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Generalization of the Curie-Weiss Model to the D-dimensional Spin System

Hyung-june Woo, Eun Kyung Lee, and Eok-Kyun Lee*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Taejon 305-701
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The critical behavior of the classical D-dimensional spin model $(D \geq 2)$, which is the intermediate model that link up the Ising $(D=1)$ and the spherical model $(D=\infty)$, is studied for the case of constant coupling interaction independent of the spin-spin distance (Curie-Weiss model). Analytical results show that the critical behavior of the present model is in quantitative agreement with the prediction of the phenomenological mean-field theory independent of D. Critical temperature is calculated to be $T_c = k/JD$. This gives a quantitative explanation of the relationship between the spin degree of freedom and the critical temperature.

Introduction

As the most symplified model of the long-range interacting spin system, meanfield theory has been used as a guide to the more realistic models[1,2]. A macroscopic hamiltonian can be made to get the thermodynamic properties that exactly match the predictions of the phenomenological mean-field theory. This so-called "Curie-Weiss Model" has been solved and discussed in the Ising case[2], in which each spin interacts with all others equally, and the spin variable can take the values of ± 1 only.

In this paper, the spin model is generalized to the D-dimensional case, in which each spin variable is a D-dimensional unit vector. This classical spin model is a realistic approximation to the quantum mechanical Heisenberg model for $D=3$ case near the critical temperature. The phase transition for $D \geq 2$ spin system is known to be given by the long-range fluctuations, whereas for the Ising case, it is done by the local defects. However, our result shows that such a difference is not reflected on the critical behavior for the present

system in which each spin interacts with all others equally, which confirms the predictions of the phenomenological mean-field theory.

Thermodynamic Properties

Our derivation of the thermodynamic properties is a direct generalization of Kac's argument[2]. But our analysis covers the case of nonzero magnetic field, without which the critical exponents β, γ and δ cannot be obtained. let us define the hamiltonian for the Curie-Weiss model in D-dimension as

$$H = -h \cdot \sum_i x_i - \frac{J}{N} \sum_i \sum_{j<i} x_i \cdot x_j, \tag{1}$$

wher h is the external field vector and x_i is the spin vector which satisfies $|x_i| = 1$. One of the great virtues of the model is that the hamiltonian can be transformed to the following form.

$$H = -\frac{J}{2N} \left| \sum_i x_i \right|^2 - h \cdot \sum_i x_i + J/2$$

$$= -\frac{J}{2N} \left| \sum_i x_i + Nh/J \right|^2 + Nh^2/2J + J/2. \tag{2}$$

The partition function Z_N is

$$Z_N = \int \cdots \int e^{-H/kT} \prod_{i=1}^{N} [s(x_i)dx_i], \tag{3}$$

where $s_i(x_i) = \delta(|x_n| - 1)/A_D$ and $A_D = 2\pi^{D/2}/\Gamma(D/2)$ is the surface area of a unit sphere in D-dimension. From (2),

$$Z_N = e^{-Nh^2/2JkT - J/2kT} \int \cdots \int \prod_{i=1}^{N} [s(x_i)dx_i]$$

$$\exp\left(-\frac{J}{2NkT} \left| \sum_i x_i + Nh/J \right|^2 \right). \tag{4}$$

Using the identity introduced by Kac in one dimensional case[2]

$$\exp(|a|^2) = \frac{1}{(2\pi)^{D/2}} \int dp \, \exp[-|p|^2/2 + 2^{1/2} a \cdot p]. \tag{5}$$

Z_N can be transformed to

$$Z_N = \frac{e^{-Nh^2/2JkT - J/2kT}}{(2\pi)^{D/2}} \int dp \, \exp[-p^2/2 + (N/JkT)^{1/2} h \cdot p]$$

$$\times \prod_{i=1}^{N} \left[\int s(x_i) dx_i e^{(J/NkT)^{1/2} p \cdot x_i} \right]$$

$$= e^{-Nh^2/2JkT - J/2kT} \frac{[\Gamma(D/2)]^N}{(2\pi)^{D/2}}$$

$$\times \int dp \, e^{-p^2/2 + (N/JkT)^{1/2} h \cdot p} [i_{D/2-1}((J/NkT)^{1/2} p)]^N, \tag{6}$$

where $i_\nu(z) = \frac{I_\nu(z)}{(z/2)^\nu}$ and $I_\nu(z)$ is the modified Bessel function. Letting $p = N^{1/2} q$,

$$Z_N = \frac{N^{D/2}}{(2\pi)^{D/2}} e^{-Nh^2/2JkT - J/2kT} [\Gamma(D/2)]^N$$

$$\times \int dq [\exp(-q^2/2 + (1/JkT)^{1/2} h \cdot q) \, i_{D/2-1}((J/kT)^{1/2} q)]^N. \tag{7}$$

