Conditions for a ferromagnetic ground state of Ising and Heisenberg models with an external magnetic field

H. P. Bader

Institut für Theoretische Physik, Eidgenössische Technische Hochschule, CH-8093 Zürich, Switzerland

R. Schilling

Institut für Physik der Universiät Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland (Received 9 March 1981; revised manuscript received 28 May 1981)

For the isotropic Heisenberg Hamiltonian with ferromagnetic nearest-, antiferromagnetic next-nearest-neighbor interactions, and an external magnetic field: $H = J_1 \sum_{n, NN} \vec{S}_n \cdot \vec{S}_{n+\delta_1}$

 $+J_2 \sum_{n,NNN} \vec{S}_n \cdot \vec{S}_{n+\delta_2} - h \sum_n S_n^z$, $J_1 < 0$, $J_2 > 0$ necessary and sufficient conditions for a ferromagnetic ground state are obtained for some Bravais lattices with periodic boundaries and arbitrary spin s. For the square and cubic lattices the sufficient conditions possess a nontrivial s dependence. These conditions are compared with the thresholds for the Ising and classical Heisenberg model. Threshold inequalities are generalized to the case $h \neq 0$. The zero-temperature magnetization and susceptibility are discussed for the classical and quantum case. For the square lattice with only 4 sites the magnetization as function of h shows a qualitatively different behavior in the quantum case for $|J_1|/J_2 < 1$ and $|J_1|/J_2 > 1$, respectively. Sufficient, necessary, and threshold conditions are also derived for the nearest-neighbor antiferromagnet and the Heisenberg model with arbitrary coupling constants (J_1, \ldots, J_r) in an external field.

I. INTRODUCTION

In three preceding papers¹⁻³ (referred to as I–III) we studied the Ising, classical, and mainly the quantum-mechanical Heisenberg model with ferromagnetic nearest-neighbor (NN) and antiferromagnetic next-nearest-neighbor (NNN) interactions.

In I and II we presented a method to derive sufficient conditions (suff. cond.) for a ferromagnetic ground state (FGS) of the quantum Heisenberg Hamiltonian for all Bravais lattices. The important feature of the results was that the suff. cond. but also the necessary conditions (nec. cond.) depended on the spin s for some lattices, e.g., the square and the cubic lattices.

The inequalities for the thresholds $\alpha^{(1s)}$, $\alpha^{(\text{Heis})}_{cl}$, and $\alpha^{(\text{Heis})}_{qm}$, which were proved in III for arbitrary lattices, allowed the prediction of an *s* dependence of $\alpha^{(\text{Heis})}_{qm}$ for lattices with $\alpha^{(\text{Heis})}_{cl} = \alpha^{(1s)}$. The results of II were in full agreement with the prediction. In the classical spin limit $s \rightarrow \infty$ the quantum and classical results became equal.

There are several reasons for extending the studies of I-III to the Heisenberg Hamiltonian with an external field:

$$H = \sum_{(nm)} J_{nm} \vec{\mathbf{S}}_n \cdot \vec{\mathbf{S}}_m - h \sum_n S_n^z , \qquad (1)$$

where \overline{S}_n is the spin operator at site *n*, J_{nm} the coupling constants, $h = \mu_B g B > 0$ and pairs are only counted once in the sums.

(i) Even for antiferromagnetic NN interactions the question for FGS gets nontrivial.

(ii) For ferromagnetic NN and antiferromagnetic NNN interactions a magnetic field will reduce the threshold condition for $|J_1|/J_2$ derived in I and II. It is of interest to investigate this reduction as function of s, the dimension, and lattice type.

(iii) In particular the ground-state magnetization and susceptibility are important.

(iv) Concerning the experimental investigation the h dependence in constrast to the $(J_1 - J_2)$ dependence is easier to measure.

