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# Three-dimensional anisotropic Ising spin model with competing two- plus four-spin interactions

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A three-dimensional anisotropic Ising spin model with nearest-neighbor interactions in all spatial directions supplemented by a four-spin interaction along one axis only is treated within a generalized mean-field approximation including short-range correlations. In obtaining the phase diagram various ordered structures are discussed. The results suggest that, besides the ferro- or antiferromagnetic and the so-called $\langle 3,1 \rangle$ phase, no additional modulated phases appear. The order-disorder transition temperature is finite everywhere, with both first- and second-order transitions present.

The concept of universality in the theory of critical phenomena is very helpful in classifying the possible critical behavior.[1] In considering the features on which the critical behavior decisively depends, one usually quotes the dimensionality of both space and order parameter, the range of interactions, etc. Recently a new class of interacting systems has been introduced that possesses multibody interactions with multiplicity $m \geq 3$. Based on exact solutions[2] evidence arises that $m$ may define new classes of universality. In other words, the critical behavior of such systems may depend explicitly on $m$. It is evident that a rich variety of possibilities may arise when different multiplicities $m, m', \ldots,$ coexist.

A second goal of such attempts is the search for simple models which exhibit—despite short-range couplings only—commensurate or incommensurate modulated structures with large periodicities. Such phases are known to exist in a number of different systems.[3] Well-known models displaying this kind of ordered structures are the three-dimensional axial next-nearest-neighbor Ising (ANNNI) model[4] and its relatives or the chiral Potts model.[5]

A very simple extension of the conventional Ising model has been proposed[6] which involves a combination of competing two- and four-body interactions. In its simplest three-dimensional (3D) version it consists of planes with familiar nearest-neighbor Ising interactions ($J_2'$), whereas different planes are coupled by a combination of two-body ($J_2$) and four-body ($J_4$) interactions. This model is now known as a $(2+4)$ model and has been the subject of several recent investigations in 1D (quantum version)[6,7] and 2D.[8–10] In the following we will consider a 3D classical version only and the Hamiltonian reads (assuming $J_2' = J_2$)

$$\mathcal{H} = -J_2 \sum_{x,y,z} S_i S_{i+1} - J_4 \sum_z \left[ \prod_{j=0}^{3} S_{i+j} \right], \tag{1}$$

where $S_i$ are Ising variables ($S_i \pm 1$) on a simple-cubic lattice. The ordered structures of this model consist—as for the 3D ANNNI model—of a series of uniformly ordered (ferromagnetic) planes staggered in the $z$ direction. For $T=0$ an (anti-) ferromagnetic and a so-called $\langle 3,1 \rangle$ phase [also denoted by $(\uparrow\uparrow\uparrow\downarrow)$ or $\langle 111\bar{1} \rangle$] are present. The latter one is a modulated structure with period four and consists of sequences of three parallel orientated planes followed by a single plane with opposite orientation. These two phases are separated by a multiphase point at $-J_4/J_2 = 0.5$, where an infinity of modulated phases have the same energy. Note, such a point is also found in the ANNNI models.[4,11] There, an infinite number of distinct modulated phases emanate from that point which are stable at finite temperatures.

The model of Eq. (1) is not solved exactly until now and one has to resort to mean-field-type approximations to obtain an idea of the phase diagram and the orders of phase transitions. A conventional (Bragg-Williams) mean-field decoupling is not well suited to four-spin interactions because the strong nearest-neighbor correlations are completely neglected. An ingenious extension of the mean-field approximation to multispin interactions has been proposed by Debierre and Turban.[12] In the presence of an $m$-spin interaction a cluster of $(m-1)$ spins is solved exactly. In addition to the ordinary order parameter $m_i = \langle S_i \rangle$ a set of $(m-2)$ near-neighbor correlation functions is introduced. Thus $(m-1)$ variational parameters are present and determine the respective free energy of the system.

 

In the case of Eq. (1) it is convenient to perform the following decouplings:[12]

$$\begin{aligned} &J_2S_1S_i \to m_iJ_2(S_1-\tfrac{1}{2}m_1)\ , \\ &J_4S_1S_iS_jS_k \to \Theta_iJ_4(S_1-\tfrac{1}{2}m_1)\ , \\ &J_4S_1S_2S_iS_j \to \Phi_iJ_4(S_1S_2-\tfrac{1}{2}\Phi_1)\ , \\ &J_4S_1S_2S_3S_i \to m_iJ_4(S_1S_2S_3-\tfrac{1}{2}\Theta_1)\ , \end{aligned} \tag{2}$$

where $\Phi_i=\langle S_iS_{i+1}\rangle$ and $\Theta_i=\langle S_iS_{i+1}S_{i+2}\rangle$ are two- and three-body local correlation functions which have to be determined self-consistently. If we are looking for (commensurate) structures with periodicity $n$ in the $z$ direction the free energy of the three-spin cluster in this approximation is equal to

$$F=\frac{1}{n}\sum_{i=1}^{n}\left[\frac{z_0}{2}J_2(m_i^2+m_{i+1}^2+m_{i+2}^2)+\tfrac{1}{2}J_2(m_{i-1}m_i+m_{i+2}m_{i+3}) + \tfrac{1}{2}J_4[\Theta_{i-3}m_i+\Theta_{i+3}m_{i+2}+\Theta_i(m_{i-1}+m_{i+3})+\Phi_{i-2}\Phi_i+\Phi_{i+1}\Phi_{i+3}]-k_BT\ln Z_i^{(3)}\right]\ , \tag{3}$$

