# Exact results of a generalized Wu model with two- and four-spin interactions

Silvia Lacková and Michal Jaščur*
*Department of Theoretical Physics and Geophysics, Faculty of Science, P. J. Šafárik University, Moyzesova 16, 041 54 Košice, Slovak Republic*
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The mixed spin-1/2 and spin-$S_B$ Ising model with two- and four-spin interactions on the honeycomb lattice is studied by the use of a generalized star-triangle transformation. The exact results for the phase diagrams, magnetization, correlation functions, internal energy, specific heat, and quadrupolar susceptibility are obtained and discussed.

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## I. INTRODUCTION

During the last two decades, there has been an increasing interest in studying Ising models with multispin interactions. The influence of multispin interactions on critical properties of various models has been theoretically studied within different methods such as the exact calculations [1–4], series expansions [5,6], renormalization-group techniques [7], and Monte Carlo simulations [8,9]. Except these accurate treatments, less sophisticated mean-field and effective-field methods have been also used to investigate the multispin effects in these systems [10–12]. Although the approximate methods usually provide rather good qualitative description of the systems with pair interactions, they can completely fail in the case of the systems with multispin interactions [13]. For this reason, the exactly solvable systems play very important role in understanding of the multispin effects. From the experimental point of view, the models with multispin interactions can be applied to various physical problems such as binary alloys [8], classical fluids [14], solid $^3$He [15], lipid bilayers [16], metamagnets [17], and rare gases [18]. Another interesting application of the model with four-spin interactions represents the paper by Chunlei [19] in which the thermodynamic properties of hydrogen bonded ferroelectrics $PbHPO_4$ and $PbDPO_4$ have been studied. Moreover, the models with four-spin interactions have been used to describe the first-order phase transition in squaric acid crystal ($H_2C_2O_4$) [10,20], as well as, in some copolymers [21]. One should notice that the authors of these studies have obtained good agreement of their theoretical predictions with the experiments. Except above-mentioned applications, we would like particularly to emphasize the recent experimental works by Köbler *et al.* [22] who have significantly contributed to our understanding of the higher-order interactions in magnetic systems. In general, the models with multispin interactions may exhibit physical peculiarities, for example, the nonuniversal critical behavior [2,3] or deviations from the Bloch's $T^{3/2}$ law at low temperatures [22].

Despite the fact that the models with higher-order interactions are much more complicated then their counterparts with pair interactions, surprisingly some of these models are exactly solvable [1–4]. One of the simplest models of this kind is a two-sublattice Ising model with pair and four-spin interaction originally introduced by Wu [1]. In this work, we will generalize this model including a crystal field and arbitrary spins $S_B$ on one sublattice, while the spins on the second one will be fixed ($S_A = 1/2$).

The outline of the present paper is as follows. In Sec. II, the relations for various physical quantities of the model with two- and four-spin interactions are derived. The most interesting numerical results are discussed in Sec. III. Finally, our main conclusions are summarized in Sec. IV.

## II. FORMULATION

In this work, we will study a mixed spin-1/2 and spin-$S_B$ Ising model on the honeycomb lattice consisting of two sublattices $A$ and $B$ that are occupied by the atoms with the spin $S_A = 1/2$ and $S_B \geqslant 1/2$, respectively. In addition to the conventional two-spin nearest-neighbor interactions — $JS_k(\mu_{k1} + \mu_{k2} + \mu_{k3})$, we consider also four body interactions — $J_4 S_k \mu_{k1}\mu_{k2}\mu_{k3}$ among any set of four spins within a unit cell of the dashed triangle as it is depicted in Fig. 1.

