Problems on Symmetry-Breaking Phase Transitions

Problem 1: *Mean-field for FM Heisenberg*

Heisenberg model with a magnetic field $\vec{B} = B\vec{e}_z$ along z direction:

$$H = \sum_{\langle i,j \rangle} J\vec{S}_i\vec{S}_j - 2\mu_B B \sum_i S_i^z \tag{1}$$

$\langle i,j \rangle$ denotes nearest-neighbor pairs of spins, we count each pair only once. Suppose that spins $\vec{S}$ have $S = \frac{1}{2}$ and $J < 0$.

1. Introduce a 'test system'

$$H^* = -2\mu_B B^* \sum_i S_i^z \tag{2}$$

that can be used to find a variational free energy that cannot be smaller than the true free energy:

$$F \leq F^* + \langle H - H^* \rangle^* = \hat{H}^* \tag{3}$$

2. Find the optimal $B^* = B_0^*$ that minimizes F^*.

3. Show that

$$k_B T_C = \frac{1}{2} z|J| \tag{4}$$

defines the critical temperature of a phase transition, with paramagnetism for $T > T_C$ and ferromagnetism for $T < T_C$.

4. Show that for $T > T_C$ and $B \to 0$,

$$\chi(T) = \frac{\partial}{\partial B} M(T,B) = 2\mu_B \frac{\partial}{\partial B} \langle S^z \rangle^* \propto \frac{1}{T - T_C} \tag{5}$$

Problem 2: *Excitations and Melting*

In symmetry-broken states, one finds characteristic excitations, which are related to eigenmodes of *deviations* from perfect order. It is plausible enough that having too many of them will be bad for this order. We will explore this issue here for phonons in a crystal, i.e. lattice vibrations that are associated with a periodic order of atoms into a (here for simplicity: Bravais) lattice. Very similar issues exist for many other ordered states, especially for broken *continuous* symmetries, where low-energy excitations with energy $\omega \to 0$ exist. (See later classes.)

Excitations with momentum $\vec{k}$ are described by phonon creation and annihilation operators $a_{\vec{k}}^\dagger$ and $a_{\vec{k}}$. For a simple mode, the operator for the vibration amplitude is

$$x = \sqrt{\frac{\hbar}{2M\omega}} \left(a^\dagger + a \right) . \tag{6}$$

As long as we stay with an *harmonic* treatment of excitations with the Hamiltonian

$$H = \hbar\omega \left(a^\dagger a \ + \frac{1}{2} \right) \tag{7}$$

its quantum-mechanical – and thus also the thermodynamic – expectation value remains 0. However, $\langle x^2 \rangle \neq 0$ and if it becomes comparable to the square of the lattice spacing, we would worry about the crystal's stability. Express $\langle x^2 \rangle$ in terms of $n = \langle \hat{n} \rangle = \langle a^\dagger a \rangle$.

Taking into account phonon/excitation modes at all available momenta, the Hamiltonian becomes just the sum

$$H = \sum_{\vec{k}} \hbar \omega_{\vec{k}} \left(a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{1}{2} \right) . \tag{8}$$

Overall expectation values are found by integrating over available momenta; as these are very dense, an integral instead of a sum is an acceptable treatment. In d spatial dimensions, we then find, e.g.,

$$\langle x^2 \rangle = \sum_{\vec{k}} \langle x^2_{\vec{k}} \rangle \approx \int \frac{\mathrm{d}^d k}{(2\pi)^d} \langle x^2_{\vec{k}} \rangle . \tag{9}$$

As $\hat{n}_{\vec{k}}$ describes the number of non-interacting phonons, its thermal expectation value is given by the Bose distribution

$$n_{\vec{k}}(T) = \frac{1}{\mathrm{e}^{\frac{\hbar \omega_{\vec{k}}}{k_B T}} - 1} . \tag{10}$$

Finally, we need to know the phonon frequency. At least for the acoustic phonons, which have to exist in every solid, and for momenta $\vec{k} \approx 0$, it grows linearly with momentum. We set here

$$\omega_{\vec{k}} \approx c |\vec{k}| \tag{11}$$

with some constant c, valid for $\vec{k} \to 0$. For low temperature $T \to 0$, only these lowest-energy phonons will have appreciable occupation numbers. Concerning *high* energies, phonon frequencies are bounded.

- First focus on the ground state $T = 0$, where we expect no excitations to be present $n_{\vec{k}}(T) = 0$.
  - Write expressions for $\langle x^2 \rangle(T)$, this will lead to an integral.
  - Estimate the integral in the three cases, paying particular attention to any potential divergence.
  - What conclusion can you draw concerning the stability of one- two- and three-dimensional lattices?
- Consider now small $T > 0$ and 1, 2 and 3 dimensions.

The situation is very similar in antiferromagnets with (broken) continuous symmetry. Ferromagnets are a slightly different story, because the classical ground state is also an eigenstate of the quantum-mechanical Hamiltonian and does not contain zero-point fluctuations. However, results at finite $T > 0$ turn out to be equivalent.