THERMAL PHASE TRANSITIONS AND GROUND STATE PHASE TRANSITIONS: THE COMMON FEATURES AND SOME INTERESTING MODELS

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Abstract

We point out the common features of the thermal phase transitions and the ground state quantum phase transitions and describe the coherent anomaly method (CAM) as a suitable tool for the theoretical treating of these collective phenomena. We use CAM for the studying of the universality of the critical exponents in the ground state phase transitions in the quantum spin Heisenberg XYZ model on the one-, two- and three dimensional lattices and present here some preliminary results.

Keywords: phase transition, ground state, mean-field, universality, XYZ model.

1 Introduction

Many interesting (and presently widely studied) physical phenomena like ferromagnetism, antiferromagnetism, superconductivity, superfluidity, etc., can be well understood in the framework of the theory of phase transitions and critical phenomena which provides a suitable qualitative and quantitative description of them. Thus, a further development and improvement of the suitable models and methods in this area is desirable.

Generally, a phase transition in a physical system is characterized by the breaking of certain symmetry of the system and the appearing of a nonzero value of some order parameter together with a singular behavior of the characteristic quantities near the critical value of the system's parameters [1], [2].

2 Thermal Phase Transitions and Ground State Phase Transitions

The physical phenomena mentioned above (ferromagnetism, superconductivity, etc.) are the examples of thermal phase transitions. The characteristic feature of these is that thermal fluctuations about an equilibrium state with thermodynamic temperature near some critical value T_c (and with critical values of external fields) induce the long-range correlations in the system together with appearing of nonzero value of some order parameter and singular behavior of the thermodynamic quantities of the system. We focus on the magnetic cooperative phenomena caused principally by the exchange interaction of the spins like ferromagnetism and antiferromagnetism, because here one can find most simple models, giving possibility to understand the phase transitions and critical phenomena more deeply. Here, the parameters characterizing an equilibrium state of the system are the temperature T of the system and an external magnetic field h.

If the temperature value T is near some T_c, and $h=0$, the thermal fluctuations induce the long-range correlations between the spins and for $T<T_c$ and $h=0$ there are two equivalent equilibrium states (instead of only one for $T>T_c$) differing only by the sign of the mean value of total spin magnetic moment, i.e. the symmetry with respect to spin flips is broken and the spontaneous magnetization (or sublattice magnetization, in case of antiferromagnetism) appears, together with the singularities of the free energy and its derivatives (magnetization, susceptibility, specific heat, etc.) as functions of the temperature and magnetic field. The typical spontaneous magnetization [3], and susceptibility [4], curves are in Fig. 1 a, b, respectively.

