



Bond diluted anisotropic quantum Heisenberg model

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ABSTRACT

Effects of the bond dilution on the critical temperatures, phase diagrams and the magnetization behaviors of the isotropic and anisotropic quantum Heisenberg model have been investigated in detail. For the isotropic case, bond percolation threshold values have been determined for several numbers of two (2D) and three (3D) dimensional lattices. In order to investigate the effect of the anisotropy in the exchange interaction on the results obtained for the isotropic model, a detailed investigation has been made on a honeycomb lattice. Some interesting results, such as second order reentrant phenomena in the phase diagrams have been found.

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1. Introduction

Quenched randomness effects are very important in modeling real materials, since consideration of these effects simulates a realistic model of real materials. Real materials have some uncontrollable defects and these defects can be modeled by introducing site dilution (randomly distributed non-magnetic atoms), bond dilution (randomly broken bonds between the magnetic atoms) or both of them into the related model. It is a well known fact that, Heisenberg model produces more realistic results than the Ising model, in order to explain the magnetic properties of real materials. Thus, it is important to work on the Heisenberg model with these quenched randomness effects. These quenched randomness effects produce different behaviors in the magnetic properties of the model, e.g. different phase transition characteristics from the pure model (i.e. the model without any quenched randomness effects).

Heisenberg model with quenched randomness effects has been studied widely by a variety of methods, such as spin-1/2 (S-1/2) isotropic Heisenberg model with bond dilution on 2D lattices with Monte Carlo (MC) simulation [1–4], anisotropic model (by means of the XXZ model) on 2D lattices with real space renormalization group (RSRG) technique [5], S-1/2 anisotropic quantum Heisenberg model with site dilution with RSRG [6], with mean field approximation (MFA) [7] and with effective field theory (EFT) [8,9]. Detailed examination of the percolation probability can be found in Ref. [10]. On the other hand, random bond distributed systems in which spin glass phases originate have been studied, e.g. discrete distribution on S-1/2 Heisenberg model with pair

approximation [11,12], density matrix product approximation [13], Gaussian distribution with imaginary time Grassmann field theory [14] and S-1 Heisenberg model with discretely distributed random bonds with exact diagonalization method [15]. Besides, both site and bond diluted systems have been studied with quantum MC on 2D lattices [16] and S-1/2 Heisenberg model with site-bond correlated dilution (which covers uncorrelated site dilution as a limit) on 2D and 3D lattices with RSRG [17] and MC [18], and also using a variational principle for the free energy [19]. All of these work are related to the isotropic Heisenberg model or XXZ model.

The aim of this work is to determine the effect of the bond dilution on the phase diagrams and the thermodynamic properties of the anisotropic quantum Heisenberg model. By anisotropy, we do not restrict ourselves with XXZ model. Namely, we want to determine the effect of the anisotropy in the exchange interaction on the phase transition characteristics not only by means of XXZ model. The method is EFT with two spin cluster approximation [20]. EFT approximation can provide results that are superior to those obtained within the traditional MFA, due to the consideration of self-spin correlations which are omitted in the MFA.

EFT for a typical magnetic system starts by constructing a finite cluster of spins which represents the system. Callen–Suzuki spin identities [21,22] are the starting point of the EFT for the one spin clusters. If one expands these identities with differential operator technique [23], multi-spin correlations appear, and in order to avoid from the mathematical difficulties, these multi-spin correlations are often neglected by using decoupling approximation (DA) [24]. Working with larger finite clusters will give more accurate results. Callen–Suzuki identities have been generalized to two spin clusters in Ref. [25] (namely EFT-2 formulation). This EFT-2 formulation has been successfully applied to a variety of systems, such as quantum S-1/2 Heisenberg ferromagnet [26,27] and antiferromagnet [28]

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systems, classical n -vector model [29,30], and spin-1 Heisenberg ferromagnet [31,32].

