General spin-$\frac{3}{2}$ Ising model in a honeycomb lattice: Exactly solvable case

N. Sh. Izmailian*
Physics Department, Rensselaer Polytechnic Institute, Troy, New York 12180-3590

N. S. Ananikian
Theoretical Division, Yerevan Physics Institute, Yerevan, 375036, Armenia
(Received 18 May 1994)

The most general spin-$\frac{3}{2}$ Ising model with up-down symmetry is investigated on a honeycomb lattice. The partition function on a surface in the space spanned by the coupling constants J, K, L, and M was found exactly. The explicit expression for the quadrupolar order parameter with the inclusion of an external crystal field of strength Δ is obtained. It is shown that this order parameter exhibits in general a simple power-law dependence on T-T_c near T_c.

Spin-1 and spin-$\frac{3}{2}$ models have been investigated carefully in two-dimensional systems. These models have become very attractive because of their simplicity and the rich fixed-point structure. A spin-1 model was introduced by Blume-Emery-Griffiths (BEG).[1] This model has been studied mostly under the molecular field[1] and renormalization group approximation.[2] Recently, Horiguchi,[3] Wu,[4] Shankar,[5] and Rosengren and Haggkvist[6] have solved exactly the BEG model for a honeycomb lattice, when $\exp(K)\cosh J=1$, where J and K are dipolar and quadrupolar interactions constants. The same result was obtained for the Bethe lattice.[7] Very recently, Kolesik and Samaj[8] proposed a systematic way for obtaining solvable cases of the general spin-1 Ising model on the honeycomb lattice.

We consider the most general spin-$\frac{3}{2}$ Ising model with nearest-neighbor interaction and up-down symmetry, which is described by the following Hamiltonian

$$-\beta H=\sum_{\langle ij\rangle}\left[JS_iS_j+KS_i^2S_j^2+LS_i^3S_j^3+\frac{M}{2}(S_iS_j^3+S_jS_i^3)\right]-\Delta\sum_i S_i^2\,, \qquad (1)$$

where $S_i=\pm\frac{1}{2},\pm\frac{3}{2}$ is the spin variable at site i and $\langle ij\rangle$ indicates summation over the nearest-neighbor pairs of sites. Here, we will not be concerned about the physical origin of these couplings (J,K,L and M); we will treat them as parameters in the calculations.

The spin-$\frac{3}{2}$ BEG model with dipolar (J) and quadrupolar (K) interactions was introduced to explain phase transition in $DyVO_4$ and its phase diagram was obtained within the mean field approximation.[9] Another spin-$\frac{3}{2}$ model was later introduced to study tricritical properties in ternary fluid mixture,[10] which was also solved in the mean field approximation. Recently, the complete phase diagram of this model with $L=M=0$ has been fully analyzed with the use of two different approaches: mean field and Monte-Carlo methods.[11] Very recently, Lipowski and Suzuki[12] have found the conditions under which the spin-$\frac{3}{2}$ Ising model with $M=0$ on the honeycomb lattice has the same partition function as the $S=\frac{1}{2}$ Ising model. The method which they used is a straightforward generalization of the method used by Kolesik and Samaj.[8] They transformed the model of Eq. (1) with $M=0$ into the three-state vertex model, and then they found the condition under which the last model is equivalent to the two-vertex model.

In this paper we derive an exact solution of the general spin-$\frac{3}{2}$ Ising model on a honeycomb lattice on a surface in the space spanned by the coupling constants J,K,L, and M. Here we use the method proposed by Wu[4] for the BEG model and developed by the authors[13] for the spin-$\frac{3}{2}$ Ising model without reference to the three-state model.

The partition function for the model given by Eq. (1) is

$$Z=\sum_{\{s\}}\exp(-\beta H)\,, \qquad (2)$$

where $\beta=1/k_BT$ and the sum is over all spin configurations.