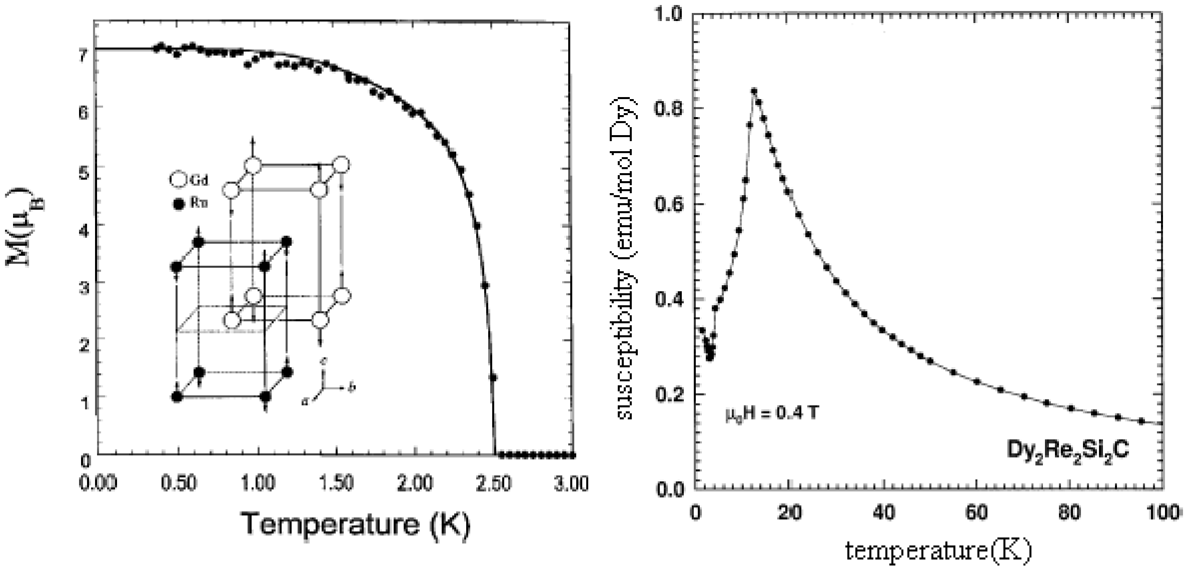

Fig. 1 *(a)* *(b)*

One can observe analogical phase transitions in quantum systems in the ground state. Here, the symmetry breaking, the long-range correlations and the nonzero value of an order parameter are induced by the quantum fluctuations of the quantity representing the order parameter about its ground state mean value. Thus, while in the description of thermal phase transitions the important parameters were the ones characterizing an equilibrium state (i.e. temperature and an external parameter), here these are the ones characterizing the ground state, i.e. the parameters characterizing the interaction itself (together with an external parameters). At the transition point, again one can observe the singular behavior of the ground state energy (as a function of these parameters) and its derivatives. In quantum spin systems, these represent e.g. the ground state mean total spin, i.e. the ground state magnetization and corresponding magnetic susceptibility. The interaction parameter (which depends on the composition of the material) dependence of these is similar as that in the Fig.1 a, b. (see e.g. [5], [6]).

Let us state several good reasons to study the models of the ground state phase transitions: it turns out that a simple model of superconductivity, the Hubbard model, in certain values of its parameters, is the same as that of antiferromagnetic quantum Heisenberg model [7] and studying its ground state properties (including the phase transitions) helps to clarify the structure of this ground state (e.g. the symmetry, the order); another reason is a rather theoretical one: the ground state critical behavior of the d-dimensional quantum spin system should be the same as that of $(d+1)$-dimensional system of classical spins [8], which means that studying the ground state phase transitions one can get an information about the critical behavior of the corresponding classical system (and vice versa).

3. Some Interesting Models

Collective behavior of many magnetic systems with dominant spin exchange interaction can be successfully described by the lattice models of interacting spin systems with exchange interaction between the spins occupying the sites of the lattice.

Probably the first (but very important) such model is the mean field (MF) model [9]. The energy of a configuration of the spins in this model is

$$E(\sigma,h) = -h_{MF}\sum_i \sigma_i, \qquad h_{MF} = h + \frac{qJ}{N-1}\sum_{(j\neq i)}\sigma_j \tag{1}$$

Here σ_i is a classical spin in the i-th site of the lattice (its value is either 1 or –1), q is a number of nearest neighbors of the site (it depends on the dimension of the lattice), J is a coupling parameter characterizing the strength of exchange interaction, N is the total number of sites on the lattice and h is the external magnetic field. Thus, in this model every spin interacts with the "mean field" of all other spins on the lattice (unlike other models, in most of which the interaction is only between the nearest neighboring spins). Given this microscopic description of the system, one can employ statistical physics to calculate thermodynamic quantities in thermal equilibrium with the temperature T:

$$f(T,h) = \lim_{N\to\infty}\frac{1}{N}(-kT\ln Z), \qquad Z = \sum_\sigma \exp\left(-E(\sigma,h)/kT\right) \tag{2}$$

$$m(T,h) = \frac{1}{Z}\sum_\sigma\left(\frac{1}{N}\sum_i\sigma_i\right)\exp(-E(\sigma,h)/kT), \qquad m_0(T) = \lim_{h\to 0} m(T,h) \tag{3}$$

$$\chi(T,h) = \frac{\partial m(T,h)}{\partial h} = -\frac{\partial^2 f(T,h)}{\partial h^2} \tag{4}$$