The Hamiltonian of the system can be written in the form

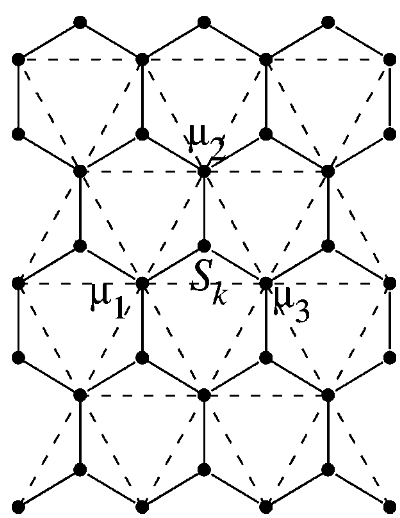


FIG. 1. Part of the honeycomb lattice representing the generalized Wu model. Spins in the center of the dashed triangle interact with their three neighbors with the pair interactions $J$ and four-spin interaction $J_4$.

*Email: jascur@kosice.upjs.sk

 

$$\mathcal{H}_h = \sum_{k \in B} \mathcal{H}_k, \tag{1}$$

where the summation is over all sites of the $B$ sublattice and the site Hamiltonian $\mathcal{H}_k$ is given by

$$\mathcal{H}_k = -J(\mu_{k1}+\mu_{k2}+\mu_{k3})S_k - J_4\mu_{k1}\mu_{k2}\mu_{k3}S_k - D(S_k)^2, \quad J>0. \tag{2}$$

In Eq. (2), the first term describes the interactions between pairs of nearest-neighbor spins, the second term represents the four-spin interaction, and the last one describes the crystal field effects on $B$ atoms only. The spin variables $\mu_{k\alpha}$ take, on the sublattice $A$, the values of $\pm 1/2$ and $S_k$, on the sublattice $B$, run over $(2S_B+1)$ values allowed for $B$ atoms with the spin $S_B$. It is easy to see that for the particular case of $J_4=0$ our model reduces to the standard mixed-spin Ising model on the honeycomb lattice, which has been exactly solved by Goncalves [23]. On the other hand, for the case of $S_B=1/2$ and $J_4 \neq 0$ we obtain the model that has originally been introduced and discussed by Wu [1]. Owing to this connection, the present model will be reffered to as the generalized Wu model.

The most important point of our calculations is the following extended star-triangle (or $Y-\Delta$) transformation (see [24] and references therein):

$$\sum_{S_k=-S_B}^{S_B} \exp[\beta J(\mu_{k1}+\mu_{k2}+\mu_{k3})S_k + \beta J_4\mu_{k1}\mu_{k2}\mu_{k3}S_k + \beta D(S_k)^2] = A\exp[\beta R(\mu_{k1}\mu_{k2}+\mu_{k1}\mu_{k3}+\mu_{k2}\mu_{k3})]. \tag{3}$$

In this transformation $A$ and $R$ represent unknown parameters of the relevant triangular lattice that can be expressed in the form [24]

$$A^4 = V_1V_2^3, \quad \beta R = \ln\frac{V_1}{V_2}, \tag{4}$$

where we have defined the functions $V_1$ and $V_2$,

$$V_1 = \sum_{n=-S_B}^{S_B} \exp(\beta D n^2)\cosh\left[\frac{n\beta J}{8}(12+\alpha)\right],$$

$$V_2 = \sum_{n=-S_B}^{S_B} \exp(\beta D n^2)\cosh\left[\frac{n\beta J}{8}(4-\alpha)\right], \quad \alpha = J_4/J. \tag{5}$$

In this way, the generalized Wu model has been transformed into the exactly solvable spin-1/2 Ising model on the triangular lattice. One should notice that the transformation (4) is rather general since it is valid for arbitrary spin values $S_B$, however, it is limited topologically. After putting the critical temperature of the spin-1/2 Ising model on the triangular lattice ($\beta_c R = R/k_B T_c = \ln 3$) into Eq. (4), we obtain the phase boundaries of the generalized Wu model, which satisfy the relation

$$\sum_{n=-S_B}^{S_B} \exp(\beta_c D n^2)\left\{3\cosh\left[\frac{n\beta_c J}{8}(4-\alpha)\right] - \cosh\left[\frac{n\beta_c J}{8}(12+\alpha)\right]\right\} = 0. \tag{6}$$