We introduce the following identity

$$\begin{aligned}\exp&\left[JS_1S_2+KS_1^2S_2^2+LS_1^3S_2^3+\frac{M}{2}(S_1S_2^3+S_2S_1^3)\right]\\&=\tfrac{1}{64}(81\alpha_0-18\alpha_1+\alpha_2)+\tfrac{1}{16}(81\beta_0-18\beta_1+\beta_2)S_1S_2+\tfrac{1}{4}(\alpha_0-2\alpha_1+\alpha_2)S_1^2S_2^2\\&\quad+(\beta_0-2\beta_1+\beta_2)S_1^3S_2^3+\tfrac{1}{4}(-9\beta_0+10\beta_1-\beta_2)(S_1S_2^3+S_2S_1^3)+\tfrac{1}{16}(-9\alpha_0+10\alpha_1-\alpha_2)(S_1^2+S_2^2)\,,\end{aligned} \qquad (3)$$

where

$$\alpha_0=\exp(\tfrac{1}{16}K)\cosh J_0\ ,\quad \beta_0=\exp(\tfrac{1}{16}K)\sinh J_0\ ,\quad J_0=\tfrac{1}{4}J+\tfrac{1}{16}M+\tfrac{1}{64}L\ ,$$
$$\alpha_1=\exp(\tfrac{9}{16}K)\cosh J_1\ ,\quad \beta_1=\tfrac{1}{3}\exp(\tfrac{9}{16}K)\sinh J_1\ ,\quad J_1=\tfrac{3}{4}J+\tfrac{15}{16}M+\tfrac{27}{64}L\ , \tag{4}$$
$$\alpha_2=\exp(\tfrac{81}{16}K)\cosh J_2\ ,\quad \beta_2=\tfrac{1}{9}\exp(\tfrac{81}{16}K)\sinh J_2\ ,\quad J_2=\tfrac{9}{4}J+\tfrac{81}{16}M+\tfrac{729}{64}L\ .$$

When $\alpha_0\alpha_2=\alpha_1^2$ and $\beta_0\beta_2=\beta_1^2$ and after simple algebraic calculations these relations can be represented as

$$\tanh^2 J_1=\tanh J_2 \tanh J_0\ ,$$
$$\exp(-4K)=\cosh(J_2-J_0)\ . \tag{5}$$

We can rewrite Eq. (3) in the following form

$$\exp\left[JS_1S_2+KS_1^2S_2^2+LS_1^3S_2^3+\frac{M}{2}(S_1S_2^3+S_2S_1^3)\right]=\alpha_0\exp[R(S_1^2+S_2^2-\tfrac{1}{2})]\left[1+4\frac{\beta_0}{\alpha_0}S_1S_2\exp[R_0(S_1^2+S_2^2-\tfrac{1}{2})]\right]\ , \tag{6}$$

where $\exp(2R)=(\cosh J_1/\cosh J_0)\exp(K/2)$ and $\exp(2R_0)=\tanh J_1/3\tanh J_0$.

Then the partition function defined by the Hamiltonian in Eq. (1) can be written as

$$Z=(\alpha_0 e^{-R/2})^E\sum_{\{s\}}\prod_{\langle ij\rangle}\{1+4\tanh J_0 S_iS_j\exp[R_0(S_i^2+S_j^2-\tfrac{1}{2})]\}\prod_i\exp(-\Delta_0 S_i^2)\ , \tag{7}$$

where E is the total number of edges, $\Delta_0=\Delta-\gamma R$ and γ is the coordination number of a lattice.

Thus, we obtain the subspace of exchange interactions in Eq. (5) where the partition function is written in the form of Eq. (7). We remark that this result is valid for any arbitrary lattice. For a honeycomb lattice $\gamma=3$ and $E=3N/2$, where N is the total number of sites. Equation (5) is the analogy of the condition $\exp(K)\cosh J=1$ obtained for the $S=1$ model by Horiguchi.[3] Note, that if $M=0$ then the condition in Eq. (5) coincides with the result obtained by Lipowski and Suzuki.[12]