This paper is organized as follows: In Section 2, we briefly present the model and formulation. The results and discussions are presented in Section 3, and finally Section 4 contains our conclusions.

2. Model and formulation

We consider a lattice which consists of N identical spins ($S=1/2$) such that each of the spins has z nearest neighbors. The Hamiltonian of the system is given by

$$\mathcal{H} = -\sum_{(ij)} (J_x^{(ij)} s_i^x s_j^x + J_y^{(ij)} s_i^y s_j^y + J_z^{(ij)} s_i^z s_j^z) \quad (1)$$

where s_i^x, s_i^y and s_i^z denote the Pauli spin operators at a site i . $J_x^{(ij)}, J_y^{(ij)}$ and $J_z^{(ij)}$ stand for the components of the exchange interaction \mathbf{J} (in other words anisotropy in the exchange interaction) between the nearest neighbor spins i and j . The sum is carried over the nearest neighbors of the lattice. The bonds between the spins i and j are randomly distributed via

$$P(\mathbf{J}^{(ij)}) = c\delta(\mathbf{J}^{(ij)} - \mathbf{J}) + (1-c)\delta(\mathbf{J}^{(ij)}) \quad (2)$$

in the bond dilution problem. The distribution given by Eq. (2) distribute bonds randomly between lattice sites as c percentage of bonds are closed and remaining $1-c$ percentage of bonds are open, i.e. c is the concentration of closed bonds in the lattice. Here δ stands for the delta function and c is a real number which is defined within the range of $0 \leq c \leq 1$. The distribution given by Eq. (2) reduces to the system with homogenously distributed bonds (i.e. pure system) for $c=1$.

We use the two spin cluster approximation as an EFT formulation, namely EFT-2 formulation [20]. In this approximation, we choose two spins (namely s_1 and s_2) and treat the interactions in this two spin cluster exactly. In order to avoid some mathematical difficulties we replace the perimeter spins of the two spin cluster by Ising spins (axial approximation) [30]. With the procedure defined in Ref. [30], we get an expression for the magnetization per spin as

$$m = \left\langle \left\langle \frac{1}{2} (s_1^z + s_2^z) \right\rangle_r \right\rangle = \left\langle \left\langle \frac{h'_+}{X'_0 \cosh(\beta X'_0) + \exp(-2\beta J_z^{(12)}) \cosh(\beta Y'_0)} \right\rangle_r \right\rangle \quad (3)$$

where $\beta = 1/(k_B T)$, k_B is Boltzmann constant and T is the temperature. The inner average bracket in Eq. (3) (which has no subscript) stands for thermal average and the outer one (which has subscript r) is for the configurational averaging which is necessary for including the effect of the random bond distribution. The parameters in Eq. (3) are given by

$$X'_0 = [(J_x^{(12)} - J_y^{(12)})^2 + h_+^2]^{1/2} \\ Y'_0 = [(J_x^{(12)} + J_y^{(12)})^2 + h_-^2]^{1/2} \quad (4)$$

$$h_+^2 = h'_1 + h'_2 \\ h_-^2 = h'_1 - h'_2 \quad (5)$$

$$h'_1 = \sum_k J_z^{(1k)} s_k^z \\ h'_2 = \sum_l J_z^{(2l)} s_l^z \quad (6)$$

where s_k^z stands for the z component of the nearest neighbor of the spin s_1 while s_l^z stands for the z component of the nearest neighbor of the spin s_2 . The sums in Eq. (6) are over the nearest neighbor sites of the sites labeled 1 and 2, respectively. The

configurational averages can be calculated via integration of the expression by using Eq. (2), over the all bonds of the treated cluster.