From this equation one can find the dependences of the critical temperature on the four-spin interaction and the crystal field parameter for arbitrary values of the spin $S_B$. Moreover, the straightforward application of Eq. (3) relates the partition function of the generalized Wu model ($\mathcal{Z}_h$) to the partition function of the spin-1/2 Ising model on the triangular lattice ($\mathcal{Z}_t$) by

$$\mathcal{Z}_h(\beta J, \beta J_4, \beta D) = A^{N/2}\mathcal{Z}_t(\beta R), \tag{7}$$

where the parameters $A$ and $R$ obviously satisfy Eq. (4) and $N$ denotes the total number of the spins on the honeycomb lattice.

In adition to the phase boundaries, we can also simply calculate some interesting physical quantities. For example, the magnetization and internal energy of the system can be directly expressed through the mean values of the spin variables (or correlation functions). Namely,

$$M_h = \frac{1}{2}(m_A+m_B),$$

$$m_A \equiv \langle \mu_{kl} \rangle_h = \frac{\mathrm{Tr}\,\mu_{kl}\exp(-\beta\mathcal{H}_h)}{\mathrm{Tr}\exp(-\beta\mathcal{H}_h)},$$

$$m_B \equiv \langle S_k \rangle_h = \frac{\mathrm{Tr}\,S_k\exp(-\beta\mathcal{H}_h)}{\mathrm{Tr}\exp(-\beta\mathcal{H}_h)}, \tag{8}$$

and

$$U_h = -\frac{J}{2}\langle S_k(\mu_{k1}+\mu_{k2}+\mu_{k3})\rangle_h - \frac{J_4}{2}\langle S_k\mu_{k1}\mu_{k2}\mu_{k3}\rangle_h - \frac{D}{2}\langle (S_k)^2\rangle_h, \tag{9}$$

where $M_h$ and $U_h$ denote the magnetization and the internal energy per one site of the generalized Wu model, respectively, and the symbol $\langle \cdots \rangle_h$ means the standard ensemble average for the system described by the Hamiltonian (1). At this stage, the main mathematical difficulty is to calculate the spin correlations included in Eqs. (8) and (9). Fortunately, these correlations can be easily obtained from the following exact Callen-Suzuki-type identity [25]

$$\langle (S_k)^p f_k \rangle_h = \left\langle f_k \frac{\sum_{S_k=-S_B}^{S_B} (S_k)^p \exp(-\beta\mathcal{H}_k)}{\sum_{S_k=-S_B}^{S_B} \exp(-\beta\mathcal{H}_k)} \right\rangle h, \quad p=1,2, \tag{10}$$

where $\mathcal{H}_k$ is given by Eq. (2) and $f_k$ represents a function of arbitrary spin variables except $S_k$. After applying one of the standard methods (for example, the differential operator technique [26]) one gets the remaining quantities in Eqs. (8) and (9)

$$m_B \equiv \langle S_k \rangle_h = 6K_1 \langle \mu_{k1} \rangle_h + 8K_3 \langle \mu_{k1}\mu_{k2}\mu_{k3} \rangle_h \quad \text{for} \quad p=1, \quad f_k=1, \tag{11}$$

$$q \equiv \langle (S_k)^2 \rangle_h = K_0 + 12K_2 \langle \mu_{k1}\mu_{k2} \rangle_h \quad \text{for} \quad p=2, \quad f_k=1, \tag{12}$$

$$\rho_h \equiv \langle S_k \mu_{k1} \rangle_h = \frac{K_1}{2} + (4K_1 + 2K_3)\langle \mu_{k1}\mu_{k2} \rangle_h \quad \text{for} \quad p=1, \quad f_k=\mu_{k1}, \tag{13}$$

$$q_4 \equiv \langle S_k \mu_{k1}\mu_{k2}\mu_{k3} \rangle_h = \frac{3K_1}{2}\langle \mu_{k1}\mu_{k2} \rangle_h + \frac{K_3}{8} \quad \text{for} \quad p=1, \quad f_k=\mu_{k1}\mu_{k2}\mu_{k3}. \tag{14}$$