We expand the first product over neighboring pairs in Eq. (7) and represent each term in the expansion by a graph drawn on the lattice. Draw a line on the edge between sites i and j if from corresponding factors one selects the term $4\tanh J_0 S_iS_j\exp[R_0(S_i^2+S_j^2-\tfrac{1}{2})]$. Draw no line if one takes the term 1. This gives a one-to-one correspondence between terms in the expansion and line configurations on the edges of the lattice. For each term in the expansion, carry out the summations $\sum_{S_i=\pm 1/2,\pm 3/2}$ for all sites. For the honeycomb lattice this can be accomplished with the use of the identity:

$$\begin{aligned}\sum_{S_i=\pm 1/2,\pm 3/2} S_i^n\exp[(nR_0-\Delta_0)S_i^2]&=2\exp\left[-\frac{\Delta_0}{4}\right][1+\exp(-2\Delta_0)]\ ,\quad n=0\\ &=\tfrac{1}{2}\exp\left[\frac{2R_0-\Delta_0}{4}\right][1+9\exp(4R_0-2\Delta_0)]\ ,\quad n=2\\ &=0\ ,\quad n=1,3\ .\end{aligned} \tag{8}$$

Here n is the number of lines with site i as an end point. It can take on values 0, 1, 2, and 3, only for the honeycomb lattice.

According to Wu[14] this fact together with Eq. (8) enable us to rewrite Eq. (7) as the partition function of a spin-$\tfrac{1}{2}$ Ising model. Introducing Ising spins $\sigma_i=\pm 1$, we can rewrite Eq. (7) as

$$Z=B^N\sum_{\sigma_i=\pm 1}\prod_{\langle ij\rangle}\left\{1+\sigma_i\sigma_j\tanh J_0\frac{1+9\exp(4R_0-2\Delta_0)}{1+\exp(-2\Delta_0)}\right\}\ , \tag{9}$$

where

$$B=\alpha_0^{3/2}[1+\exp(-2\Delta_0)]\exp\left[-\frac{3R+\Delta_0}{4}\right]\ . \tag{10}$$

Now the right-hand side of Eq. (9) gives precisely the high-temperature expansion of a spin-$\tfrac{1}{2}$ Ising partition function $Z_{\rm Ising}(K_1)$ whose nearest-neighbor interaction is K_I with

$$\tanh K_I=\frac{1+9\exp(4R_0-2\Delta_0)}{1+\exp(-2\Delta_0)}\tanh J_0\ . \tag{11}$$

Thus, we obtain the exact equivalence

$$Z=B^{N}(\cosh K_I)^{-3N/2}Z_{\text{Ising}}(K_I)\ , \tag{12}$$

where $Z_{\text{Ising}}(K_I)$ is the partition function of a spin-$\frac{1}{2}$ Ising model on the honeycomb lattice with interaction $-k_BTK_I$. In other words, the spin-$\frac{1}{2}$ Ising model is a special case of the spin-$\frac{3}{2}$ Ising model. The free energy for the spin-$\frac{1}{2}$ Ising model on the honeycomb lattice in the limit of an infinite lattice is well known,[15] and after some algebra we obtain, in the large N limit, the free energy for the spin-$\frac{3}{2}$ Ising model

$$-\beta f=\ln 2B+\frac{1}{16\pi^2}\int_0^{2\pi}d\theta\int_0^{2\pi}d\varphi \ln\{1+3u^4-2u^2(1-u^2)[\cos\theta+\cos\varphi+\cos(\theta+\varphi)]\}\ , \tag{13}$$

with $u=\tanh K_I$. B and K_I are given by Eqs. (10) and (11), respectively.

That is, we have solved the spin-$\frac{3}{2}$ Ising model exactly on the surface represented by Eq. (5) in the four-dimensional space spanned by the coupling constants J_0, J_1, J_2, and K. For arbitrary values of J_0 and J_2, Eq. (5) determines a unique set of values of K and J_1 for which the model can be solved exactly.