where $f(T,h)$ is the free energy per one site of the lattice, Z is the partition function, $m(T,h)$ is the magnetization, $m_0(T)$ is the spontaneous magnetization (becoming nonzero for temperature values under the critical one) and $\chi(T,h)$ is the magnetic susceptibility. Sums over σ are over all possible spin configurations on the lattice. This way, for $m(T,h)$ in the MF model one can derive the self-consistency relation

$$m = \tanh\left(\frac{qJm+h}{kT}\right) \tag{5}$$

Detailed analysis of (5) and of the free energy $f(T,h)$ shows that in the neighborhood of the point $T=T_c=qJ/k$, $h=0$ the free energy, the magnetization and the susceptibility exhibit singular behavior of the form:

$$f(T,0) \propto (T-T_c)^{2-\alpha} \tag{6a}$$

$$m_0(T) \propto (T_c-T)^{\beta} \qquad \text{for } T<T_c \tag{6b}$$

$$\chi(T,0) \propto (T-T_c)^{-\gamma} \qquad \text{for } T>T_c \tag{6c}$$

$$\chi(T,0) \propto (T_c-T)^{-\gamma'} \qquad \text{for } T<T_c \tag{6d}$$

where α, β, γ, γ′ are called the critical exponents. For MF model, there is

$$\alpha = 0, \qquad \beta = 1/2, \qquad \gamma = \gamma' = 1 \tag{7}$$

the same critical temperature and exponents one can obtain also from the Landau theory by expanding the free energy in the neighborhood of the critical point into a power series in order parameter (in this case, the magnetization)

$$f(T,h,m) = a_0(T) + a_2(T)m^2 + a_4(T)m^4 + \ldots - mh \tag{8}$$

and by examining the (global) minima of this function [1]. When h=0, the critical point is indicated by the appearance of two symmetric global minima and a nonzero value of the magnetization (compared to one global minimum above the critical temperature). At this point, the single global minimum becomes a local maximum and the second derivative of f with respect to m becomes zero, which yields the critical temperature. The MF critical exponent values are interesting, because, according to the renormalization group calculations [1], for the lattices with the dimension $d \geq 4$ these values correctly describe critical behavior of classical spin system with short range interaction.

The critical exponents (i.e. the character of critical singularities) are universal for a broad range of collective phenomena. For spin systems with short range interaction the universality means that the critical exponents depend only on the spatial dimensionality of the system and on the symmetry of the system (they are independent e.g. of the details of interaction). However, there are several models, for which the universality hypothesis doesn't hold [9]. We focus on the ground state of the quantum Heisenberg XYZ model, characterized by the energy operator

$$H = -\sum_{(i,j)} (J_1\sigma_i^1\sigma_j^1 + J_2\sigma_i^2\sigma_j^2 + J_3\sigma_i^3\sigma_j^3) - \sum_i (h_1\sigma_i^1 + h_2\sigma_i^2 + h_3\sigma_i^3) \tag{9}$$

where $\sigma_i^{1,2,3}$ are the spin operators on the i-th site of the lattice, and $h_{1,2,3}$ are the magnetic field components. The first sum is over all pairs of the nearest neighboring spins. In one dimension with zero external field, the ground state energy of this model is known as an explicit function of the coupling parameters J_1, J_2, J_3. The points of phase transition are given by the singularities of this function at the border $-J_3=J_1$ of the "basic parameter region" [5] $-J_3 \geq J_1 \geq |J_2|$. Its singular part and the order parameter (we take $(h_1, h_2, h_3) = (h, 0, 0)$) in the neighborhood of the critical point are [9], [10]

$$E_{\sin g} = (4\pi/\mu) J_1 \sin\mu \cot(\pi^2/2\mu)\, p^{\pi/\mu} \tag{10a}$$

$$\left\langle \frac{1}{N}\sum_i \sigma_i^1 \right\rangle \approx (\pi/\mu)\, p^{(\pi-\mu)/4\mu} \tag{10b}$$

