Transverse Ising model with arbitrary spin

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An effective-field theory that has recently been used for studying higher-spin Ising models is herein extended to the transverse Ising model with an arbitrary spin S. The general formulation for evaluating the transition line in the Ω-T space and relevant statistical-mechanical quantities is derived. Numerical results are performed and analyzed for the particular cases $S=\frac{3}{2}$ and $S=2$.

I. INTRODUCTION

The Ising model with a transverse field Ω is described by the Hamiltonian

$$\mathcal{H}=-\tfrac{1}{2}\sum_{i,j} J_{ij}S_i^zS_j^z-\Omega\sum_i S_i^x \ , \tag{1}$$

where the S_i^x, S_i^z are the components of quantum spin-S operators, J_{ij} is the exchange interaction, and the first summation is over all nearest-neighbor pairs.

The model (1) for the case $S=\frac{1}{2}$ has been extensively investigated for many years by the use of various techniques. In fact, the model is useful for the study of cooperative phenomena and phase transitions in many systems including order-disorder ferroelectrics, induced moment ferromagnets, and cooperative Jahn-Teller systems (see Ref. 1 and references therein). On the other hand, transverse Ising models for spin S higher than $S=\frac{1}{2}$ have also received some attention, especially for $S=1$. As far as we know, however, only a few works have made contact with the quantum transverse spin-S Ising model.[2,3] Very recently, we have introduced a framework for treating Ising systems with higher-spin values.[4] The formulation can be extended to the spin-S transverse Ising model.

In this work, we shall discuss via the formulation the transverse Ising models with an arbitrary spin S on the basis of generalized but approximated Callen relation, derived by Sá Barreto, Fittipaldi, and Zeks.[5] The relation has been successfully applied to a number of interesting physical systems, such as (pure or disordered) spin-$\frac{1}{2}$, spin-1 (Refs. 6 and 7) or mixed spin-$\frac{1}{2}$ and spin-1 (Ref. 8) transverse Ising models. The outline of this paper is as follows. The formulation of the problem is given in Sec. II. The relations for obtaining phase diagram, magnetization curves, internal energy, and specific heat are presented in Sec. III. Finally, some numerical results are discussed in Sec. IV.

II. FORMULATION

The starting point for the statistics of our spin system is the relation proposed by Sá Barreto, Fittipaldi, and Zeks;[5]

$$\langle f_i A_i\rangle=\left\langle f_i\frac{\mathrm{Tr}_{\{i\}}A_i\exp(-\beta\mathcal{H}_i)}{\mathrm{Tr}_{\{i\}}\exp(-\beta\mathcal{H}_i)}\right\rangle \ ; \quad \beta=\frac{1}{k_BT} \ , \tag{2}$$

where the operator A_i is a spin operator function at a site i, and $\mathrm{Tr}_{\{i\}}$ denotes to take a partial trace for the site i. f_i represents an arbitrary function of spin variables except S_i^z and S_i^x at a site i and $\langle \cdots \rangle$ denotes the canonical ensemble average. Then, the total Hamiltonian (1) is separated into two parts:

$$\mathcal{H}=\mathcal{H}_i+\mathcal{H}' \ , \tag{3}$$

where $\mathcal{H}_i$ includes all the parts of $\mathcal{H}$ associated with the site i, and $\mathcal{H}'$ represents the rest of the Hamiltonian and does not depend on any spin operators of the site i. Although relation (2) has been derived approximately, we emphasize that it reproduces the exact identity for the Ising limit ($\Omega=0$) and the approximation introduced reveals it to be very appropriate for high dimensional lattice.[5-8]

By the use of (2), the longitudinal and transverse site magnetizations for the spin-S transverse Ising model are given by, on putting $f_i=1$,

$$\langle S_i^z\rangle=\left\langle\frac{\theta_i}{E_i}f_S(\theta_i)\right\rangle \ , \tag{4}$$

$$\langle S_i^x\rangle=\left\langle\frac{\Omega}{E_i}f_S(\theta_i)\right\rangle \ , \tag{5}$$

with

$$\theta_i=\sum_j J_{ij}S_j^z \tag{6}$$

and

$$E_i=\sqrt{\Omega^2+\theta_i^2} \ , \tag{7}$$

where the function $f_S(x)$ depends on the value of S. The explicit form of $f_S(x)$ can be found by means of the way described in the Appendix. This is to say, it is given by

