Static properties of infinite-range anisotropic spin Hamiltonians

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The thermodynamic properties of systems described by means of infinite-range anisotropic spin Hamiltonians depending on the total spin and its z component are exactly evaluated. XY-type, Ising-type, and intermediate-type states can be exhibited at different temperature ranges. A certain family of Hamiltonians containing quadratic and quartic terms is studied in detail.

I. INTRODUCTION

A general treatment of isotropic infinite-range spin Hamiltonians was recently proposed by the present authors.[1] This formalism was applied to the treatment of quadratic magnetostriction,[2] singlet ground-state ferromagnetism,[3] and re-entrant ferromagnetism.[4] The equivalence of infinite-range and mean-field theories[5–7] enabled the generalization of this formalism, allowing the application to a very broad class of many-body Hamiltonians,[8] which contains the spin systems as a special case.

The anisotropic Heisenberg Hamiltonian[9] was recently considered by Lee and co-workers.[10–12] They studied the static and dynamic properties of the infinite-range Hamiltonian

$$\mathscr{H}=-N(J\hat{S}^2-\lambda\hat{S}_z^2)\ . \tag{1}$$

Here N is the number of spins and $\hat{S}^2=\hat{S}_x^2+\hat{S}_y^2+\hat{S}_z^2$, where $\hat{S}=\hat{S}_{\rm total}/N$. It was revealed that for this Hamiltonian the only possible values of $\langle\hat{S}_z\rangle$ were 0 and $S=\lim_{N\to\infty}(\langle S^2\rangle)^{1/2}$, which means that either $\langle\hat{S}_z^2\rangle$ or $\langle(\hat{S}_x^2+\hat{S}_y^2)\rangle$ vanishes. In order to investigate the possibility of observing situations in which $\langle\hat{S}_z\rangle$ obtains intermediate values, which correspond to the magnetization being tilted relative to the main crystallographic axis, we propose to investigate more general anisotropic infinite-range spin Hamiltonians.

II. GENERAL FORMULATION

For the isotropic infinite-range spin Hamiltonian $\mathscr{H}=NH(\hat{S}^2)$ whose eigenvalues, in the thermodynamic limit, are $NH(S^2)$, the availability of the degeneracy function[7,13] enables the evaluation of the maximum term in the canonical partition function, resulting in the equation

$$S=\sigma B_\sigma\left[-\beta\sigma\frac{\partial H}{\partial S}\right]\ , \tag{2}$$

where σ is the elementary spin and B_σ is the Brillouin function.

Considering a tetragonal lattice in which the two directions perpendicular to the main axis are equivalent, the spin Hamiltonian we introduce will be of the form $\mathscr{H}=NH(\hat{S}^2,\hat{S}_z)$. The commutativity of $\hat{S}^2$ and $\hat{S}_z$ enables the specification of the energies in terms of the corresponding quantum numbers, S,S_z. The degeneracy of a state specified by S,S_z is given, in the thermodynamic limit, by the same degeneracy function used in the isotropic case,

$$\Omega(N,S)\simeq\Omega(N,S,S_z)\simeq\exp[-N(\mu S+\ln C)]\ ,$$

where

$$C=\sinh(\mu/2)/\sinh[\mu(\sigma+\tfrac{1}{2})] \tag{3}$$

and

$$S=\sigma B_\sigma(\sigma\mu)\ .$$

We now evaluate the values of S,S_z corresponding to the maximum term of the canonical partition function

$$Z=\sum_S\sum_{S_z}Z_{S,S_z}=\sum_S\Omega(N,S)\sum_{S_z}\exp[-\beta NH(S,S_z)]\ . \tag{4}$$

The maximum with respect to S_z corresponds to the minimum of $H(S,S_z)$ with respect to S_z. This minimum occurs either within the range $-S<S_z<S$, and is then given by $\partial H/\partial S_z=0$, or on the boundary, $|S_z|=S$. In either case $S_z=S_z(S)$. After substitution of this relation in Eq. (4) we evaluate the maximum term with respect to S, obtaining

$$S=\sigma B_\sigma\left[-\beta\sigma\frac{dH}{dS}\right]\ , \tag{5}$$

where

$$\frac{dH}{dS}=\frac{\partial H}{\partial S}+\frac{\partial H}{\partial S_z}\frac{\partial S_z}{\partial S}\ .$$

The approach developed by Lee and co-workers[10–12] for the Hamiltonian (1) with $\sigma=\frac{1}{2}$ can be viewed as a more rigorous derivation of a special case of this result. The three possible types of solutions are as follows.

