Statistical physics 2, homework 1

October 11, 2018

1. **Mean field free energy of the ferromagnetic Ising model**
   Consider the Ising model:
   $$H/k_BT = \mathcal{H} = -K\sum_{(i,j)} \sigma_i\sigma_j - h\sum_i \sigma_i \ ,$$
   with $K = J/k_BT$ and $h = \mu_B B/k_BT$.

   - Assume that each spin points upwards with a probability $p_\uparrow = (1+m)/2$, while they point downwards with a probability $p_\downarrow = (1-m)/2$, but otherwise they are independent. Thus $\langle\sigma_i\rangle = m$ for each spin, independently.
   - Compute $\langle\mathcal{H}\rangle$ with this Ansatz. Determine also the configurational entropy and show that the conditional free energy density reads
     $$f(m,T,h) = -\frac{\kappa}{2}m^2 - hm + \frac{1+m}{2}\ln\left(\frac{1+m}{2}\right) + \frac{1-m}{2}\ln\left(\frac{1-m}{2}\right) \ .$$
     with $\kappa = Kz = T_C/T$.
   - Derive the mean field equations by taking the minimum of $f(m,T,h)$ w.r.t. m.
   - Expand now $f(m,T,h)$ in m to fourth order and show that
     $$f(m,\tau,h) \approx \frac{\tau}{2}m^2 - hm + \frac{1}{12}m^4 \ ,$$
     with $\tau = (T_C - T)/T_C$ the reduced temperature.

2. **Ising antiferromagnet in magnetic field:**

   - Construct the Hamiltonian of the Ising *antiferromagnet* on the two-dimensional square lattice with a (dimensionless) nearest neighbor interaction K and external field, h.
   - Divide the lattice onto two sublattices, and assume that the magnetizations on them are m_1 and m_1, respectively. Express then the expectation value of the energy in the mean field limit.
   - Express the entropy in terms of m_1 and m_1, and construct the approximate conditional free energy density f of the system.
   - Derive the mean field equations, and analyze its solutions for $h = 0$ and $h \neq 0$.
   - Construct the $T - h$ phase diagram close to the critical point.

3. **Ising model with isotropic next-nearest-neighbor interactions:**

   - Write down the Hamiltonian for the Ising model with next-nearest-neighbor interactions on the two-dimensional square lattice. Let $J_1{>}0$ be the nearest, and J_2 the next-nearest-neighbor neighbor coupling constant
   - Calculate the average effective field in the mean-field limit!
   - Write the mean field for $J_2{>}0$. Discuss the difference to the nearest-neighbor Ising
   - Consider $J_2{<}0$. Determine the sublattices for the antiferromagnetic interactions. Derive the free energy for this case.

4. **Mean field for the 3 state, Potts model**
   The dimensionless Hamiltonian of the three state Potts model is
   $$H/k_BT = \mathcal{H} = -K\sum_{(i,j} \delta_{\sigma_i,\sigma_j} - h\sum_i \delta_{\sigma_i,1}$$
   where $\sigma_i \in \{-1, 0, +1\}$, and the magnetic field is in the $+1$ direction.

- Assume that the probability of finding a spin in state $+1$ is x, the other two state have the probability $(1-x)/2$, and each spin is otherwise independent from the others.
- Derive the average mean field energy of the system as a function of x. (Hint: Consider the probability of each nearest neighbor configuration, and show that $\langle \delta_{\sigma_i,1} \rangle = 1$ and $\langle \delta_{\sigma_i,\sigma_j} \rangle = (3x^2+1-2x)/2$.)
- Write down the configurational entropy of a given spin.
- Derive the conditional free energy.
- Define the magnetization as $m = x - 1/3$, and express the Taylor series of the free energy around $m = 0$. Show that there is a third order therm in m. (This indicates a *first* order phase transition.)

5. **Lattice gas**
   - Consider a two-dimensional lattice gas on a square lattice
   - If two particles are next to each other there is an energy of $-J$ due to attraction between the particles.
   - Derive the energy of the system.
   - Derive the entropy of the system.
   - Write down the free energy of the system show the similarities and differences to the Ising model

6. **Mean field theory of a classical ferromagnetic Heisenberg model**
   Consider a lattice with coordination number z, and a vector spin model with nearest neighbor interactions:
   $$H/k_BT \equiv \mathcal{H} \equiv -K \sum_{(i,j} \overline{\sigma}_i \cdot \overline{\sigma}_j - \sum_i \overline{h} \cdot \overline{\sigma}_i \ ,$$
   with $\overline{\sigma}$ now denoting vectors of unit length.
   - Compute first the magnetization $\overline{m} \equiv \langle \overline{\sigma} \rangle$ of a single spin in an external field $\overline{h}$.
   - Assume that $\overline{h}||\overline{e}_z$. Now calculate the effective field on a given spin, and derive the selfconsistency equation for $\overline{m}$.
   - Show that this implicit equation may have one or three solutions, and derive the critical temperature.
   - Derive the susceptibility close to T_C.