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$$
\begin{aligned}
f_S(x)&=\tfrac{1}{2}\tanh(\tfrac{1}{2}\beta y) \quad \text{for } S=\tfrac{1}{2}\ ,\\
f_S(x)&=\frac{2\sinh(\beta y)}{2\cosh(\beta y)+1} \quad \text{for } S=1\ ,\\
f_S(x)&=\frac{3\sinh(\frac{3}{2}\beta y)+\sinh(\frac{1}{2}\beta y)}{2\cosh(\frac{3}{2}\beta y)+2\cosh(\frac{1}{2}\beta y)} \quad \text{for } S=\tfrac{3}{2}\ ,\\
f_S(x)&=\frac{4\sinh(2\beta y)+2\sinh(\beta y)}{2\cosh(2\beta y)+2\cosh(\beta y)+1} \quad \text{for } S=2\ ,
\end{aligned}
\tag{8}
$$

and so on, where the parameter y is defined by

$$y=\sqrt{\Omega^2+x^2}\ . \tag{9}$$

At this place, one should notice that the standard mean-field theory is given by replacing the operator θ_i in (4) and (5) with the averaged value $\langle\theta_i\rangle$;

$$\langle S_i^z\rangle=\frac{\langle\theta_i\rangle}{\bar{E}_i}f_S(\langle\theta_i\rangle)\ , \tag{10}$$

$$\langle S_i^x\rangle=\frac{\Omega}{\bar{E}_i}f_S(\langle\theta_i\rangle)\ , \tag{11}$$

with

$$\bar{E}_i=\sqrt{\Omega^2+(\langle\theta_i\rangle)^2}\ . \tag{12}$$

As discussed for spin-$\frac{1}{2}$ and spin-1 (Refs. 6 and 7) transverse Ising models, Eqs. (4) and (5) can be rewritten, by introducing the differential operator technique, as

$$\langle S_i^z\rangle=\langle\exp(\theta_i\nabla)\rangle F_S(x)|_{x=0} \tag{13}$$

and

$$\langle S_i^x\rangle=\langle\exp(\theta_i\nabla)\rangle H_S(x)|_{x=0}\ , \tag{14}$$

where $\nabla=\partial/\partial x$ is a differential operator and the functions $F_S(x)$ and $H_S(x)$ are defined by

$$F_S(x)=\frac{x}{\sqrt{\Omega^2+x^2}}f_S(x)\ , \tag{15}$$

$$H_S(x)=\frac{\Omega}{\sqrt{\Omega^2+x^2}}f_S(x)\ . \tag{16}$$

Now, for spin-$\frac{1}{2}$ and spin-1 transverse Ising models the expectation value $\langle\exp(\theta_i\nabla)\rangle$ has been transformed into a convenient form for the mathematical treatments by introducing the exact Van der Waerden identity, such as

$$\exp(aS_i^z)=\cosh\left[\frac{a}{2}\right]+2S_i^z\sinh\left[\frac{a}{2}\right] \quad \text{for } S=\tfrac{1}{2}\ , \tag{17}$$

where a is a parameter. However, for a general spin S higher than $S=1$ the Van der Waerden identity has a complicated form and hence the mathematical treatment becomes extremely complicated when it is introduced into (13) and (14). Furthermore, the exact Van der Waerden identity has a form depending on S and hence the formulation must be given in a form depending on S, as noted in Refs. 4 and 11. In the previous work,[4] therefore, we have introduced the generalized but approximated Van der Waerden identity, namely

$$\exp(aS_i^z)=\cosh(\eta a)+\frac{S_i^z}{\eta}\sinh(\eta a)\ , \tag{18}$$

with

$$\eta^2\equiv\langle(S_i^z)^2\rangle\ , \tag{19}$$

which is valid for any spin value S. In particular, for $S=\frac{1}{2}$ (18) reduces to the exact one (17), since the parameter η is given by $\eta=\frac{1}{2}$. In fact the framework based on (18) has given reasonable results for various physical quantities in comparison with those based on the exact Van der Waerden identities.[4,9] Thus, (13) and (14) can be transformed, by the use of (18), into the forms