The coefficients $K_0 - K_3$ depend on the exchange parameters, the crystal field and the spin value, and they are given by

$$K_0 = \frac{1}{4}[G_{S_B}(3J/2 + \alpha J/8) + 3G_{S_B}(J/2 - \alpha J/8)],$$

$$K_1 = \frac{1}{4}[F_{S_B}(3J/2 + \alpha J/8) + F_{S_B}(J/2 - \alpha J/8)],$$

$$K_2 = \frac{1}{4}[G_{S_B}(3J/2 + \alpha J/8) - G_{S_B}(J/2 - \alpha J/8)],$$

$$K_3 = \frac{1}{4}[F_{S_B}(3J/2 + \alpha J/8) - 3F_{S_B}(J/2 - \alpha J/8)], \tag{15}$$

where the functions $G_{S_B}(x)$ and $F_{S_B}(x)$ have been defined as

$$G_{S_B}(x) = \frac{\sum_{n=-S_B}^{S_B} n^2 \exp(n^2 \beta D)\cosh(\beta n x)}{\sum_{n=-S_B}^{S_B} \exp(n^2 \beta D)\cosh(\beta n x)} \tag{16}$$

and

$$F_{S_B}(x) = \frac{\sum_{n=-S_B}^{S_B} n \exp(n^2 \beta D)\sinh(\beta n x)}{\sum_{n=-S_B}^{S_B} \exp(n^2 \beta D)\cosh(\beta n x)}. \tag{17}$$

To complete our calculations, we have to find out the spin correlations on the r.h.s of Eqs. (11)–(14). Because all these correlations include only the spins of the sublattice $A$, we may determine them directly from the definition. In fact, using the transformation (3) one easily proves the equality [27]

$$\langle f(\mu_{ki}, \mu_{kj}, \ \ldots, \ \mu_{k\ell}) \rangle_h = \langle f(\mu_{ki}, \mu_{kj}, \ \ldots, \ \mu_{k\ell}) \rangle_t, \tag{18}$$

where $f$ represents a function that depends only on the spin variables $\mu_{ki}$ of the sublattice $A$. The subscripts $h$ and $t$ mean that the relevant averaging is related to the honeycomb and triangular lattice, respectively. Consequently, from Eq. (18) one obtains relations

$$\langle \mu_{k1} \rangle_h = \langle \mu_{k1} \rangle_t, \quad \langle \mu_{k1}\mu_{k2} \rangle_h = \langle \mu_{k1}\mu_{k2} \rangle_t,$$
$$\langle \mu_{k1}\mu_{k2}\mu_{k3} \rangle_h = \langle \mu_{k1}\mu_{k2}\mu_{k3} \rangle_t, \tag{19}$$

that complete our calculations, since the spin correlations on the triangular lattice are well known [27]. Apart from the quantities discussed above, we are also able to get the specific heat and the quadrupolar susceptibility of the system under investigation that are, respectively, defined as follows:

$$C_h = \left(\frac{\partial U_h}{\partial T}\right), \quad \chi_T = \left(\frac{\partial q}{\partial D}\right)_T. \tag{20}$$

## III. NUMERICAL RESULTS AND DISCUSSION

We start our discussion with the investigation of the ground-state properties of the generalized Wu model. It is worth noticing that in addition to the ground-state energy $U_h$, we will also analyze the exchange parameter $R$ for $T \to 0$ because the spin configurations on the sublattice $A$ and consequently also the number of possible phases essentially depend on the sign of $R$. At first, we summarize our findings for integer values of $S_B$. In this case we have found that if $D/J \geqslant -1$ then the exchange parameter $R$ changes its sign as follows:

$$R > 0 \quad \text{for} \quad \alpha > -4,$$
$$R = 0 \quad \text{for} \quad \alpha = -4,$$
$$R < 0 \quad \text{for} \quad \alpha < -4. \tag{21}$$