Now, we consider the critical behavior of our model. Since the second derivative of the free energy in Eq. (13) diverges logarithmically at $u=u_c=1/\sqrt{3}$, the spin-$\frac{3}{2}$ Ising model will exhibit a first-order transition if $u>u_c$, a second-order transition if $u=u_c$ and no transition at all $u<u_c$. The important thermodynamic properties of this model are summarized as follows. A second-order phase transition occurs at a temperature T_c determined by

$$\frac{\tanh J_0+\tanh J_2\exp(-2\Delta_0)}{1+\exp(-2\Delta_0)}=\frac{1}{\sqrt{3}}\ , \tag{14}$$

where $\Delta_0=\Delta-3R$ and R is a function of J_0 and J_2 in subspace of Eq. (5):

$$\exp(-4R)=\frac{\cosh J_0}{\cosh J_2}\cosh^{5/4}(J_2-J_0)\ . \tag{15}$$

The critical condition given by Eqs. (14) and (15) gives us the λ-surface Ising-type transition (logarithmic specific heat singularity) in spin-$\frac{3}{2}$ model in the space spanned by the Δ, J_0, and J_2.

We have solved the model exactly for arbitrary values of J_0 and J_2, the λ-surface of critical points in Eq. (14), defined only in the two regions on the (J_0,J_2) plane:

$$\text{(i)}\ 0\le\tanh J_0\le 1/\sqrt{3}\ \text{ and }\ 1/\sqrt{3}\le\tanh J_2\le 1\ , \tag{16}$$

$$\text{(ii)}\ 0\le\tanh J_2\le 1/\sqrt{3}\ \text{ and }\ 1/\sqrt{3}\le\tanh J_0\le 1\ . \tag{17}$$

Note, that for each set of values of J_0 and J_2, Eq. (14) determines a unique value of Δ, except the intersect point of two regions (i) and (ii), for which Δ is an arbitrary. Thus, the λ surface in Eq. (14) contained the nontrivial λ line of critical points given by

$$J_0=J_2=\operatorname{arctanh}(1/\sqrt{3})\ \text{ and }\ \Delta-\text{arbitrary}\ , \tag{18}$$

in which, as it is shown below, the model exhibits the critical behavior different from the critical behavior elsewhere on the λ surface. Also, we must remark, that for $M=0$ we recover the previously reported exactly solvable case,[12] which is located in the region (i) given by Eq. (16).

This model has an order parameter (quadrupolar moment) p defined by

$$p=\frac{1}{N}\sum_{i=1}^{N}\langle S_i^2\rangle=Z^{-1}\sum_{\{s\}}S_i^2\exp(-\beta H)\ . \tag{19}$$

This order parameter can also be defined by the variation of the free energy with Δ. It is now straightforward, although tedious, to compute the quadrupolar moment p through direct differentiation of Eq. (13). We found that

$$p=\frac{5}{4}-\frac{1-\exp(-2\Delta_0)}{1+\exp(-2\Delta_0)}+\frac{\exp(-2\Delta_0)}{1+\exp(-2\Delta_0)}\frac{\tanh J_2-\tanh J_0}{\tanh J_0+\tanh J_2\exp(-2\Delta_0)}\left[\frac{1-2u^2}{1-u^2}+I\right]\ , \tag{20}$$

with

$$I=\begin{cases}\dfrac{(3u^2-1)(1+u^2)}{u}\dfrac{K(q)}{2\pi}\ , & \text{if } u^2>\frac{1}{3}\ ,\\[2ex] \dfrac{4u^2(3u^2-1)(1+u^2)}{(1-u^2)^{3/2}(1+3u^2)^{1/2}}\dfrac{K(q_0)}{2\pi}\ , & \text{if } u^2<\frac{1}{3}\ .\end{cases} \tag{21}$$

Here $q^2=(1-u^2)^3(1+3u^2)/16u^6$ and $qq_0=1$.

Furthermore $K(q)$ is the complete elliptic integral defined by

$$K(q)=\int_0^{\pi/2}(1-q^2\sin^2\theta)^{-1/2}d\theta\ . \tag{22}$$

That is, we have been able to exactly evaluate the order parameter p on the subspace Eq. (5). The phase transition occurs at $q=1$ or $u=u_c=1/\sqrt{3}$. While $K(q)$ diverges as $\ln|T-T_c|$ when $q\to 1$, it can be seen from Eqs. (20) and (21) that

$$p\to p_\lambda+|T-T_c|\ln|T-T_c|\ . \tag{23}$$

Hence, p is continuous at T_c and $\partial p/\partial T$ diverges logarithmically near T_c.