$$\langle S_i^z\rangle=\left\langle\prod_j\left[\cosh(J_{ij}\eta\nabla)+\frac{S_j^z}{\eta}\sinh(J_{ij}\eta\nabla)\right]\right\rangle F_S(x)|_{x=0}\ , \tag{20}$$

$$\langle S_i^x\rangle=\left\langle\prod_j\left[\cosh(J_{ij}\eta\nabla)+\frac{S_j^z}{\eta}\sinh(J_{ij}\eta\nabla)\right]\right\rangle H_S(x)|_{x=0}\ . \tag{21}$$

On the other hand, for a spin S higher than $S=\frac{1}{2}$ one has to evaluate the parameter η. It can be derived in the same way as $\langle S_i^z\rangle$ and $\langle S_i^x\rangle$ by the use of (2);

$$
\begin{aligned}
\eta^2&\equiv\langle(S_i^z)^2\rangle\\
&=\langle\exp(\theta_i\nabla)\rangle G_S(x)|_{x=0}\\
&=\left\langle\prod_j[\cosh(J_{ij}\eta\nabla)+(S_j^z/\eta)\sinh(J_{ij}\eta\nabla)]\right\rangle G_S(x)|_{x=0}\ .
\end{aligned}
\tag{22}
$$

Here, the function $G_S(x)$ also depends on the spin value S and for $S=1$, $\frac{3}{2}$, and 2 it is, respectively, given by

$$
\begin{aligned}
G_S(x)&=\frac{\Omega^2+(x^2+y^2)\cosh(\beta y)}{[1+2\cosh(\beta y)]y^2}\ ,\\
G_S(x)&=\frac{3(y^2+2x^2)\cosh(\frac{3}{2}\beta y)+(y^2+6\Omega^2)\cosh(\frac{1}{2}\beta y)}{[4\cosh(\frac{3}{2}\beta y)+4\cosh(\frac{1}{2}\beta y)]y^2}\ ,\\
G_S(x)&=\frac{3\Omega^2+(3\Omega^2+2y^2)\cosh(\beta y)+2(y^2+3x^2)\cosh(2\beta y)}{[2\cosh(2\beta y)+2\cosh(\beta y)+1]y^2}\ ,
\end{aligned}
\tag{23}
$$

where y is defined by (9). For the derivation of these functions, see also the Appendix.

When the right-hand side of (20), (21), and (22) is expanded, the multispin correlation functions may be obtained. The simplest approximation, and one of the most frequently adopted, for their treating is based on introducing the following decoupling approximation:

$$\langle S_j^z S_k^z \cdots S_l^z \rangle \cong \langle S_j^z \rangle \langle S_k^z \rangle \cdots \langle S_l^z \rangle \tag{24}$$

for $j \neq k \neq \cdots \neq l$. In fact, for $\Omega=0.0$ the decoupling approximation corresponds to the Zernike approximation of spin-$\frac{1}{2}$ model.[10] Using the approximation (24) and taking into account the fact that J_{ij} is given by J for nearest neighbors, the longitudinal and transverse magnetizations as well as the parameter η are given by

$$m_z \equiv \langle S_i^z \rangle = \left[\cosh(J\eta\nabla) + \frac{m_z}{\eta}\sinh(J\eta\nabla)\right]^z F_S(x)|_{x=0} , \tag{25}$$

$$m_x \equiv \langle S_i^x \rangle = \left[\cosh(J\eta\nabla) + \frac{m_z}{\eta}\sinh(J\eta\nabla)\right]^z H_S(x)|_{x=0} , \tag{26}$$

and

$$\eta^2 \equiv \langle (S_i^z)^2 \rangle = \left[\cosh(J\eta\nabla) + \frac{m_z}{\eta}\sinh(J\eta\nabla)\right]^z G_S(x)|_{x=0} , \tag{27}$$

where z is the coordination number.

III. THERMODYNAMICAL PROPERTIES

A. Phase diagram

In this section, let us investigate the phase diagram (or transition temperature) of a spin-S transverse Ising model. In a finite transverse field the S_i^z component of the system is disordered at high temperatures, but below a transition temperature T_c it orders, so that $m_z \neq 0$ and the direction of the moment changes continuously, although there is an order with $m_x \neq 0$ at all temperatures.