(a) The XY solution. The minimum with respect to S_z occurs at $S_z=0$. In this case $\partial S_z/\partial S=0$.

(b) The intermediate solution. The minimum occurs within the range $0<|S_z|<S$. In this case $\partial H/\partial S_z=0$.

(c) The Ising solution. The minimum occurs at $S_z=S$. In this case $\partial S_z/\partial S=1$.

The designation XY and Ising is due to Dekeyser and Lee.[10] In both cases (a) and (b)

$$\frac{dH}{dS}=\frac{\partial H}{\partial S}\,, \tag{6}$$

whereas in case (c)

$$\frac{dH}{dS}=\frac{\partial H}{\partial S}+\left.\frac{\partial H}{\partial S_z}\right|_{S_z=S}\,. \tag{7}$$

In order to clarify this procedure it may be helpful to note that what is really happening is that S_z and S are coupled through the restriction $|S_z|\le S$. The two variables S and $\sigma_z=S_z/S$ vary over the mutually independent ranges $0\le S\le S_{\max}$ and $-1\le\sigma_z\le 1$. When the Hamiltonian is expressed in terms of these variables $H(S,\sigma_z)=H(S,S\sigma_z)$ we have

$$S=\sigma B_\sigma\left[-\beta\sigma\frac{dH}{dS}\right],\quad \frac{dH}{dS}=\frac{\partial H}{\partial S}+\frac{\partial H}{\partial S_z}\sigma_z$$

and σ_z is determined by minimization of $H(S,\sigma_z)$, resulting in the expressions (6) or (7) for the appropriate cases.

For the Hamiltonian considered by Lee and coworkers,[10–12] Eq. (1), $\partial H/\partial S_z=2\lambda S_z$, so that the minimum with respect to S_z can only occur at $S_z=0$ ($\lambda>0$) or $S_z=S$ ($\lambda<0$), corresponds to the XY- and Ising-type solutions, respectively. In the former case $dH/dS=-2JS$, whereas in the latter $dH/dS=-2(J-\lambda)S$. For these two cases Eq. (5) becomes the generalization to arbitrary σ of Eqs. (16c) and (23), respectively, of Ref. 10. In order to obtain the intermediate solution, corresponding to $0<|S_z|<S$, i.e., $S_z^2>0$, $S_x^2+S_y^2>0$, we must consider a more general Hamiltonian, containing higher powers of the spin operators. In the following section we consider a Hamiltonian containing quartic terms in the spin.

III. A QUARTIC ANISOTROPIC SPIN HAMILTONIAN

We shall now introduce, in addition to S^2, the two quartic terms $(S_x^2+S_y^2)^2$ and S_z^4. In terms of S^2 and S_z we obtain

$$H=aS^2/2+bS_z^2/2+c(S^2-S_z^2)^2/4+dS_z^4/4\,. \tag{8}$$

We shall only be interested in choices of the Hamiltonian parameters (a,b,c,d) resulting in intermediate-type solutions ($0<|S_z|<S$) at least over some temperature range. For large S_z, the dominant term is $(c+d)S_z^4$, whereas the behavior near $S_z=0$ is determined by $\partial^2H/\partial S_z^2\,|_{S_z=0}=b-cS^2$. The behavior of the Hamiltonian as a function of S_z can be of one of the four types presented in Fig. 1. Only behavior of type II can exhibit the intermediate solution.

The minimum is obtained for $S_z^2=(cS^2-b)/(c+d)$, provided that this value is not larger than S^2, which results in the condition $dS^2+b>0$. The four restrictions $c+d>0$, $b-cS^2<0$, $dS^2+b>0$, and $S^2<\sigma^2$ result in a division of the space of the parameters b,c,d into the three relevant regions presented in Fig. 2.