Using Eq. (23) together with Eqs. (20) and (14) we found p_λ as functions of J_0 and J_2,

$$p_\lambda = \frac{5}{4} - \frac{\tanh J_2 + \tanh J_0 + \sqrt{3}(\tanh J_2 \tanh J_0 - 1)}{2(\tanh J_2 - \tanh J_0)} . \tag{24}$$

This is the λ surface of Ising-type phase transition at T_c in three-dimensional space spanned by p_λ, J_0, and J_2.

Note, that critical behavior of the order parameter p_λ given by Eqs. (23) and (24) is valid everywhere, except of the λ line of critical points given in Eq. (18), where as it is easy to see from Eqs. (6) and (11), $K_I = J_0$ and hence $u = \tanh K_I$ do not depend on Δ. Therefore, the variation of the free energy given in Eq. (13) with Δ, does not contain the divergence part. This leads to the simple expression for the order parameter p_λ given by

$$p_\lambda = \frac{5}{4} - \frac{1-\exp(-2\Delta)}{1+\exp(-2\Delta)} . \tag{25}$$

Thus, we see that in the λ line given in Eq. (18) the phase transition is not marked with the logarithmic divergence in the order parameter p_λ. Really the phase transition is associated with the logarithmic divergence in the specific heat.

In summary, we have used the method proposed by Wu[4] and developed by the authors[13] for obtaining the exact solution for spin-$\frac{3}{2}$ Ising model in the honeycomb lattice. In particular, we have developed the analytical expressions for the free energy per spin, the quadrupolar moment and the λ surface of Ising-type phase transition in the parameter space of our model. In principle, this method can also be used for the description of Ising models with higher values of spin on lattice sites with larger values of the coordination number in a lattice. In particular, our results suggest that the equivalence of the most general spin-$\frac{3}{2}$ Ising model with a spin-$\frac{1}{2}$ Ising model can be extended to the square lattice, for which very few exact results are available. Note that this result cannot be obtained for the special ($M=0$) spin-$\frac{3}{2}$ Ising model on the square lattice. Details will be reported elsewhere.

This research was supported in part by Soros Foundation grant awarded by the American Physical Society, Grant No. 211-5291 YPI of the German Bundasminsterium fur Forschung and Technologie, and CAST grant program of the National Academy of Sciences USA. One of us (N.Sh.I.) wishes to thank G.-C. Wang for the hospitality extended to him at the Rensselaer Polytechnic Institute where a portion of this work was carried out.

---

*On leave from Theoretical Division, Yerevan Physics Institute, Yerevan, 375036, Armenia.

[1] M. Blume, V. J. Emery, and R. B. Griffiths, Phys. Rev. A **4**, 1071 (1971).

[2] A. N. Berker and M. Wortis, Phys. Rev. B **14**, 4946 (1976).

[3] T. Horiguchi, Phys. Lett. **113A**, 425 (1986).

[4] F. Y. Wu, Phys. Lett. A **116**, 245 (1986).

[5] R. Shankar, Phys. Lett. A **117**, 365 (1986).

[6] A. Rosengren and R. Haggkvist, Phys. Rev. Lett. **63**, 660 (1989).

[7] A. R. Avakian, N. S. Ananikian, and N. Sh. Izmailian, Physica A **172**, 394 (1991).

[8] M. Kolesik and L. Samaj, Int. J. Mod. Phys. **6**, 1529 (1992).

[9] J. Sivardiere and M. Blume, Phys. Rev. B **5**, 1126 (1972).

[10] S. Krinsky and D. Mukamel, Phys. Rev. B **11**, 399 (1975).

[11] F. C. Sa Barreto and O. F. de Alcantara Bonfim, Physica A **172**, 378 (1991).

[12] A. Lipowski and M. Suzuki, Physica A **193**, 141 (1993).

[13] N. S. Ananikian and N. Sh. Izmailian (unpublished).

[14] F. Y. Wu, J. Math. Phys. **15**, 687 (1974).

[15] I. Syozi, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 1.