On the other hand, for $D/J < -1$ we have

$$R > 0 \quad \text{for} \quad \alpha > -8D/J - 12,$$
$$R = 0 \quad \text{for} \quad 12D/J + 4 \leqslant \alpha \leqslant -8D/J - 12,$$
$$R < 0 \quad \text{for} \quad \alpha < 12D/J + 4. \tag{22}$$

Already at this stage it is clear that in the regions of positive values of $R$, the ground state of our system will be ordered. In the regions where $R=0$, we expect the appearance of the paramagnetic phase ($D_1$) and finally, for $R<0$ a more complicated disordered phase ($D_2$) can be observed since in this case our model is transformed on the antiferromagnetic triangular lattice. A simple examination of the possible spin configurations reveals the existence of $2S_B$ ordered phases

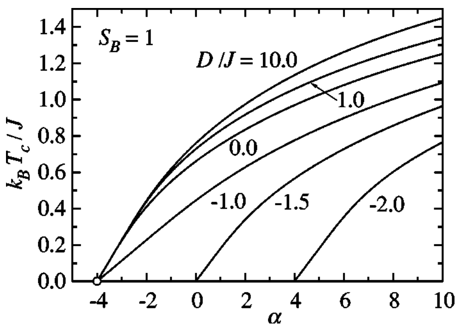


FIG. 2. Phase diagrams of the generalized Wu model with two- and four-spin interactions for $S_B=1$ and different values of the crystal-field parameter $D/J$.

(to be denoted as $O_1, O_2, \ldots, O_{2S_B}$). All these phases are ferromagnetic ones with $m_A=1/2$ and different values of $m_B$ that depend on the crystal field and four-spin interactions. The regions of stability for the relevant ordered phases can be found in the usual way, i.e., by comparing their ground-state energies. In order to clarify the behavior of the ground-state phases, we will now analyze one representative case with $S_B>1$. This choice is related to the fact that for $S_B>1$ more than three ordered phase appear in the system that allows one to make very general conclusions. For the sake of simplicity, we will investigate only the stability of three typical ferromagnetic phases $O_1$, $O_2$, and $O_3$ that are present in any system with $S_B>1$. According to our notation, the sublattice magnetization $m_B$ of these phases is, respectively, given by $m_B(O_1)=S_B$, $m_B(O_2)=S_B-1/2$ and $m_B(O_3)=S_B-1$. Similarly, the ground-state energies of these phases are given by

$$U_h(O_1)=-3JS_B/4-J_4S_B/16-DS_B^2/2,$$

$$U_h(O_2)=-3J(2S_B-1)/8-J_4(2S_B-1)/32 -D(S_B^2-S_B+1/2)/2,$$

or

$$U_h(O_3)=-3J(S_B-1)/4-J_4(S_B-1)/16-D(S_B-1)^2/2.$$

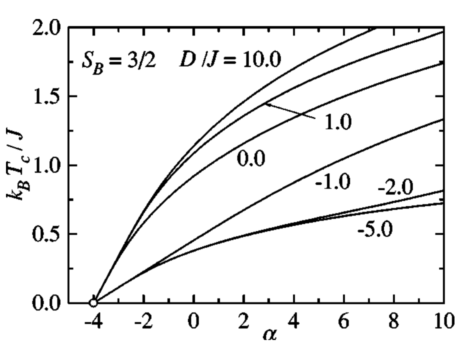


FIG. 3. Phase diagrams of the generalized Wu model with two- and four-spin interactions for $S_B=3/2$ and different values of the crystal-field parameter $D/J$.

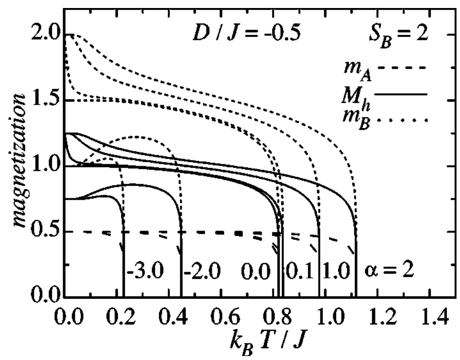


FIG. 4. Temperature dependences of the total magnetization $M_h$ (full lines), sublattice magnetization $m_A$ (dashed lines), and $m_B$ (dotted lines) for the generalized Wu model with $D/J=-0.5$ and different values of the four-spin interaction.