In order to study the phase diagram, we must expand the right-hand side of (25) and (27). Retaining only term linear in m_z, we find

$$m_z = zA_1 m_z + O(m_z^3) \tag{28}$$

and

$$\eta^2 = B_1 + O(m_z^2) , \tag{29}$$

with

$$A_1 = \frac{1}{\eta}\sinh(J\eta\nabla)\cosh^{z-1}(J\eta\nabla)F_S(x)|_{x=0} , \tag{30}$$

$$B_1 = \cosh^z(J\eta\nabla)G_S(x)|_{x=0} , \tag{31}$$

where the coefficients A_1 and B_1 can be easily calculated by applying a mathematical relation

$$\exp(a\nabla)\Gamma(x) = \Gamma(x+a) . \tag{32}$$

The second-order phase-transition line is then determined by solving the coupled equations

$$1 = zA_1 , \tag{33}$$

$$\eta^2 = B_1 . \tag{34}$$

Now, let us examine the statistical accuracy of the present formulation by taking the special case of $S=\frac{1}{2}$ and $\Omega=0.0$. For $S=\frac{1}{2}$, as noted above, the parameter $\eta=\frac{1}{2}$. Furthermore, when $\Omega=0.0$, the function $F_S(x)$ reduces to

$$F_s(x) = \tfrac{1}{2}\tanh(\tfrac{1}{2}\beta x) . \tag{35}$$

Thus, (33) is given by

$$1 = z\sinh(\tfrac{1}{2}J\nabla)\cosh^{z-1}(\tfrac{1}{2}J\nabla)\tanh(\beta_c x)|_{x=0} , \tag{36}$$

with $\beta_c = (k_B T_c)^{-1}$, which is nothing but the equation for spin-$\frac{1}{2}$ Ising model in the Zernike approximation.[10] The solution of (36) is given by

$$\frac{4k_B T_c}{J} = 5.073 \quad \text{for } z=6 , \tag{37}$$

which is superior to the standard mean-field result ($4k_B T_c/J = 6$).

B. Internal energy and specific heat

The internal energy U is given by

$$\frac{U}{N} = -\frac{1}{2}\langle \theta_i S_i^z \rangle - \Omega \langle S_i^x \rangle , \tag{38}$$

where N is the number of magnetic atoms. Here, by substituting $f_i = \theta_i$ into (2), the first term of (38) can be written as

$$\langle \theta_i S_i^z \rangle = \left[\frac{\partial}{\partial y}\langle \exp(y\theta_i) \rangle\right]_{y=\nabla} F_S(x)|_{x=0} . \tag{39}$$

The expression $\langle \exp(y\theta_i) \rangle$ can be evaluated by the same way as that of m_z and m_x, namely by introducing the decoupling approximation (24). After this procedure, one obtains

$$\langle \theta_i S_i^z \rangle = zJ\eta\left[\sinh(J\eta\nabla) + \frac{m_z}{\eta}\cosh(J\eta\nabla)\right] \times \left[\cosh(J\eta\nabla) + \frac{m_z}{\eta}\sinh(J\eta\nabla)\right]^{z-1} \times F_S(x)|_{x=0} . \tag{40}$$

It is clear that for the evaluation of internal energy U we must know m_z, m_x, and η. Then, these quantities can be easily obtained by solving (25)–(27) numerically.

Finally, the magnetic contribution to the specific heat can be determined from the relation

$$C = \frac{\partial U}{\partial T} . \tag{41}$$

TABLE I. Numerical values of the critical transverse field Ω_c for different lattices.

