Anisotropic exchange-interaction model: From the Potts model to the exchange-interaction model

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A spin model called the anisotropic exchange-interaction model is proposed. The Potts model, the exchange-interaction model, and the spin-$\frac{1}{2}$ anisotropic Heisenberg model are special cases of the proposed model. Thermodynamic properties of the model on the bcc and the fcc lattices are determined by the constant-coupling approximation.

I. INTRODUCTION

Consider a spin-S system on a lattice described by the Hamiltonian

$$H=-J\sum_{\langle ij\rangle}[(1-\alpha)\delta(S_{iz},S_{jz})+\alpha P_{ij}]\ , \tag{1}$$

where J is the coupling constant, α is a parameter, and the summation is over nearest-neighbor pairs of sites. S_{iz} is the z component of the spin $\mathbf{S}_i$ and $\delta(S_{iz},S_{jz})$ is the Kronecker δ function. The operator P_{ij} is the Schrödinger exchange operator[1] which has the property that it permutes the spin variables $\mathbf{S}_i$ and $\mathbf{S}_j$. For general spins, Eq. (1) reduces to the $(2S+1)$-state Potts model[2] and the spin-S exchange-interaction (EI) model,[3] when $\alpha=0$ and 1, respectively. For $S=\frac{1}{2}$ and for general values of α, Eq. (1) is the same as the spin-$\frac{1}{2}$ anisotropic Heisenberg model,[4] of which the Ising model and the Heisenberg model are special cases. The Potts model and the EI model are generalizations of the Ising and the Heisenberg models, respectively, to higher spin systems which contain spin multipole interactions.[5] It is appropriate to call the new model the anisotropic exchange-interaction (AEI) model, as the model described by Eq. (1) is a generation of the spin-$\frac{1}{2}$ anisotropic Heisenberg model to general spins.

The Potts model has been a subject of continuous research interest in the past two decades.[6,7] The anisotropic Heisenberg model has also been extensively studied.[7–9] Critical behaviors of these models are generally understood. For the EI model, however, little is known about its properties.[10–13] Recently, it has been shown that the Potts model and the EI model have exactly the same thermodynamic properties in the mean-field approximation (MFA).[5] The EI model is a quantum spin model, while the Potts model is a classical one. Their properties should be quite different. The purpose of this work is to study the properties of the ferromagnetic ($J>0$) AEI model for $0\le\alpha\le1$. From this study we can see how thermodynamic properties change as the system varies from the Potts model to the isotropic EI model.

We will investigate the AEI model by using the constant-coupling approximation (CCA), which has been recently applied to the isotropic EI model.[14] In Sec. II, the ground states of the AEI model and the CCA are described. Thermodynamic properties of the ferromagnetic AEI model on the body-centered-cubic (bcc) and the face-center-cubic (fcc) lattice are presented and discussed in Sec. III.

II. GROUND STATES AND THE CONSTANT-COUPLING APPROXIMATION

The Hamiltonian of the AEI model, Eq. (1), can be expressed in terms of spin multipole moments[5,11] $Q_m^{(l)}$. That is,

$$H=-J\sum_{\langle ij\rangle}\sum_{l=0}^{2S}A(S,l)\left[Q_0^{(l)}(\mathbf{S}_i)Q_0^{(l)}(\mathbf{S}_j)+\alpha\sum_{m\neq0}Q_m^{(l)}(\mathbf{S}_i)Q_m^{(l)}(\mathbf{S}_j)\right]\ , \tag{2}$$