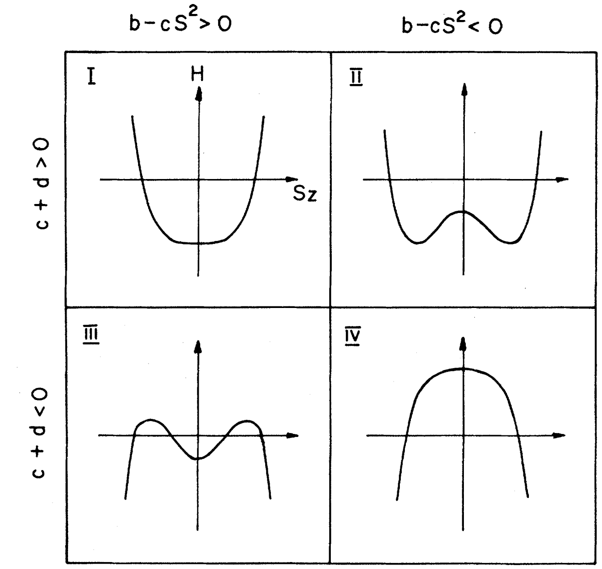

FIG. 1. Types of behavior of the Hamiltonian, Eq. (8), with respect to S_z.

The expressions for dH/dS for each one of the three types of solution are as follows.

(a) $S_z=0$: $dH/dS=aS+cS^3$,

(b) S_z intermediate: $dH/dS=[a+bc/(c+d)]S+cd/(c+d)S^3$,

(c) $S_z=S$: $dH/dS=(a+b)S+dS^3$.

For a Hamiltonian of the form $H=C_1S^2/2+C_2S^4/4$, i.e., $dH/dS=C_1S+C_2S^3$, the condition for a monotonic dependence of S on the temperature (second-order transition) is[1]

$$C_2/C_1<3[(2\sigma+1)^2+1]/\{20[\sigma(\sigma+1)]^2\}\equiv\psi_\sigma,\quad C_1<0\,.$$

A sufficient condition for all the transitions among the different types of solutions to be of second order is

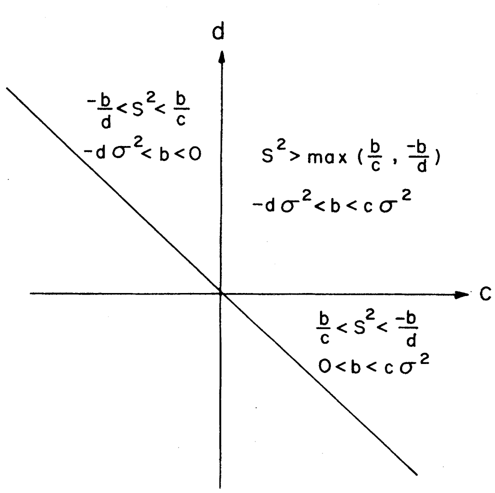

FIG. 2. Regions of parameter space exhibiting intermediate-type solutions.

TABLE I. Behavior of the solutions in the asymptotic regimes.

$c+d>0$	$S_z=0$	intermediate	$S_z=S$
$S\to 0$	$b>0$	$b=0$	$b<0$
$S\to\sigma$	$b-c\sigma^2>0$	$b-c\sigma^2<0$	$b-c\sigma^2<0$
		$b+d\sigma^2>0$	$b+d\sigma^2<0$

$$c/a<\psi_\sigma,\quad cd/[a(c+d)+bc]<\psi_\sigma,\quad b/(a+b)<\psi_\sigma$$
$$a<0,\quad a+bc/(c+d)<0,\quad a+b<0\ . \tag{9}$$

All these conditions can be satisfied for a sufficiently large value of $|a|$. In order to restrict the number of cases we consider numerically, we shall only present quantitative results corresponding to parameter choices satisfying these conditions.