$$m = \left\langle \int d\mathbf{J}^{(12)} P(\mathbf{J}^{(12)}) \prod_{k,l} d\mathbf{J}^{(1k)} d\mathbf{J}^{(2l)} P(\mathbf{J}^{(1k)}) P(\mathbf{J}^{(2l)}) \frac{h'_+}{X'_0 \cosh(\beta X'_0) + \exp(-2\beta J_z^{(12)}) \cosh(\beta Y'_0)} \right\rangle \quad (7)$$

where product is taken over the nearest neighbors of the sites 1 and 2. If we perform the integration concerning the bond between the sites 1 and 2 then we get the following expression,

$$m = \left\langle \int \prod_{k,l} d\mathbf{J}^{(1k)} d\mathbf{J}^{(2l)} P(\mathbf{J}^{(1k)}) P(\mathbf{J}^{(2l)}) h'_+ \times \left[\frac{c}{X''_0} \frac{\sinh(\beta X''_0)}{\cosh(\beta X''_0)} (\beta X''_0) + \exp(-2\beta J_z) \cosh(\beta Y''_0) + \frac{1-c}{h'_+} \frac{\sinh(\beta h'_+)}{\cosh(\beta h'_+) + \cosh(\beta h'_-)} \right] \right\rangle \quad (8)$$

where

$$X''_0 = [(J_x - J_y)^2 + h_+^2]^{1/2} \\ Y''_0 = [(J_x + J_y)^2 + h_-^2]^{1/2} \quad (9)$$

Eq. (8) can be written in terms of the differential operators using differential operator technique [23] and it is found as

$$m = \left\langle \int \prod_{k,l} d\mathbf{J}^{(1k)} d\mathbf{J}^{(2l)} P(\mathbf{J}^{(1k)}) P(\mathbf{J}^{(2l)}) \exp(h_1' \nabla_x) \exp(h_2' \nabla_y) \right\rangle f(x, y)|_{x=0, y=0} \quad (10)$$

where

$$f(x, y) = \frac{c z_+}{X_0 \cosh(\beta X_0) + \exp(-2\beta J_z) \cosh(\beta Y_0)} + (1-c) \frac{\sinh(\beta z_+)}{\cosh(\beta z_+) + \cosh(\beta z_-)} \quad (11)$$

and

$$X_0 = [(J_x - J_y)^2 + z_+^2]^{1/2} \\ Y_0 = [(J_x + J_y)^2 + z_-^2]^{1/2} \\ z_+ = x + y, \quad z_- = x - y. \quad (12)$$

In Eq. (10), the parameters $\nabla_x = \partial/\partial x$ and $\nabla_y = \partial/\partial y$ are the usual differential operators in the differential operator technique. Differential operators act on an arbitrary function via

$$\exp(a \nabla_x + b \nabla_y) g(x, y) = g(x + a, y + b) \quad (13)$$

with any constant a and b .

Now let us assume that each of s_1 and s_2 has number of z_0 distinct nearest neighbors and both of them have z_1 common nearest neighbors. This means that, in Eq. (6), the two sums have number of z_1 common terms. If we take the integration in Eq. (10) with the help of Eqs. (2) and (6) and using DA [24] we get an expression,

$$m = \langle [A_x + m B_x]^{z_0} [A_y + m B_y]^{z_0} [A_{xy} + m B_{xy}]^{z_1} \rangle f(x, y)|_{x=0, y=0} \quad (14)$$

for the magnetization. The coefficients are defined by

$$A_x = c \cosh(J_z \nabla_x) + (1-c), \quad B_x = c \sinh(J_z \nabla_x) \\ A_y = c \cosh(J_z \nabla_y) + (1-c), \quad B_y = c \sinh(J_z \nabla_y) \\ A_{xy} = c \cosh[J_z (\nabla_x + \nabla_y)] + (1-c), \quad B_{xy} = c \sinh[J_z (\nabla_x + \nabla_y)]. \quad (15)$$

With the help of the Binomial expansion, Eq. (14) can be written as

$$m = \sum_{p=0}^{z_0} \sum_{q=0}^{z_0} \sum_{r=0}^{z_1} C'_{pqr} m^{p+q+r} \quad (16)$$

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