where $A(S,l)$ are constants and $Q_m^{(l)}$ are normalized in the way that $\operatorname{Tr}A(S,l)Q_m^{(l)}Q_{m'}^{(l')}=\delta_{l,l'}\delta_{m,m'}$. The summation $\sum_{m\neq0}$ sums over $m=\pm l,\pm(l-1),\ldots,\pm1$. When J and α are positive, the system is ordered ferromagnetically at low temperatures. For $\alpha=1$, it is known[11] that for any pure single-spin state $|\phi\rangle$, $\Phi=|\phi(\mathbf{S}_1)\rangle|\phi(\mathbf{S}_2)\rangle\cdots|\phi(\mathbf{S}_N)\rangle$ is a ground state with ground-state energy $E_0=-zNJ/2$, where N is the number of sites and z is the coordination number of the lattice. For $0\le\alpha<1$, Φ is a ground state with $E_0=-zNJ/2$ only when $|\phi\rangle$ is an eigenstate of S_z, to be denoted as $|\pi\rangle$ hereafter. (Since $\langle\pi|Q_m^{(l)}|\pi\rangle=0$ for $m\neq0$.) The system is Potts-like with $2S+1$ degenerate ground states. The symmetries of the ground states are quite different for $\alpha=1$ and for $\alpha<1$.

In the MFA, a pair interaction $Q_m^{(l)}(\mathbf{S}_i)Q_m^{(l)}(\mathbf{S}_j)$ is replaced by a single-spin term $\langle Q_m^{(l)}\rangle Q_m^{(l)}$. For the Potts-like ordering, the $2S+1$ eigenstates of the single-spin Hamiltonian are $|\pi\rangle$, and the thermal average $\langle Q_m^{(l)}\rangle=0$ for $m\neq0$.[5] The last term in Eq. (2) does not contribute to the mean-field Hamiltonian. Therefore, thermodynamic properties of the AEI model are independent of α for $0\le\alpha\le1$.

In the CCA, both the single-spin and the two-spin Hamiltonians are considered. The single-spin Hamiltonian $H_{cc}^{(1)}$ of the AEI model is also independent of α when $0\le\alpha\le1$. Following the previous study[14] for the isotropic EI model we have

$$H_{cc}^{(1)}(\mathbf{S})=-Jzh\rho_\pi(\mathbf{S})+Jz\epsilon/2\ , \tag{3}$$

where h is the effective field, ϵ is a constant operator, and ρ_π is the single-spin density matrix for the spin $\mathbf{S}$ to be in the pure state $|\pi\rangle$. Let $K=J/kT$, the free energy in units of J, $F_{cc}^{(1)}/J$, associated with the single-spin Hamiltonian is

$$F_{cc}^{(1)}/J=-K^{-1}\ln \mathrm{Tr}\{\exp[-H_{cc}^{(1)}/kT]\}$$
$$=-K^{-1}\ln[\exp(Kzh)+2S]+z\epsilon/2\ . \tag{4}$$

The two-spin Hamiltonian in the CCA is given by

$$\begin{aligned}H_{cc}^{(2)}&=-J(1-\alpha)\delta_{12}-J\alpha P_{12}+(z-1)/(2z)[H_{cc}^{(1)}(\mathbf{S}_1)+H_{cc}^{(1)}(\mathbf{S}_2)]\\&=-J(1-\alpha)\delta_{12}-J\alpha P_{12}-J(z-1)h[\rho_\pi(\mathbf{S}_1)+\rho_\pi(\mathbf{S}_2)]/2+J(z-1)\epsilon\\&\equiv H_2(J,\alpha,h)+J(z-1)\epsilon\ ,\end{aligned} \tag{5}$$

where δ_{12} is the shorthand notation for $\delta(S_{1z},S_{2z})$.