	Ω_c/J				
	Present	PA Ref. 3	Present	PA Ref. 3	SE Ref. 2
z	$S=\frac{3}{2}$	$S=\frac{3}{2}$	$S=2$	$S=2$	$S=2$
3	3.737	3.0	5.211	4.0	
4	5.253	4.5	7.233	6.0	
6	8.261	7.5	11.245	10.0	11.598
8	11.261	10.5	15.250	14.0	15.600
12	17.260	16.5	23.252	22.0	23.325

IV. NUMERICAL RESULTS AND DISCUSSION

In this section, we shall show some typical results for the spin-$\frac{3}{2}$ and spin-2 transverse Ising models. At first, in Figs. 1(a) and 1(b) there are presented the phase diagrams in the Ω-T space for the honeycomb, square, and simple cubic lattices. From these figures we can see that the effect of a transverse field on the critical temperature in the higher-spin transverse Ising systems is very similar to that of the spin-$\frac{1}{2}$ transverse Ising model. Namely, the critical temperature gradually decreases from its Ising value at $\Omega=0$ and rapidly vanishes when the transverse field approaches some critical value Ω_c. Our estimations of Ω_c are collected in Table I. For comparison, there are also listed the "pair-approximation" (PA) results[3] and series-expansions results (SE).[2] As we can see, our results are in much better agreement with series-expansion estimations than those of pair approximation. We can also

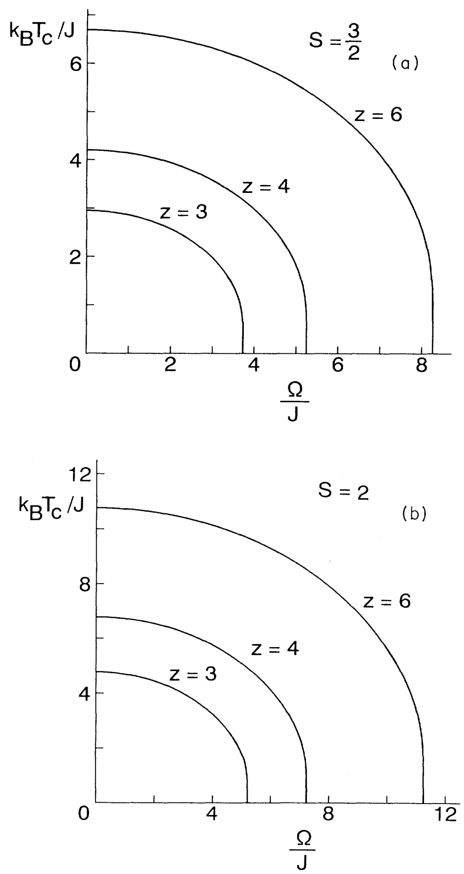

FIG. 1. (a) The phase diagram of the spin-$\frac{3}{2}$ transverse Ising model for the honeycomb, square, and simple cubic lattices. (b) The phase diagram of the spin-2 transverse Ising model for the honeycomb, square, and simple cubic lattices.

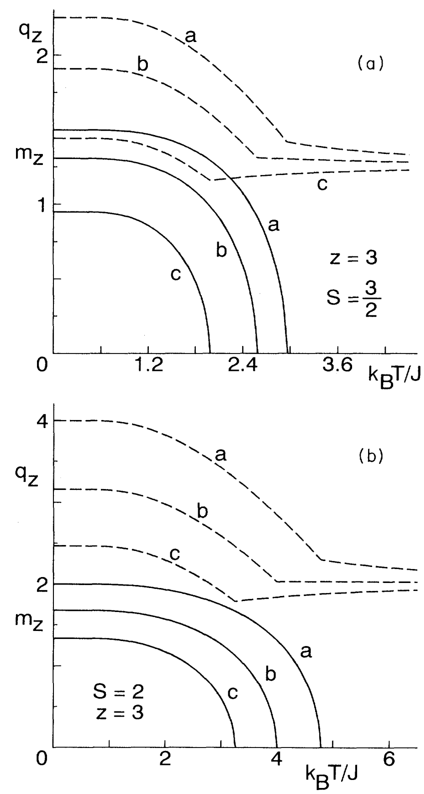

FIG. 2. (a) The temperature dependences of the longitudinal magnetization m_z (solid line) and q_z (dashed line) for the spin-$\frac{3}{2}$ transverse Ising model on the honeycomb lattice, when the transverse field Ω is selected as $\Omega/J=0.001$ for curve a, $\Omega/J=2.0$ for curve b, $\Omega/J=3.0$ for curve c. (b) The temperature dependences of the longitudinal magnetization m_z (solid line) and q_z (dashed line) for the spin-2 transverse Ising model on the honeycomb lattice, when the transverse field Ω is selected as $\Omega/J=0.001$ for curve a, $\Omega/J=3.0$ for curve b, $\Omega/J=4.0$ for curve c.