$$p \approx \frac{|J_3^2 - J_1^2|}{16(J_1^2 - J_2^2)} \qquad \cos\mu = \frac{J_2}{J_1}, \qquad 0 < \mu < \pi \tag{10c}$$

where $\langle . \rangle$ is the ground state mean value. Clearly, the critical exponents of the singular part of the ground state energy and of the magnetization (in the x direction) depend on the coupling parameters J_1, J_2, J_3 i.e. they are not universal. The aim of our work is to check if universality in the XYZ model is restored for the two- and three-dimensional lattice. To reach the aim, we use the coherent anomaly method (CAM) developed by Suzuki [11]. CAM is based on the construction of the sequence of suitable MF-type approximations from which it is possible to obtain the true critical value of a parameter like temperature or coupling parameter, and the corrections to the MF critical exponents. For the quantum XYZ model, we construct this sequence as a sequence of variational approximations [12]. Each of these is characterized by the “trial function” $|\psi_L(x)\rangle$ containing free parameter(s) x (L is the degree of approximation). The ground state energy approximation is then a global minimum of the function

$$E_L(J,h,x) = \langle \psi_L(x) | H | \psi_L(x) \rangle / \langle \psi_L(x) | \psi_L(x) \rangle \tag{11}$$

(for given J_1, J_2, J_3, h) with respect to x. The MF critical behavior is then obtained similarly to the Landau theory-by expanding $E_L(J, h, x)$ in J, h, x, (two of the coupling parameters are fixed here, the true critical exponents will turn to depend on them) near the critical point $(J_c^{(L)},0,0)$. and examining the global minima. According to CAM, the MF approximation sequence should be such that, $J_c^{(L)} \xrightarrow[L\to\infty]{} J_c$ where J_c is the true critical temperature and the prefactors of the MF singularities (i.e. the proportionality coefficients in expressions similar to (6)) exhibit coherent anomaly, for example, the spontaneous ground state magnetization (e.g. for J_1, J_3 fixed) is:

$$m_0(J_2,L) \equiv \langle \psi_L(x) | \frac{1}{N}\sum_i \sigma_i^1 | \psi_L(x) \rangle \Big/ \langle \psi_L(x) | \psi_L(x) \rangle \tag{12a}$$

$$m_0(J_2,L) \approx \overline{m}_0(L,J_1,J_3)(J_{2c}^{(L)} - J_2)^{1/2} \tag{12b}$$

$$\overline{m}_0(L,J_1,J_3) = a(J_1,J_3,J_{2c}^{(L)})(J_{2c}^{(L)} - J_{2c})^{-\varphi} \tag{12c}$$

By determining parameters J_{2c} and φ in (12c) one can get the true critical value of J_2 and the true critical exponent $\beta=1/2-\varphi$.

4. Preliminary results

So far we have been doing calculations for the one dimensional case (when they are complete they will be compared to the exact results): we have constructed the suitable trial function having symmetry properties necessary for description of the phase transition and parameterized such that it allows for the disordered as well as for the ordered (i.e. with a nonzero magnetization) ground state. On the L-th degree of approximation it is an $N/2L$-folded tensor product of vectors of the form

$$\sum_{i=1}^{2^{2L-1}-1} \left[x_i (e_i + e_{2^{2L}+1-i}) \right] + e_{2^{2L-1}} + e_{2^{2L-1}+1} \tag{13}$$

where $\{e_i\}_{i=1}^{2^{2L}}$ is the basis of 2^{2L}-dimensional Euclidean space at each site of the chain. For L=1, 2, 3 we have calculated the approximate critical lines (Fig. 3b). The calculations were done with J_1=1, J_3 fixed and we were searching for the global minima for various values of J_2, looking for $J_{2c}^{(L)}$. It can be found as in Landau theory, but for L>1 it had to be found numerically, because the equations are too complicated to be solved analytically. The calculations were programmed in FORTRAN, using the MINUIT routine of the CERN program library to find the minima. The results agree with those obtained with the help of Mathematica package [13], the calculations programmed in FORTRAN were much quicker. The approximate critical lines obviously approach the true critical line shown in Fig. 3a, which is a promising result from the CAM point of view. At the point J_1=1, J_2=1, J_3=-1 they touch the true critical line, which means that our trial function is suitable in the neighborhood of this point.

