Statistical Mechanics - 2019-2 - Problem set 3

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Deadline: 05/11

1. **(Blume-Capel model)** Consider a system of N spin-1 particles placed in a one-dimensional lattice and subject to the Hamiltonian

$$H = -J \sum_{i=1}^{N} S_z^i S_z^{i+1} - D \sum_{i=1}^{N} (S_z^i)^2, \tag{1}$$

where $S_z = \text{diag}(1, 0, -1)$ is the z component of the spin-1 operator for each particle. You may assume, for concreteness, that $J > 0$ and $D > 0$. Discuss the equilibrium properties of this system. Among other things, study the quadrupole moment

$$Q = \frac{1}{N} \Big\langle \sum_{i=1}^{N} (S_z^i)^2 \Big\rangle. \tag{2}$$

2. **Landau theory for discontinuous transitions:** Consider a system described by a real order parameter m with Z_2 symmetry ($m \to -m$). In class we discussed how to expand the Landau free energy close to the critical point. In order to respect the Z_2 symmetry, the expansion could contain only even terms. Hence, it would look like

$$f(m) = \frac{a}{2} m^2 + \frac{b}{4} m^4 + \frac{c}{6} m^6. \tag{3}$$

In class we stopped at the quartic term because we were assuming that $b > 0$. However, if $b < 0$ then we need to go one order further in order to get a thermodynamically stable theory (we hence assume that $c > 0$. If not, we have to keep going...). We also continue to assume that $a \sim T - T_c$, so that it changes sign at the critical point.

   (a) Assume $b < 0$. Make plots of $f(m)$ for 4 different cases: $a < 0$, $0 < a < a_1$, $a_1 < a < a_0$ and $a > a_0$. Here a_0 and a_1 are defined as

$$a_0 := \frac{b^2}{4c}, \qquad a_1 := \frac{3b^2}{16c}. \tag{4}$$

   Keep these plots in mind to get some intuition as to what is happening.

   (b) Show that if $a > a_0$ the only minimum is at $m = 0$.

   (c) If $a < a_0$, two new minima appear at $m \neq 0$. However, show that for $a_1 < a < a_0$ these will be local, instead of global. They therefore correspond to **metastable states**: they are not global minima, but there is nonetheless a barrier separating them from the true minimum, so that it would require some energy to remove the system from them.

   (d) Show that the minima with $m \neq 0$ become global ones when $a < a_1$. This is the critical point for a discontinuous transition: when a reaches a_1 the system will jump abruptly from $m = 0$ to the state with $m \neq 0$. This is fundamentally different from the situation we studied in class, where m varied continuously.

   (e) Show that if $a < 0$ then the local minimum at $m = 0$ disappears completely.

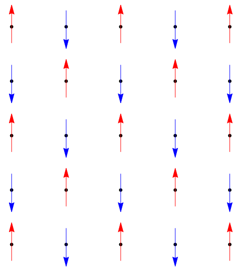
   (f) Sketch how the magnetization should look like as a function of a.

3. **Mean-field theory for anti-ferromagnetic systems**

Consider a system of N spins on a d-dimensional hypercubic lattice and described by the anti-ferromagnetic Ising model

$$H = J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^z, \tag{5}$$

with $J > 0$. I also introduced a site-dependent magnetic field h_i. This will just be used for bookkeeping below and in the end we can set $h_i = h$. The important difference with respect to the model we studied in class is the plus sign in front of the first term. This means that the spins tend to align *anti-parallel* to each other (up-down-up-down-...). The ground-state of the model is then divided into two **sub-lattices**, A and B, one with all spins pointing up and the other with all spins pointing down (see figure). Note also how spins in one sub-lattice only interact with the spins from the other sub-lattice.



(a) Perform a mean-field approximation by writing $\sigma_i^z = m_i + \delta\sigma_i^z$, where $m_i = \langle\sigma_i^z\rangle$. However, differently from how we did in class, assume now that m_i can take on two different values, m_a and m_b, depending on which sub-lattice the spin resides.

(b) Compute the partition function and the free energy.

(c) You can compute the magnetization in each sub-lattice by notting that the individual magnetization of each spin is given by $m_i = \langle\sigma_z^i\rangle = -\frac{\partial F}{\partial h_i}$. Show that m_a and m_b must satisfy the Curie-Weiss equations

$$\begin{aligned} m_a &= \tanh(-2\beta J d m_b + \beta h) \\ m_b &= \tanh(-2\beta J d m_a + \beta h) \end{aligned} \tag{6}$$

(d) Solve these equations for $h = 0$ in the vicinity of the critical point. Assume $m_b = -m_a$ and $|m_a| \ll 1$. Show that there is indeed a phase transition and find the critical temperature. This is called the **Néel Temperature** T_N.

(e) Let $M = m_a + m_b$ denote the total magnetization. Compute the susceptibility at zero field for $T > T_N$, $\chi = \partial M/\partial h$. Show that it can be written as

$$\chi = \frac{\partial M}{\partial h} = \frac{C}{T + T_N}$$

where C is a constant. This result is used experimentally all the time. It offers a simple way of knowing, if you are in a paramagnetic phase, if the material is anti-ferromagnetic or ferromagnetic. In the ferromagnetic case we saw in class that $\chi \propto 1/(T - T_c)$. Hence, a curve of χ^{-1} vs. T should be a straight line which, if we extrapolate to low temperatures, will intercept the horizontal axis at a positive value. Conversely, in the anti-ferromagnetic case, $\chi \propto 1/(T + T_N)$. The plot will therefore also be a straight line, but the extrapolation will intercept the horizontal axis at a *negative* point.