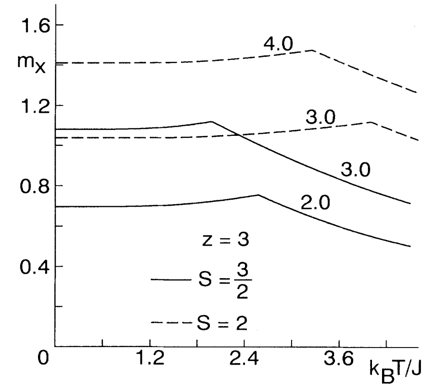

FIG. 3. The temperature dependences of the transverse magnetization m_x for the spin-$\frac{3}{2}$ (solid line) and spin-2 (dashed line) transverse Ising model on the honeycomb lattice. The number accompanying each line means the value of the transverse field (Ω/J).

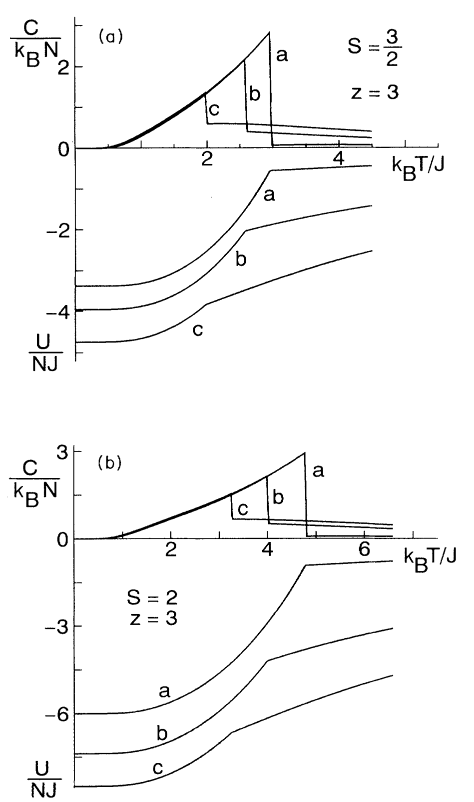

FIG. 4. (a) The temperature dependences of the internal energy U and magnetic specific heat C for the spin-$\frac{3}{2}$ transverse Ising model on the honeycomb lattice. The transverse field Ω is fixed at the same values as in Fig. 2(a). (b) The temperature dependences of the internal energy U and magnetic specific heat C for the spin-2 transverse Ising model on the honeycomb lattice. The transverse field Ω is fixed at the same values as in Fig. 2(b).

see that the value of Ω_c increases with the increasing spin value S. This finding is also in agreement with other works.

In Figs. 2(a), 2(b), and 3, the temperature dependences of the longitudinal and transverse magnetizations as well as the parameter q_z ($q_z \equiv \eta^2$) for the honeycomb lattice are depicted, when the transverse field is fixed at some typical values. Again, these quantities display qualitatively the same behavior as the case of spin-$\frac{1}{2}$ (or spin-1) transverse Ising model.[6,7] Finally, in Figs. 4(a) and 4(b) there are plotted the temperature dependences of the internal energy (U) and magnetic specific heat (C) for the same systems as in Figs. 2. As far as we know, these quantities (for $S>1$) have not been reported in the literature. We can see that, if the transverse field increases, then the absolute value of internal energy in the systems increases holding the same qualitative features as in the pure higher-spin Ising model.[9] On the other hand, the magnetic specific heat is gradually depressed by increasing of the transverse field strength Ω. It can also be seen that the jump at the critical temperature gradually disappears with the increasing value of Ω.