Fig. 4a, b, c show the ground state spontaneous magnetization for L=1, 2, 3, as function of J_2, $J_2 < J_{2c}^{(L)}$, for J_3=-1, -0.9, -0.8 respectively. It exhibits the MF behavior, the next step will be to calculate the prefactors (12b), check the coherent anomaly property of our sequence of approximations, find the corrections to the MF critical exponents and compare them with the exact solution.

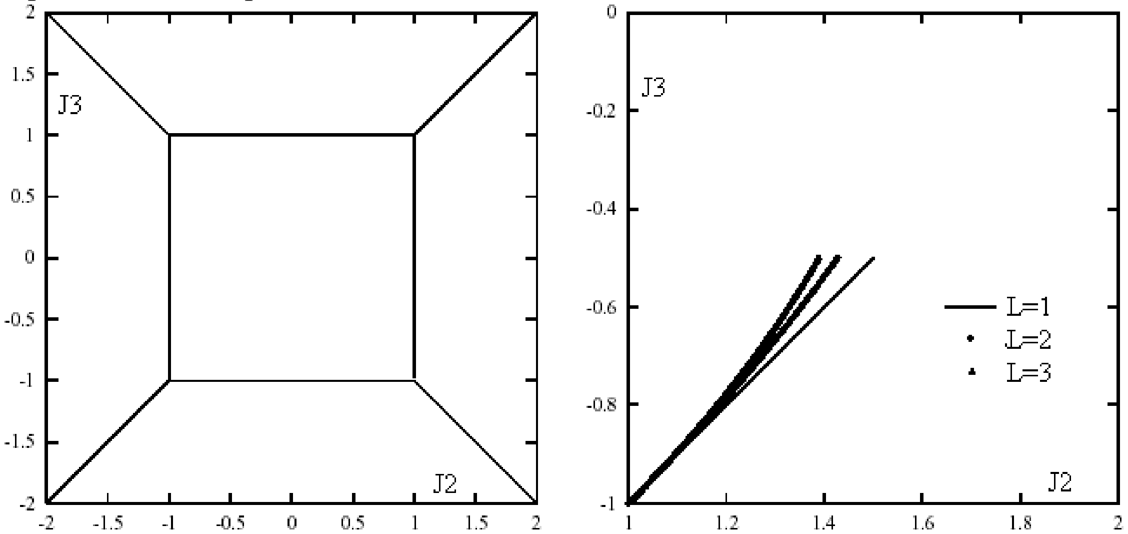

Fig. 3 *(a)* *(b)*

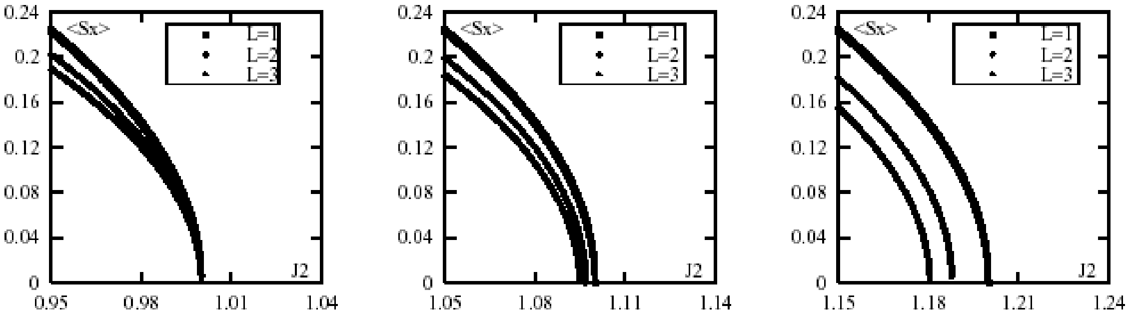

Fig. 4 *(a)* *(b)* *(c)*

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