The free energy per pair of spins associated with the two-spin Hamiltonian is

$$F_{cc}^{(2)}/J=-K^{-1}\ln \mathrm{Tr}\{\exp(-H_2/kT)\}+(z-1)\epsilon$$
$$\equiv -K^{-1}\ln Z(K,\alpha,h)+(z-1)\epsilon\ . \tag{6}$$

Let $X=\exp[(z-1)hK]$, it can be shown that

$$\begin{aligned}Z&=\mathrm{Tr}\{\exp(-H_2/kT)\}\\&=2S\cosh(K\alpha)[2X+2S-1]\\&\quad+\exp(K)[X^2+2S]\ .\end{aligned} \tag{7}$$

The free energy per site of the system[14] is then given by

$$F_2=(z/2)F_{cc}^{(2)}-(z-1)F_{cc}^{(1)}\ . \tag{8}$$

For a given temperature T, the stable value of h is the one which has the lowest free energy F_2. In general, there are three characteristic temperatures: T_m, T_c, and T_0 (with $T_m>T_c>T_0$). At high temperatures $T>T_m$, the minimum of F_2 occurs at $h=0$. When $T_m>T>T_0$, F_2 has two minima and one maximum. The lowest free energy occurs at $h=0$ for $T>T_c$ and at $h>0$ for $T<T_c$. The two minima which occur at $h=0$ and h_c, respectively, have the same value at the temperature T_c, which is a first-order phase-transition temperature. At low temperatures $T<T_0$, F_2 has a maximum at $h=0$ and a minimum at $h>0$. We have determined the stable values of h numerically for various α and T for the bcc and fcc lattices. The order parameter q $[=\langle Q_0^{(l)}\rangle/\langle\pi|Q_0^{(l)}|\pi\rangle]$ is then obtained[14] by

$$q=[\exp(Kzh)-1]/[\exp(Kzh)+2S]\ ,$$

and the per site internal energy in units of J for the ferromagnetic AEI model is given by

$$\begin{aligned}U/NJ&=(-z/2)\mathrm{Tr}\{[(1-\alpha)\delta_{12}+\alpha P_{12}]\exp(-\beta H_2)\}/Z\\&=-(z/2)\exp[-(z-1)\epsilon K](\exp(K)\{\exp[2(z-1)hK]+2S\}\\&\qquad+2S\alpha\sinh(\alpha K)\{2\exp[(z-1)hK]+2S-1\})/Z\ .\end{aligned} \tag{9}$$

III. RESULTS AND DISCUSSIONS

It can be shown analytically that in the CCA the inverse phase-transition temperature $K_c(=J/kT_c)$ of the AEI model satisfies the equation

$$[(2S)^{(z-2)/z}-1]\exp(K_c)=(2S-1)\cosh(\alpha K_c)\ . \tag{10}$$

Transition temperatures of the bcc lattice ($z=8$) and the fcc lattice ($z=12$) obtained by the CCA are shown in Figs. 1 and 2, respectively, for several spins. The transition temperature T_c is a decreasing function of α as the model is more symmetric when $\alpha=1$. It can be shown that $dT_c/d\alpha=0$ for $\alpha=0$. It means that T_c does not change when the system changes from a classical spin model ($\alpha=0$) to a quantum spin one ($\alpha=0^+$). The transition temperature decreases more rapidly when $\alpha\approx 1$. The parameter α changes the universality class of the Hamiltonian. If we let $R=(1-\alpha)/\alpha$, the scaling hypothesis[15] implies that $T_c(R)-T_c(0)\sim(R)^{1/\varphi}$, where φ is the crossover exponent. In the CCA, each T_c versus α plot has a finite slope at $\alpha=1$. That is, $\varphi=1$ for all spins and for all lattices. Although the CCA provides good estimates of T_c, it predicts the same critical exponents ($\varphi=1$) as the mean-field theory.