V. CONCLUSION

In this work we have developed a simple approximate theory for studying the transverse Ising models with an arbitrary spin. The statistical accuracy of the present method is nearly the same as that of the Zernike approximation for the spin-$\frac{1}{2}$ Ising model. Within the simplest (or Zernike) approximation, we have shown how the spin-$\frac{1}{2}$ or spin-1 transverse Ising model based on the identity of Sá Barreto, Fittipaldi, and Zeks can be extended to the spin-S transverse Ising model. The approximation can be of course improved to the better (or Bethe-Peierls) approximation, if one uses the correlated effective-field approximation.[12] Moreover, on the basis of present formulation the effective-field renormalization-group method, such as Ref. 13, may be developed and applied to study the critical phenomena of the spin-S transverse Ising model. Because of its mathematical simplicity, the present framework based on (24) will probably have a wider applicability than others methods, especially when one wants to get whole temperature-dependences of magnetic properties in the spin-S transverse Ising model.

In the previous sections we have shown and discussed some typical results for spin-$\frac{3}{2}$ and spin-2 systems on the honeycomb lattice. On the basis of our analysis, we can conclude that effects of the transverse field in the higher-spin Ising systems are very similar to those of the spin-$\frac{1}{2}$ case. Owing to the mathematical simplicity and versatility of our formulation, we hope that this method will be potentially very useful for studying and understanding more complicated physical systems in the presence of a transverse field.

APPENDIX

In this appendix, let us show how Eqs. (4), (5), and (22) can be derived for an arbitrary spin S.

From (1), we may write $\mathcal{H}_i$ as

$$\mathcal{H}_i = -\theta_i S_i^z - \Omega S_i^x \ , \tag{A1}$$

where θ_i is defined by (6). In order to diagonalize the form of (A1), we shall use a rotational transformation as follows:

$$S_i^z = S_i^{z\prime}\cos(\phi_i) - S_i^{x\prime}\sin(\phi_i) \ , \tag{A2}$$

$$S_i^x = S_i^{z\prime}\sin(\phi_i) + S_i^{x\prime}\cos(\phi_i) \ , \tag{A3}$$

with

$$\cos(\phi_i) = \frac{\theta_i}{E_i}, \quad \sin(\phi_i) = \frac{\Omega}{E_i} \ , \tag{A4}$$

where E_i is defined by (7). By the use of the transformations (A2) and (A3), $\mathcal{H}_i$ can be rewritten as

$$\mathcal{H}_i = -E_i S_i^{z\prime} \ . \tag{A5}$$

From (2) one can obtain, for $f_i = 1$,

$$\langle S_i^z \rangle = \left\langle \cos(\phi_i) \frac{\mathrm{Tr}_{\{i\}} S_i^{z\prime} \exp(\beta E_i S_i^{z\prime})}{\mathrm{Tr}_{\{i\}} \exp(\beta E_i S_i^{z\prime})} \right\rangle \ , \tag{A6}$$

$$\langle S_i^x \rangle = \left\langle \sin(\phi_i) \frac{\mathrm{Tr}_{\{i\}} S_i^{z\prime} \exp(\beta E_i S_i^{z\prime})}{\mathrm{Tr}_{\{i\}} \exp(\beta E_i S_i^{z\prime})} \right\rangle \ , \tag{A7}$$

$$\langle (S_i^z)^2 \rangle = \left\langle \cos^2(\phi_i) \frac{\mathrm{Tr}_{\{i\}} (S_i^{z\prime})^2 \exp(\beta E_i S_i^{z\prime})}{\mathrm{Tr}_{\{i\}} \exp(\beta E_i S_i^{z\prime})} \right\rangle + \left\langle \sin^2(\phi_i) \frac{\mathrm{Tr}_{\{i\}} (S_i^{x\prime})^2 \exp(\beta E_i S_i^{z\prime})}{\mathrm{Tr}_{\{i\}} \exp(\beta E_i S_i^{z\prime})} \right\rangle \ . \tag{A8}$$

These equations can be easily calculated by the use of the following matrices:

$$\langle \sigma | S_i^{z\prime} | \sigma' \rangle = \sigma \delta_{\sigma,\sigma'} \ , \tag{A9}$$

$$\langle \sigma | S_i^{x\prime} | \sigma' \rangle = \langle \sigma' | S_i^{x\prime} | \sigma \rangle = \tfrac{1}{2} \delta_{\sigma',\sigma-1} [(S+\sigma)(S-\sigma+1)]^{1/2} \ , \tag{A10}$$

where δ is the Kronecker δ function and σ can take $2S+1$ values allowed for a spin S, namely $\sigma = -S, -S+1, \ldots, S-1, S$.

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