Some further results which can be obtained analytically involve the behavior close to the highest critical temperature and at very low temperatures. As $S\to 0$ the intermediate solution is only possible if $b=0$. Otherwise $\partial^2H/\partial S_z^2\,|_{S_z=0,S>0}=b$, which means that $S_z=0$ if $b>0$ and $S_z=S$ if $b<0$. As $S\to\sigma$, if $b-c\sigma^2>0$ then $S_z=0$. For $b-c\sigma^2<0$, the intermediate solution will be obtained if $b+d\sigma^2>0$, and $S_z=S$ otherwise. These results are summarized in Table I.

The possible sequences of transitions that can be obtained upon lowering the temperature (starting from the highest critical temperature) can be specified by the values obtained by S_z [0, intermediate (I), or S], as follows: 0;0,I,S;0,I;I;S,I,0;S,I;S.

IV. NUMERICAL EXAMPLES

For the simplest case, $\sigma=\frac{1}{2}$, the equation to be solved is as follows:

$$S=\tfrac{1}{2}\tanh\left[-\left[\frac{dH}{dS}\right]\Big/2\tau\right],\quad \tau=kT$$

which can also be written in the form

$$\tau=-\left[\frac{dH}{dS}\right]\Big/\ln[(1+2S)/(1-2S)]\ .$$

The following parameter choices were made.

(i) $a=-1$, $b=\frac{1}{32}$, $c=0.5$, $d=-0.25$. Checking the various conditions derived in the preceding section we find that we have three critical temperatures corresponding to second-order transitions according to the sequence 0,I,S. The second and third transitions occur for $S=0.25$ and $S=\sqrt{2}/4$, respectively. The numerical results are shown in Fig. 3(a).

(ii) $a=-1$, $b=-\frac{1}{32}$, $c=-0.25$, $d=0.5$. This choice of parameters corresponds to the sequence S,I,0 and is presented in Fig. 3(b).

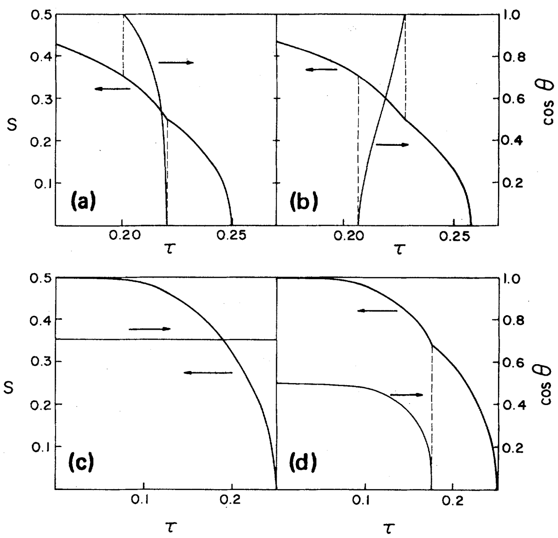

FIG. 3. Magnetization (S) and its orientation relative to the z axis ($\cos\theta=S_z/S$). (a) $a=-1$, $b=\frac{1}{32}$, $c=0.5$, $d=-0.25$; 0,I,S sequence. (b) $a=-1$, $b=-\frac{1}{32}$, $c=-0.25$, $d=0.5$; S,I,0 sequence. (c) $a=-1$, $b=0$, $c=d=1$; I sequence. (d) $a=-1$, $b=\frac{1}{8}$, $c=d=1$; 0,I sequence.

(iii) $a=-1$, $b=0$, $c=d=1$. In this case S_z obtains the intermediate value $S/\sqrt{2}$ over the whole range of temperatures; see Fig. 3(c).

(iv) $a=-1$, $b=\frac{1}{8}$, $c=d=1$. This case corresponds to the sequence 0,I; see Fig. 3(d).

V. CONCLUSIONS

The formalism for the treatment of the infinite-range anisotropic spin Hamiltonian with axial symmetry was presented. It constitutes a rather straightforward extension of the isotropic case. Three types of solutions are obtained: an XY-type solution for which the magnetization lies in the XY plane, an intermediate-type solution, for which the magnetization is tilted relative to the z axis, and an Ising-type solution, for which the magnetization is parallel to the z axis. Some analytical and numerical results were presented for a family of Hamiltonians containing quadratic and quartic terms.

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