7. **Correlations on a three-spin cluster**
   Consider three Ising spins described by the following Hamiltonian:
   $$H = -J(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1).$$
   - Enumerate all states of the spins and compute and list their Boltzmann weights.
   - Now evaluate the expectation values $\langle \sigma_1\sigma_2 \rangle$, $\langle \sigma_1 \rangle$ and $\langle \sigma_2 \rangle$.
   - Sketch the behavior of the correlation function C_{12} as a function of temperature. (Hint: You may plot this function also numerically, and compute its value for small and large temperatures.)

8. **Critcal exponents from Landau theory**
   Consider the Landau free energy density:
   $$f(M, B, T) = \frac{a}{2}M^2 + \frac{b}{4}M^4 - BM$$
   with $a = \alpha(T - T_C)$, and $b(T)$ a positive constant.
   - Derive the equation determining $M(B, T)$.
   - Analyze this equation, and derive the critical exponents, β, δ, and γ.
   - Having found the solution $M(T)$ for $B = 0$ now compute and plot $f(T)$. Determine the value of α, too.

9. Landau theory with cubic terms
   - Consider a Landau model with cubic term:
     $$f = f_0 + \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4$$
     where we assume that $y > 0$.

- Show that we do not have $m \to -m$ symmetry
- Find the possible equilibrium solutions for $h = 0$
- Find out which one of them is stable
- Plot the possible states of the free energy as function of m ($h = 0$)
- Show that the order parameter makes a jump at the transition point and that there is a hysteresis

10. **Landau free energy density with M^6 terms**
    Consider the Landau free energy density:

$$f(M, T) = \frac{a}{2}M^2 + \frac{b}{4}M^4 + \frac{c}{4}M^6.$$

- Find the equilibrium solutions for M.
- Discuss the number of real solutions in different regimes.
- Draw the schematic form of the free energy in each regime.
- Evaluate the transition points.
- Locate the first order transition point
- Derive the entropy
- Evaluate the latent heat at the first order transition as $L = T\Delta s$

11. **Landau theory of an Ising domain wall**
    Consider the one dimensional Landau free energy:

$$F(M(z), T) = \int \mathrm{d}z \, \Big(\frac{\kappa}{2}(\partial_z M)^2 + \frac{a}{2}M^2(z) + \frac{b}{4}M^4(z)\Big).$$

- Derive the Euler-Lagrange equation describing the spatial dependence of $M(z)$.
- Assume now that $a = a(T) < 0$, i.e. that $T < T_C$. Introduce the dimensionless length scale, $\tilde{z} \equiv z/\xi$ and the dimensionless magnetization $\tilde{m} \equiv M(z)/M_0$ with $\xi \equiv \sqrt{\kappa/|a|}$ the correlation length and $M_0 = \sqrt{-a/b}$ the equilibrium magnetization. Rewrite the Euler-Lagrange equation for $\tilde{m}(\tilde{z})$.
- Show that the $\epsilon(\tilde{z}) \equiv \frac{1}{2}(\partial_{\tilde{z}}\tilde{m})^2 + \frac{1}{2}\tilde{m}^2(z) - \frac{1}{4}\tilde{m}^4(z)$ is a constant independent of z. (Hint: Show that $\partial_{\tilde{z}}\epsilon(\tilde{z}) = 0$). What is the value of this constant for a solution, which has $M(z = \pm\infty) = M_0$?
- Now use the previous result to derive a simple differential equation for $\tilde{m}(\tilde{z})$.
- Solve this differential equation and show that its solution has the form $\tilde{m}(\tilde{z}) = \tanh(\tilde{z}/\sqrt{2})$.

12. **Critical scaling of the Landau free energy density**
    Consider the Landau free energy density:

$$f(M(z), T, B) = \frac{a}{2}M^2 + \frac{b}{4}M^4 - BM.$$

- Determine the equilibrium values of the order parameter
- Calculate the exponent β: $m \propto \tau^\beta$ (where $\tau = T_c - T$
- Calculate the exponent δ: $m \propto h^{1/\delta}$
- Calculate the exponent γ: $\chi \propto \tau^{-\gamma}$