The Hamiltonian of the EI model ($\alpha=1$) is spherically symmetric. It is known[16] that such a system cannot have a phase transition for lattice dimensionality $d\le 2$. In the CCA the lattice parameter involved is the coordination number z, instead of the dimensionality d. The CCA (Ref. 14) predicts that the EI model has a phase transi-

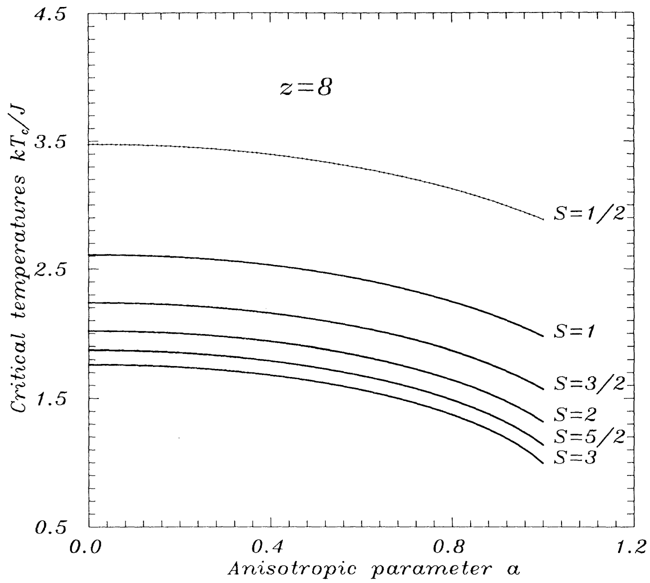

FIG. 1. Critical temperatures kT_c/J of the bcc lattice ($z=8$) plotted against α for several spins.

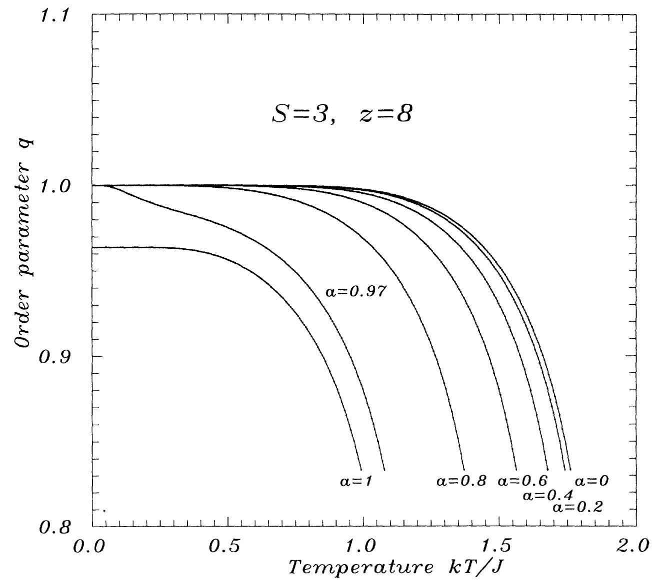

FIG. 3. Thermal variations of the order parameter q for several values of α. $z=8$.

tion only when $z>2\ln(2S)/\ln[4S/(2S+1)]$. This result is probably incorrect for large spins. For $0\le\alpha<1$ (Potts-like) the CCA predicts a phase transition for $z>2$ (i.e., $d>1$). We think that this is qualitatively correct. But the transition temperatures predicted by the CCA are less accurate for small values of z (say $z\le 6$).

Thermal variations of the order parameter q for $S=3$ and $z=8$ (bcc lattice) are plotted in Fig. 3 for various values of α. As $T\to 0$, the parameter q is not saturated $[q(T\to 0)<1]$ for $\alpha=1$; but for $0\le\alpha<1$, $q(T\to 0)=1$. The nonsaturation of the order parameter is a main drawback of the CCA. But the drastic change of $q(T\to 0,\alpha)$ near $\alpha=1$ gives an indication that $\alpha<1$ and $\alpha=1$ belong to different universality classes. The nonsaturation of q is more evident for larger spins and for small values of z. At the transition temperature we find that the discontinuity of the order parameter is $q_c=(2S-1)/2S$. This result is independent of α and is the same as that obtained by the MFA and the Oguchi[17] method. We expect that q_c should be smaller[12] than $(2S-1)/2S$ and should depend on α. More studies on q_c are needed.

