Problem 1 – 3 pts. The spontaneous magnetization of a ferromagnet in the mean field theory is:

\[ m = B_s \left( \frac{3S \ m}{S + 1 \ \tau} \right), \]

where \( m = M(T)/M(T=0) \) and \( \tau = T/T_c \), and

\[ B_s(x) = \frac{2S + 1}{2S} \coth \left( \frac{2S + 1}{2S} x \right) - \frac{1}{2S} \coth \left( \frac{1}{2S} x \right). \]

Show that in the \( T \to 0 \) limit:

\[ m = 1 - \frac{1}{S} \exp \left( -\frac{3}{S + 1} \frac{T_c}{T} \right) + \ldots \]

The above expression was found not to describe the results of observations correctly – the observed decrease of \( m \) with \( T \) just above the absolute zero is much more rapid. This is often quoted as an argument stressing that the mean field theory is only an approximation, and should be used with caution, especially, when discussing subtle effects – which doesn’t change the fact that the MFT is a very useful model. Hints: show that for \( y \gg 1 \), \( \coth(y) = 1 + 2 \exp(-2y) + \ldots \), and use it to determine the asymptotic behavior of the \( B_s(x) \) function for large arguments.

Problem 2 – 4 pts. Use the small-argument expansion of \( \coth(y) \) (Hint: up to the cubic term) to show that when \( T \) approaches the \( T_c \) value from below, then:

\[ m^2 = \frac{10}{3} \frac{(S + 1)^2}{(S + 1)^2 + S^2} \frac{T_c - T}{T_c}, \]

which means that:

\[ m \propto (T_c - T)^{\frac{1}{2}}. \]

This is another known drawback of the MFT, because experiments and some more advanced theoretical models show that for Heisenberg magnets the exponent is not \( \frac{1}{2} \), but it’s value is close to \( \frac{1}{3} \).

Problems 3 & 4 - 8 pts. each. An interesting problem in stat mech is finding the average thermal energy of a system of rigid rotators at temperature \( T \). It’s not an abstract problem because such rotators really exist – the simplest incarnation is a gas of diatomic molecules, e.g., H₂, HCl. The molecules have translational, rotational and vibrational degrees of freedom. The latter usually get activated only at pretty high temperatures – so at lower temperatures the molecules may indeed be treated with a good approximation as rigid dumbbell-shaped rotators.

The problem is additionally interesting in that it may be approached on the grounds of classical formalism, or quantum formalism. It’s therefore quite instructive to solve the problem both ways and to compare the solutions.

Classical rotator: A diatomic molecule can be thought of as a “dumbbell” that may be either an “even” one (both atoms have the same mass, as is the case, e.g., in H₂), or an “uneven” one (atoms of different masses – e.g. HCl). Let’s consider an “uneven” dumbbell, which is a more general case. In the figure, such a “dumbbell” is shown schematically, and the meaning of
the symbols used later on is explained. The molecule rotates about its mass center $c$. The total energy is the sum of the energy of the precessional motion, in which the atoms follow the circular orbits shown in the figure with velocity $d\phi/dt$, and the energy of the “end-over-end” rotation with velocity $d\theta/dt$. The moment of inertia $I$ is defined as:

$$I = m_A r_A^2 + m_B r_B^2 = \frac{m_A m_B}{m_A + m_B} (r_A + r_B)^2.$$ 

In order to calculate the partition function, we need to express the energy in terms of generalized coordinates. For that, we can use the two angular coordinates, $\theta$ and $\phi$, and the angular momenta associated with the angular velocities $d\phi/dt$ and $d\theta/dt$ – let’s denote them, respectively, as $P_\phi$ and $P_\theta$. Show that in terms of these generalized coordinates the total rotational kinetic energy can be written as:

$$\epsilon = \frac{1}{2I} \left( P_\theta^2 + \frac{P_\phi^2}{\sin^2 \theta} \right).$$

Now, use:

$$Z_{\text{rot}} = \frac{1}{\hbar^2} \int_0^{2\pi} \int_0^\pi \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp \left( -\frac{\epsilon}{kT} \right) dP_\theta dP_\phi d\theta d\phi,$$

and proceed with the calculations to obtain the average rotational energy and the heat capacity as a function of $T$. Before making the calculations, think of what you expect to obtain for $\langle \epsilon \rangle$ and $C$, and then check whether the calculated results agree with the expected one.

**Quantum rotator:** The energy eigenstates for a quantum rotator (one can find them in the usual way, by solving the time-independent Schrödinger equation) are:

$$\epsilon_J = J(J + 1) \frac{\hbar^2}{8\pi^2 I} = J(J + 1) k \Theta_r,$$

where

$$\Theta_r \equiv \frac{\hbar^2}{8\pi^2 I k}.$$
The degeneracy of each $J$ level is given by:

$$g_J = 2J + 1$$

Find the general expression for the partition function, and then again find the mean energy and the specific heat as functions of $T$. The problem cannot be solved analytically for an arbitrary temperature, some approximations need to be used. At very low temperatures (what is the condition for that?) only the first two terms in the partition sum are important. Neglecting other terms, one can obtain relatively simple expressions for $\langle \epsilon \rangle$ and $C$. At high temperatures the sum can be replaced by an integral.

For one of those $T$ regions (which one?) you certainly expect to obtain the same result as from the classical approach. Are the results indeed the same?