which also reacts to the magnetic field. By expanding the free energy in powers of m_s as before, we now find (don't do it yourself)

$$f_h(m_0, m_\mathrm{s}) = c_0(m_0) + \tfrac{1}{2}c_2(m_0)m_\mathrm{s}^2 + \tfrac{1}{4}\left[c_4(m_0) - 2\phi(m_0)\right]m_\mathrm{s}^4 + \tfrac{1}{6}\tilde{c}_6(m_0)m_\mathrm{s}^6,$$

where $m_0 = m_0(T, h)$ is a solution of equation (4). The function $\phi(m_0) = \frac{k_\mathrm{B} T m_0}{(1-m_0^2)^2(\alpha_m/k_\mathrm{B}T)+1}$ describes the change to $c_4(m_0)$ caused by the coupling of the staggered magnetisation to the magnetic field. Also $c_6(m_0)$ is changed to $\tilde{c}_6(m_0)$, but we do not consider its exact form here, since it is enough to consider that it is positive.

The phase diagram for the magnetisation $m(T)$ versus temperature is given in Figure 3.

(j) **(0.5)** There are first-order phase transitions between the paramagnetic phase (P) and the mixed phase, and between the antiferromagnetic phase (AF) and the mixed phase. How can one calculate the transition temperatures $T(m)$ of these phase transitions? Only describe the steps that have to be done, without calculating explicitly.

(k) **(0.4)** For the first-order phase transition, draw sketches of the free energy: (i) below the transition temperature, (ii) at the transition temperature, (iii) above the transition temperature. Indicate clearly the differences between the three sketches.
(iv) Draw also a qualitative sketch of the order parameter as function of the temperature and indicate clearly the transition temperature in your sketch.

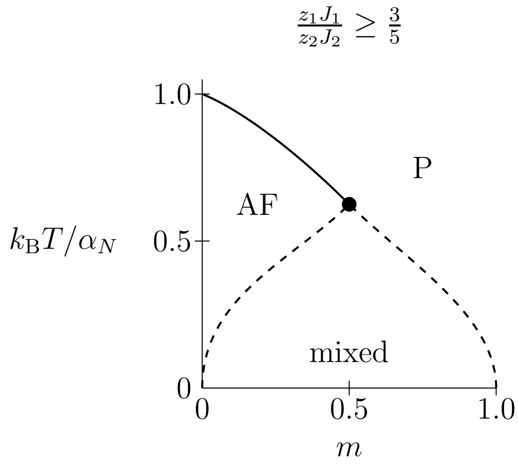

Figure 3: Phase diagram of a metamagnet. On the horizontal axis, we have the magnetisation m and on the vertical axis the scaled temperature $k_{\mathrm{B}}T/\alpha_N$. The antiferromagnetic, paramagnetic (normal), and mixed phases are indicated by AF, P, and mixed, respectively. In the mixed phase, the material consists of regions which are antiferromagnetic and regions which are paramagnetic (normal). Phase transitions of first order are indicated by dotted curves, and those of second order by solid curves. Here, the phase diagram is given for the case that $\frac{z_1 J_1}{z_2 J_2} \geq \frac{3}{5}$.

(l) **(0.4)** Repeat the steps of part (k), but now for a second-order phase transition.

(m) **(0.5)** The material $\mathrm{FeCl_2}$ is known to exhibit a tricritical point if $\frac{z_1 J_1}{z_2 J_2} \geq \frac{3}{5}$. What is a *tricritical point*? For $0 < \frac{z_1 J_1}{z_2 J_2} < \frac{3}{5}$, the phase diagram changes and there is a critical point, which is similar to the critical point in the phase diagram of water, where the transition line between the liquid and gas phases terminates. Discuss what happens around a critical point in terms of a possible symmetry change of the different phases.

Formulas

- Maxwell-Boltzmann distribution: $g(\varepsilon) \propto \exp(-\varepsilon/k_B T)$
- Planck distribution: $f(E) = \frac{1}{e^{\beta E}-1}$
- Fermi-Dirac and Bose-Einstein distributions: $f(E) = \frac{1}{e^{\beta(E-\mu)}\pm 1}$, where the sign $+$ stands for fermions and the sign $-$ stands for bosons.
- Gaussian integral: $\int_{-\infty}^{+\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}$
- Stirling's approximation: $\log(n!) \approx n \log n - n$