$z_0$ being the number of nearest neighbors in a plane ($z_0=4$), $Z_i^{(3)}$ the exact three-spin cluster partition function, and $k_B$ the Boltzmann constant.

For a given periodicity $n$ there are $3n$ coupled equations to be solved, and the equilibrium structure $\bar{n}$ is assumed to be given by

$$\bar{n}=\min_{\{n\}}F(n,T,J_2,J_4)\ , \tag{4}$$

similar as in other problems with competing interactions.[11] In two important cases the equations greatly simplify: (a) uniformly ordered [ferromagnetic (FM)] phase: $m_i=m$, $\Phi_i=\Phi$, and $\Theta_i=\Theta$ for all $i=1\ldots n$, and (b) disordered [paramagnetic (PM)] phase: $m_i=\Theta_i=0$; here the free energy depends on $\Phi$ only.

In order to explore the presence of different periodicities we have investigated various structures with particular emphasis on the FM phase and the $\langle 3,1\rangle$ phase produced by the $J_4$ term.[13] Besides these two phases we have looked for structures[14] of types $(n_\uparrow,n_\downarrow)$ and $(n_\uparrow,\downarrow)$ (or $\langle n,n\rangle$ and $\langle n,1\rangle$), $n\geq 3$. The former are known to appear in the phase diagram of the 3D ANNNI model.[4] To test our procedure we have calculated also the phase diagram of this model. We found almost identical results compared to those yielded with other methods.

In the following we shall present the results of computations of the phase diagram for the case $J_2>0$, $J_4<0$. (For $J_2<0$ the FM phase transforms into an antiferromagnetic phase without change of any transition line.) In Fig. 1 we present the phase diagram in the $(T,\kappa)$ plane, $\kappa=-J_4/J_2$. For $\kappa=0$ the critical temperature for the PM$\to$FM transition satisfies $T_c(\kappa=0)/J_2<6$, signaling a small improvement compared with the conventional mean-field approximation. For finite $\kappa$ the PM$\to$FM transition line is convex downwards. One can show that $T_c(\kappa)-T_c(0)=-a\kappa$, $a>0$ for small $\kappa$, as it should be, because a $J_4<0$ weakens the FM phase. For larger $\kappa$ the transition line exhibits a shallow minimum at $\kappa\approx 1$ and raises again with increasing $\kappa$. A Bragg-Williams approximation would yield a constant transition temperature. Unlike the 2D (Ref. 9) and the 1D quantum version of the (2+4) model,[6] but in accordance with the 3D ANNNI model,[4] the disordered (PM) phase does not extend down to $T=0$.

The FM phase passes over into the $\langle 3,1\rangle$ phase along a transition line starting vertically from the multiphase point at $\kappa=0.5$. In accordance with the results for the 2D version[6,8,9] *no other* phases are found to be stable. The FM phase penetrates between the PM and the $\langle 3,1\rangle$ phases, demonstrating the possibility of a transition from a high-temperature uniformly ordered to a low-temperature modulated phase. Such a feature is similar to one observed in an $S=1$ generalized ANNNI model.[11] Since this propery does not appear in 2D, it may well be characteristic for the 3D (2+4) model. In addition, the FM phase persists for large $\kappa$ but is metastable, whereas for the ANNNI model it disappears completely above a