By comparing $U_h(O_1)$, $U_h(O_2)$, and $U_h(O_3)$ one finds that for $\alpha>-12+8(1-2S_B)D/J$ is the stable phase $O_1$, for $\alpha<-12+8(1-2S_B)D/J$ is the stable phase $O_3$, and for $\alpha=-12+8(1-2S_B)D/J$ all three phases coexist, thus a first-order phase transition is possible. Of course, the similar behavior appears also at lower values of $\alpha$ where other phases ($O_4$, $O_5, \ldots$) become stable (or coexist). It is also clear that if we make the four-spin interaction weak enough a disordered phase will appear in the system. In fact, in agreement with Eqs. (21) and (22) one finds in the relevant regions the paramagnetic phase $D_1$ or another disordered phase $D_2$, which is expected to manifest different physical properties in comparison with the standard paramagnet. Moreover, one can expect that the disordered phase $D_2$ can also exist at finite temperatures. This implies the possibility of a phase transition between $D_1$ and $D_2$. We believe that this conjecture can be verified by Monte Carlo simulations in the relevant region.

To complete our considerations, we would like to emphasize that the foregoing discussion is fully applicable also for the generalized Wu model with arbitrary half-integer values of $S_B$ taking into account a small modification. Namely, we have to account for the fact that in the case of half-integer values of $S_B$ the sign of the parameter $R$ is given by Eq. (21), regardless of the value of $D$.

Now, we will proceed further with the investigation of the finite-temperature phase diagrams of generalized Wu model.

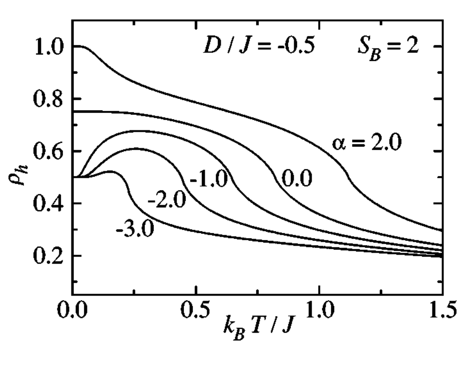


FIG. 5. Temperature variations of the two-spin correlation function $\rho_h$ for the same parameters as in Fig. 4.

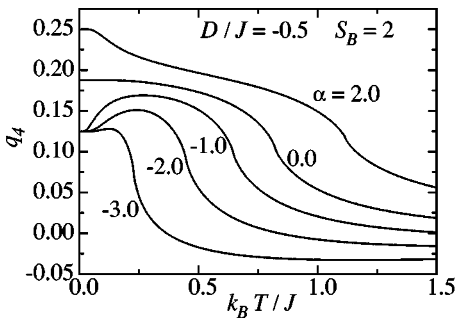


FIG. 6. Temperature variations of the four-spin correlation function $q_4$ for the same parameters as in Fig. 4.

In order to illustrate typical phase boundaries, we have depicted in Figs. 2 and 3 the dependences of the critical temperature $k_B T_c/J$ versus $\alpha$ for selected values of $D/J$. Since the phase diagrams depend also on the spin $S_B$, we have analyzed two representative systems, namely, $S_B = 1$ and $S_B = 3/2$. As we can see, the critical temperature in both cases decreases monotonically from its maximum value (at $\alpha \to \infty$) and vanishes at a certain characteristic value of the parameter $\alpha$ (to be denoted as $\alpha_0$). We have found that in the case of $S_B = 1$ the parameter $\alpha_0$ is given by

$$\alpha_0 = \begin{cases} -4 & \text{for} \quad D/J \geqslant -1 \\ -8D/J - 12 & \text{for} \quad D/J < -1 , \end{cases} \tag{23}$$

