Advanced Statistical Physics

TD1 The Blume-Capel model

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The Blume-Capel model is intended to reproduce the relevant features of superfluidity in He^3-He^4 mixtures [1, 2, 3]. In this study, we will consider infinite range, mean-field like interactions between the relevant variables. With this choice, the phase diagram can be obtained analytically both within the canonical and the microcanonical ensembles [4, 5] and the analysis enables one to get a better understanding of the effect of the non-additivity on the thermodynamic behaviour of the model.

The Blume-Capel model is defined as follows [1, 2, 3]. On each site of a complete graph one places a spin-1 variable, $S_i = \pm 1, 0$. Each spin is coupled to all others with the same strength $J_0 > 0$. The Hamiltonian is given by

$$H = -\frac{J_0}{2} \sum_{i \neq j} s_i s_j + \Delta \sum_i s_i^2 \tag{1}$$

with $\Delta > 0$. Let us start by analysing the parameter dependence in the Hamiltonian.

Energetic analysis

Consider the case $\Delta = 0$.

1. Which kind of order favours the exchange J_0? What is the model obtained and what does it describe?
2. How does one need to scale J_0 to ensure a reasonable thermodynamic, $N \to \infty$, limit and the extensivity of the energy? Call the new relevant coupling parameter J.
3. What is the nature of the phase transition expected in this case? (We will derive it below.)

Consider now $\Delta \neq 0$.

1. What is the role played by this parameter?
2. Which are the two states that you may expect to be ground states, in the canonical ensemble, at zero temperature? Find the relation between the parameters Δ, J where the preferred one changes. Discuss the result.

The canonical ensemble.

1. Write the partition function.
2. Think about introducing the auxiliary variable $x = N^{-1} \sum_i s_i$, as it is usually done in the study of the fully-connect Ising model. In this case, in which the spins take values ± 1,0, which is the difficulty encountered?
3. Use an alternative method, the Hubbard-Stratonovich identity or Gaussian decoupling, to render the expression in the exponential of the partition sum, local in the spin variable. Perform the sum over the spin variables explicitly.
4. Identify the "Ginzburg-Landau" free-energy density as a function of x and call it $\tilde{f}(x)$.
5. Show, in the $N \to \infty$ limit, that the saddle-point value of x is equal to the spontaneous magnetisation per spin m.
6. Identify the extrema of the Ginzburg-Landau free-energy function and study their stability.
7. Set up the Taylor expansion of the Ginzburg-Landau free-energy function around $x = 0$ and find the critical line on which the coefficient of the quadratic term vanishes and the one of the quartic term remains larger than zero. This is the *second order phase transition* ending at a tricritrical point $(\Delta/J,\, T/J)_c$ where the two coefficients vanish. Prove that the canonical tricritical point is located at $J/(2\Delta) = 3/\ln 16 \simeq 1.0820$, $\beta J = 3$.
8. The *first order phase transition* corresponds to the parameters $(\Delta/J,\, T/J)$ on which $\tilde{f}(\beta J,\, \beta\Delta,\, x \neq 0) = \tilde{f}(\beta J,\, \beta\Delta,\, x = 0)$. Find the line with a numerical solution of the corresponding equation.
9. Use a graphical facility to plot the Ginzburg-Landau free-energy function as a function of x for various values of the control parameters βJ and $\beta\Delta$. Confirm the results found in the previous two items for the critical lines from the visual inspection of the evolution of $\tilde{f}(x)$.
10. Draw the *canonical phase diagrams* in the $(\Delta/J,\, T/J)$ plane.

The microcanonical ensemble.

A microscopic configuration is determined by the number of spins taking value $+1$, that we call N_+, number of spins taking value -1, that we call N_-, and the number of spins taking value 0, that we call N_0. We will now study the macroscopic observables as functions of these number.

1. Write a constraint that relates N_+, N_-, N_0 to the total number of spins N.
2. Write the total magnetisation, $M = \sum_i s_i$, the quadrupole moment $Q = \sum_i s_i^2$, the total energy as functions of N_+, N_-, N_0.
3. Calculate the number of microscopic configurations, Ω, that are compatible with the macroscopic occupation numbers N_+, N_-, N_0.
4. Using Stirling's approximation, compute the entropy $S = k_B \ln \Omega$ and write it as a function of $m = M/N$, $q = Q/N$ and $e = E/N$. Note that one of this intensive parameters is absent from $s = S/N$.

5. We will fix the energy and look for the equilibrium magnetisation density values that render the entropy maximal.

   In the paramagnetic phase $m = 0$ and the Taylor expansion of $s(m,e)$ around this value has negative quadratic and quartic coefficients. The second order phase transition occurs when the coefficient of the quadratic term vanishes while the one of the quartic term remains negative.

   The tricritical point is located at the parameters such that the two coefficients vanish. The microcanonical tricritical point is located at $J/(2\Delta) \simeq 1.0813$, $\beta J = 3.0272$. This has to be compared with the canonical tricritical point located at $J/(2\Delta) \simeq 1.0820$, $\beta J = 3$.

In conclusion the microcanonical critical line extends beyond the canonical one.

Références

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