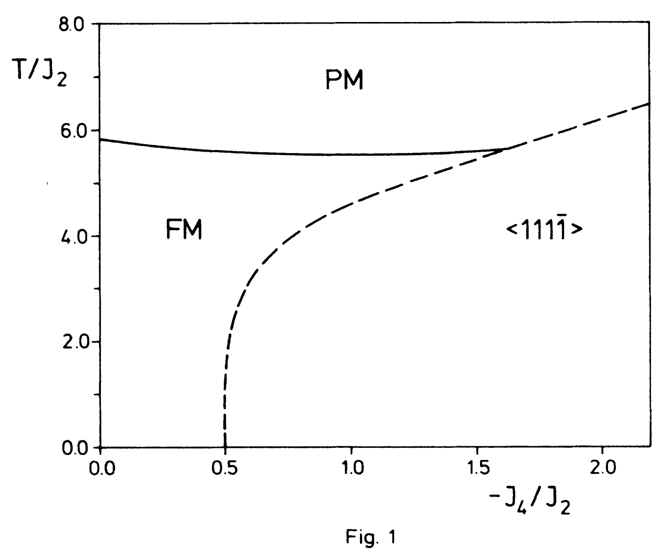


FIG. 1. Phase diagram of the 3D (2+4) model. PM denotes the disordered (paramagnetic) and FM the ferromagnetic phase. The $\langle 3,1\rangle$ or $\langle 111\bar{1}\rangle$ phase is a periodic structure consisting of three parallel orientated planes followed by a single one with opposite orientation. The solid line refers to a second-order transition, the dashed line to a first-order transition.

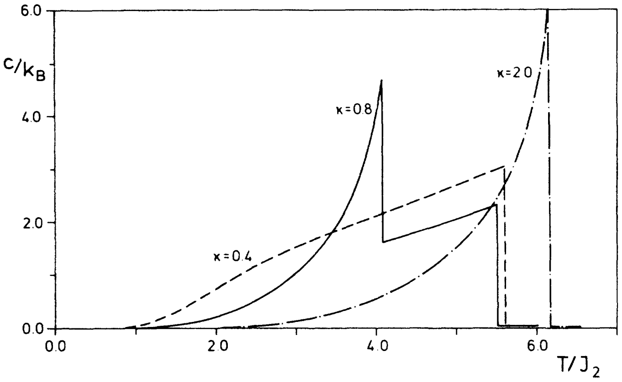


FIG. 2. Specific heat $c/k_B$ as a function of temperature for three distinct values of $\kappa=-J_4/J_2$. Note the different orders of transition.

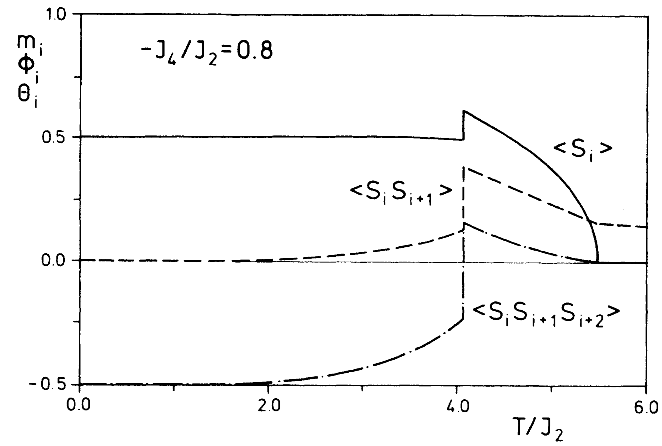


FIG. 3. Order parameters $m_i=\langle S_i\rangle$ and local correlation functions $\Phi_i=\langle S_iS_{i+1}\rangle$ and $\Theta_i=\langle S_iS_{i+1}S_{i+2}\rangle$ as a function of temperature for $\kappa=-J_4/J_2=0.8$. In the case of modulated phases the average over a period is given.

certain value of $\kappa$.

The transition line between the disordered and the FM phase is second order, whereas the transitions from PM and FM phases to the $\langle 3,1\rangle$ phase are *always* first order. This is clearly seen in Fig. 2 where the specific heat is plotted as a function of temperature and different $\kappa$. For instance, for $\kappa=0.8$ we see both transitions: the first-order one with a $\delta$-function-like singularity ($\langle 3,1\rangle\rightarrow$FM), the second-order one shows a discontinuity (FM$\rightarrow$PM). In Fig. 3 we present the behavior of the three correlation functions $m(T)$, $\Phi(T)$, and $\Theta(T)$ for $\kappa=0.8$. All of them exhibit strong discontinuities at the first-order transition temperature. (It is worth noting that $\Phi$ and $\Theta$ cannot be obtained within the conventional mean-field approximation.) The point where all three phases merge looks like some sort of bicritical point where first- and second-order transition lines meet with a discontinuous slope of the transition line at that point.[15]

In summary we have shown that the 3D $(2+1)$ model exhibits only two ordered phases. The order-disorder transition temperature is always finite, but the order of transition changes from first to second order. We expect the generalized mean-field approximation to yield a qualitatively correct phase diagram. However, application to 2D would yield a similar diagram, which is obviously not correct.

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[14]The two chosen subsets of modulated structures are reasonable but evidently not complete. Since none of these investigated phases appears to be stable, we concluded that other types of stable modulated structures do not exist either.

[15]Note that this point is *not* a conventional Lifshitz point [R. M. Hornreich, M. Luban, and S. Shtrikman, Phys. Rev. Lett. **35**, 1678 (1975)] which occurs, e.g., in the 3D ANNNI model,[4] as in our model no phases with continuously varying wave number occur.