Applying the Laplace's method for large N,

$$Z_N = \frac{N^{D/2}}{(2\pi)^{D/2}} e^{-Nh^2/2JkT - J/2kT} [\Gamma(D/2)]^N$$

$$\times max_{(q)} [\exp(-q^2/2 + (1/JkT)^{1/2} h \cdot q) i_{D/2-1}((J/kT)^{1/2} q)]^N, \tag{8}$$

where in the maximum function q is allowed to vary freely in the D-dimensional space. It is obvious that this maximum occurs for q parallel to h. Thus the free energy per spin f becomes in the thermodynamic limit,

$$-f/kT = \lim_{N \to \infty} \frac{1}{N} \ln Z_N = -h^2/2JkT + \ln \Gamma(D/2)$$

$$+ max_{(0 \le q \le \infty)} [F_D(q)], \tag{9}$$

where

$$F_D(q) = -q^2/2 + (1/JkT)^{1/2} hq + \ln i_{D/2-1}((J/kT)^{1/2} q). \tag{10}$$

The maximum of $F_D(q)$ is determined by
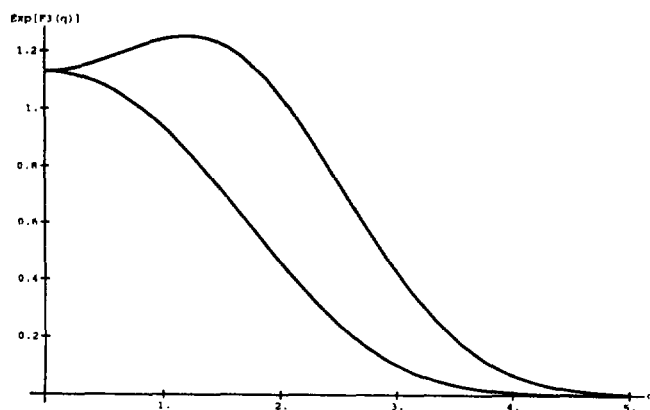
$$F_D'(q_M) = -q_M + (1/JkT)^{1/2} h$$

Figure 1. Numerical plot of $\exp(F_3(q))$ in (10). The upper and lower curve corresponds to the case of $T^* = 1/4$ and $T^* = 1/2$, respectievely. Note that $T_c^* = 1/2$ in this case.

$$+ \frac{i_{D/2-1}'((J/kT)^{1/2} q_M)}{i_{D/2-1}((J/kT)^{1/2} q_M)} (J/kT)^{1/2} = 0 \tag{11}$$

and

$$-f/kT = -h^2/2JkT + \ln \Gamma(D/2) + F_D(q_M). \tag{12}$$

Since the magnetization $m = -\left(\frac{\partial f}{\partial h}\right)$ is related to the value of q_M by $q_M = h(1/JkT)^{1/2} + m(J/kT)^{1/2}$, m is determined by

$$m = \frac{i_{D/2-1}'((Jm/kT + h/kT))}{i_{D/2-1}((Jm/kT + h/kT))} = \frac{I_{D/2}(Jm/kT + h/kT)}{I_{D/2-1}(Jm/kT + h/kT)}. \tag{13}$$

In series representation, the spontaneous magnetization m_0 satisfies

$$m_0 \sum_{s=0}^{\infty} \frac{(Jm_0/2kT)^{2s}}{s! \Gamma(s+D/2)} \left(1 - \frac{J/2kT}{s+D/2} \right) = 0. \tag{14}$$