and in the case of half-integer values of $S_B = 3/2$ we have obtained $\alpha_0 = -4$ for arbitrary values of the crystal-field parameter. Here one should notice that the values of $\alpha_0$ for $S_B = 1$ and $S_B = 3/2$ are, respectively, valid for arbitrary integer and half-integer values of $S_B$ and they are in agreement with the ground-state analysis. We have also observed that further increase of $S_B$ does not bring any qualitative results for the system. In fact, it is easy to verify that the systems with integer values of $S_B$ ($S_B \geqslant 2$) exhibit qualitatively the same behavior as the system with $S_B = 1$ and the systems with half-integer values of $S_B$ ($S_B \geqslant 5/2$) display very similar behavior as that with $S_B = 3/2$. One should also mention that the model under investigation belongs to the same universality class as the usual spin-1/2 planar Ising model.

In addition to the phase diagrams, we have also studied the temperature dependences of some thermodynamic quantities and we have obtained some interesting results that can not be observed in the original Wu's model. In order to demonstrate these findings, we have selected the system with $S_B = 2$ in which all characteristic behaviors are clearly manifested. At first in Fig. 4, the thermal variations of the sublattice and total magnetization are shown for $D/J = -0.5$. The corresponding two- and four-spin correlation functions are depicted in Figs. 5 and 6. As one can see, the sublattice magnetization $m_A$ exhibits the standard dependence that is usually observed in the planar Ising model with pair interactions only. On the other hand, the sublattice magnetization $m_B$ displays for negative values of $\alpha$ a broad maximum at low-temperature region. The phenomenon is clearly related

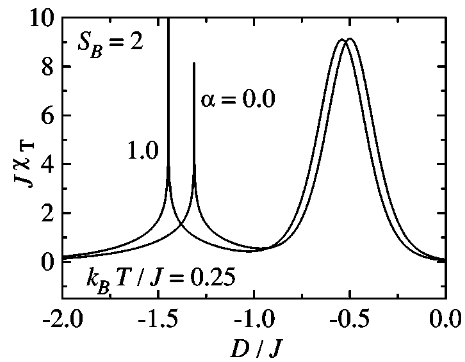


FIG. 7. Crystal-field dependences of the quadrupolar susceptibility $\chi_T$ for $S_B = 2$, $k_B T/J = 0.25$ and two values of $\alpha$ ($\alpha = 0.0$, $\alpha = 1.0$).

to the thermal spin excitations on the sublattice $B$. These excitations, in fact, form the characteristic dependences of the total magnetization (see Fig. 4) and those of the correlation functions (see Figs. 5 and 6).

Finally, in Fig. 7, the quadrupolar susceptibility $\chi_T$ as a function of the crystal-field parameter $D/J$ for $\alpha = 0.0$ and $\alpha = 1.0$ has been plotted at the fixed temperature $k_B T/J = 0.25$. The results indicate that $\chi_T$ diverges at critical point (similarly as the longitudinal susceptibility) and has a sharp peak (maximum) in the region of abrupt spin excitations on the sublattice $B$. Thus the behavior of the quadrupolar susceptibility can be used to identify the second-order phase transition at finite temperatures, as well as, the first-order phase transition at the ground state.

## IV. CONCLUSION

In this work, we have studied the generalized Wu model with two- and four-spin interactions. Applying the standard star-triangle transformation, we have derived the exact equations for the phase diagrams and other relevant thermodynamic quantities. Apart from the trivial finding of the universality in the critical region, we have also obtained some interesting results far from the criticality. As we have discussed in the previous sections, some of the results differ from those of the standard planar Ising models and the physical origin of the effects follows from the competition between the crystal field, exchange interactions, and temperature.

Although the present calculations provide the complete exact solution to the model, there still remain some open problems, for example, the existence of two different disordered phases. Despite the fact that we have presented some arguments that support this idea, the problem requires further investigation and we assume that it can be definitely resolved using large-scale Monte Carlo simulations.

## ACKNOWLEDGMENT

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