We have calculated the internal energy U of the AEI

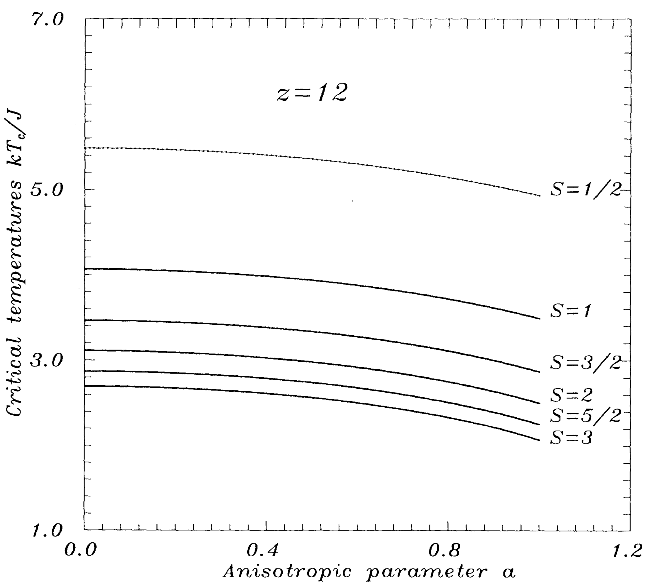

FIG. 2. Critical temperatures kT_c/J of the fcc lattice ($z=12$) plotted against α for several spins.

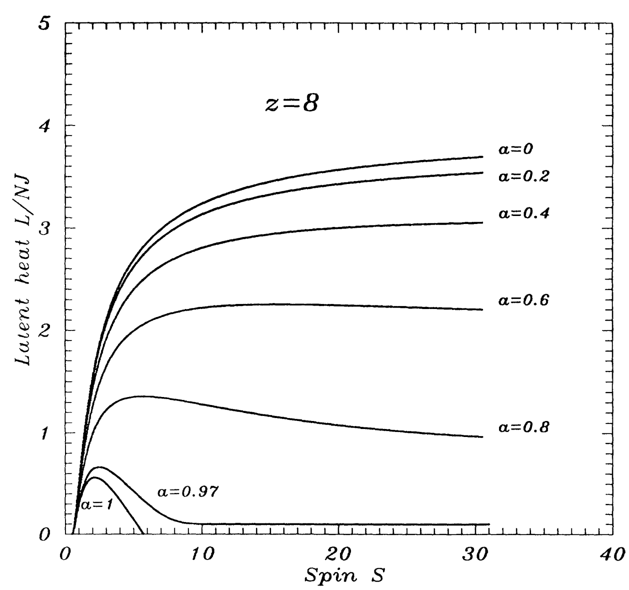

FIG. 4. Latent heats of the bcc lattice L/NJ vs S for several values of α.

model on the bcc and the fcc lattices. The discontinuities of U at T_c, i.e., the latent heats are shown in Fig. 4 for the bcc lattice. From the spin dependence of the latent heat, we also see a drastic change between $\alpha<1$ and $\alpha=1$. The curve for $\alpha=1$ terminates at $S_{\max}$ [($S_{\max}$ is the solution of $z=2\ln(2S)/\ln[4S(2S+1)]$). For $S>S_{\max}$, there is no phase transition. For $\alpha\neq1$ a phase transition exists for any spin. We emphasize that the CCA results are reasonably good for the bcc and the fcc lattices for small spins, say $S\leq3$. The CCA results become poor for small z and for large S, especially when $\alpha\approx1$.

In this work we only study the AEI model for $0\leq\alpha\leq1$. When $\alpha>1$ the ground states of the system are different from those for $\alpha=1$ and $\alpha<1$. In the limit $\alpha\gg1$, the AFI model reduces to the XY model when $S=\frac{1}{2}$; and for other spins, the limiting cases of the AEI model have not been considered before. It is of theoretical interest to study thermal properties of the AEI model for $\alpha>1$.

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