It is easily seen that nonzero solution can occur only if $J/kT \ge D$. Figure 1 shows the numerical plot of $\exp(F_D(q))$, in which nonzero maximum corresponds to the case of $J/kT \ge D$. Thus the critical temperature $T_c^* = JT_c/k = 1/D$. Also from (14), we see that near the critical point,

$$m_0^2 \sim (1 + 2/D)(1 - T/T_c), \tag{15}$$

from which the exponent $\beta = 1/2$ is obtained. The curvature of the $m - h$ isotherm is obtained by substituting the value of the critical temperature into (14) and assuming small h and m. The result is $m \sim h^{1/3}$ and the exponent $\delta = 3$. To find the susceptibility $\chi = \frac{\partial m}{\partial h}\Big|_{h=0}$, we differentiate both sides of (13) with respect to h, set $h = 0$, and again use (13) with $h = 0$ and the recurrence relations of the modiofied Bessel function to get

$$\chi = \frac{(-m_0^2 + 1)/kT + (D-1)kT/J}{(m_0^2 - 1)J/kT + + D}. \tag{16}$$

Since $m_0 \to 0$ as $J/kT \to D$, we see that

$$\chi \sim \frac{1}{JD} (T/T_c - 1)^{-1} \tag{17}$$

and χ diverges at the critical temperature $T_c^* = 1/D$ with the

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critical exponent $\gamma = 1$. The specific heat $C = T^2 \frac{\partial^2 f}{\partial T^2}$ can be obtained from (12) using (10), (11), and (13) in terms of the spontaneous magnetization m_0 as

$$C = \frac{m_0^2}{m_0^2 + \frac{T}{T_c} - 1} \tag{18}$$

This is nonzero only $T < T_c$. But from (15), the limiting value of C at $T = T_c$ is seen to be $C = D/2 + 1$. Therefore, the specific heat does not diverge at the critical point but has a jump discontinuity, from which we deduce the exponent $\alpha = 0$.

Discussion

The generalization of the Curie-Weiss model to the D-dimensional spin system shows the critical behavior that is predicted by the phenomenological mean-field theory. This is supported by the above direct calculation of the critical exponents; $\alpha = 0$, $\beta = 1/2$, $\gamma = 1$, and $\delta = 3$. Therefore the spin dimensionality has no essential effect on the critical behavior of the model, the only difference being the critical temperature. It is worth noting that the critical temperature can be scaled to unity by assuming the length of each spin vector as $|x_i| = D^{1/2}$.

The fact that the critical temperature is inversely proportional to the spin dimension D is the manifestation of the decrease of the ordered phase stability with the incresing degree of freedom of the spin vector. As $D \to \infty$, the critical temperature approaches zero and no ordered phase exists in this limit. This infinite-dimensional spin system is closely related to the spherical model[3], in which it is shown that there is no spontaneous magnetization in the one-dimensional lattice system.

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Theoretical Studies on the Photochemical Reaction of Psoralen. Photocycloaddition of Angelicin with Thymine

Ja Hong Kim, Sung Ho Sohn*, Gae Soo Lee*, Kee Soo Yang, and Sung Wan Hong†

Department of Chemistry Education, Chonbuk National University, Chonju 560-750
*Department of Chemistry, Chonnam National University, Kwangju 500-757
†Department of Chemistry, Woosuk University, Wanju 565-800

A semiempirical methods (PM3-CI-UHF. etc.) for the evaluation of ground and excited state electronic structures of psoralens are applied to angelicin with thymine. The photocycloaddition reaction of angelicin with thymine were deduced to be formed by their preferable HSOMO-LUMO interactions. The photoadduct was inferred to be a C_4-cycloaddition product with the stereochemistry of *cis-anti* formed through [2+2] addition reaction between the 3,4 double bonds of angelicin and the 5,6-double bond of thymine.

Introduction

The relative reactivity of the photoexcited states of angelicin for C_4-cycloaddition reaction is very interesting from the physical and chemical point of view on the photoexcited states. Natural products with a linear structure such as a psoralens, or with a non-linear structure, like angelicin are well known photosensitizing agent and have been used in the photochemotherapy of psoriasis and vitiligo[1,2]. Psoralens and their congeners are known to photoreact with purine and pyrimidine bases, free in DNA, upon irradiation with long wave length UV light (320-380 nm). Various physiological actions such as skin erythma on human and guinia pig skin, mutagenic and lethal effect in bacteria, in activation of DNA viruses, and inhibition of tumor transmitting capacity of various tumor cells have been attributed to this photoreaction[3].

The family of furocoumarin derivatives known as psoralen, angelicin has been actively investigated with regard to their ability of act as dermal photosensitizing agents and as probes of nucleic acid structure and fuction[4,5]. The biological activity of psoralen is primarily the result of covalent bonding with nucleic acid, especially DNA. Monoaddition at 3,4 positions results in a low-lying triplet state for the photoadduct. The low-lying triplet state is probably unreactive with respect to the second photocycloaddition because of its rapid relaxation to the ground state. On the other hand, monoaddition at 4',5'-positions yields a relatively long-lived singlet state[6]