The zero-temperature magnetization and susceptibility as functions of *h* follow from the ground-state energy. This was investigated during the last 15 years for the corresponding classical Heisenberg-and-Ising model.⁴⁻¹² Let us summarize some results of these works. For the classical Heisenberg model with energy $E = \sum_{(nm)} J_{nm} \vec{S}_n \cdot \vec{S}_m - h \sum_n S_n^2$ and periodic boundaries Broughton and Mullin⁴ calculated the ground state and ground-state energy generalizing the Luttinger-Tisza method. From their results follows immediately the threshold condition for FGS:

$$\frac{h}{s} > J(0) - J(\vec{k}_0) ,$$

$$J(\vec{k}_0) = \min_{\vec{k}} J(\vec{k}) , \qquad (2)$$

where $J(\vec{k}) = \sum_{m} J_{nm} e^{i \vec{k} \cdot (\vec{R}_{n} - \vec{R}_{m})}$ is the Fourier transform of the coupling constants. This condition

<u>24</u>

2570

©1981 The American Physical Society

is equal to the spin-wave stability condition (SWSC) as shown in Sec. II. Therefore the SWSC in Tables I and III are also the classical threshold conditions. For the Ising model (spin s) with magnetic field, conditions for FGS were studied up to second- or higher-neighbor interactions.⁵⁻¹² The results for the threshold conditions are presented in Tables I and III. Actually they can also be derived as described in paper II Sec. IV.

It is easily seen that the threshold conditions for the Ising and the classical Heisenberg model are always of the form

$$\frac{h}{s} > f(\{J_{nm}\})$$

where f is s independent. For the quantum case there may be a nontrivial s dependence, i.e., f depends on s.

For the quantum case, concerning the ground-state properties, mainly the magnetization and susceptibility as functions of h, there are only few exact results. The most important is the work by Griffiths¹³ investigating the infinite NN-antiferromagnetic Heisenberg chain with $s = \frac{1}{2}$.

The purpose of this paper is to study the influence of an external magnetic field on some ground-state properties extending the results of I–III. We consider only systems with periodic boundaries.

In Sec. II we begin with the simplest nontrivial case, the NN antiferromagnet in a magnetic field, called the (J,h) model. An extension to systems up to *r* th-neighbor interactions $[(J_1, \ldots, J_r, h) \mod l]$ is suggested. The conditions thus derived are not stringent if one or more of the couplings are ferromagnetic. However, they can be improved. We demonstrate this procedure in Sec. IV for the simplest case, the $(-|J_1|, J_2, h) \mod l$. In Sec. V. we study the zero temperature magnetization and susceptibility for the same model. Section VI presents a

generalization of the threshold inequalities and the study of the nontrivial spin dependence, which is helpful for the discussion of the results.

II. NECESSARY AND SUFFICIENT CONDITIONS FOR FGS OF THE (J,h) MODEL

In this section we drive conditions for FGS for the following Hamiltonian:

$$H = J \sum_{n, NN} \vec{S}_n \cdot \vec{S}_{n+b_1} - h \sum_n S_n^z, \quad J > 0, \quad h > 0 \quad . \tag{3}$$

A. Necessary conditions

Using the one-magnon energies we get

$$\frac{h}{s} > J(0) - J(\vec{k}), \text{ for all } \vec{k} \neq 0 , \qquad (4)$$

as nec. cond., which coincides with condition (2). Thus as in I and II the SWSC does not lead to a nontrivial spin dependence. Discussion of (4) leads to the nec. cond. presented in Table I.

B. Sufficient conditions

Decomposing Hamiltonian (3) into cell operators

$$H^{(m)} = \tilde{J} \sum_{1 \leq i < j \leq m} \vec{S}_i \cdot \vec{S}_j - \tilde{h} \sum_{i=1}^m S_i^z$$

as described in I and II, we get for suff. cond. using $H^{(2)}$

$$\frac{h/s}{J} > 2z_1 \tag{5}$$

for all lattices. z_1 is the number of NN. Using $H^{(m)}$ with m > 2 for the hexagonal and fcc lattice, which

TABLE I. Threshold values for FGS for the (J,h) Ising, classical and quantum Heisenberg model. The classical and quantum thresholds are valid for N_i even (except for the hexagonal lattice, where N_i is a multiple of 3). N_i is the number of sites in directions of the primitive vectors. For other N_i the classical thresholds (which are necessary in the quantum case) differ in order $(1/N_i)^2$ from the above values.

Dimension	Lattice	Classical and quantum thresholds $\frac{h/s}{J}$	Ising thresholds $\frac{h/s}{J} = z_1$
. 1	Linear	4	2
2	Square	8	4
2	Hexagonal	9	6
3	Cubic P	12	6
3	Cubic I	16	8
3	Cubic F	16	12

<u>24</u>

are better adapted to the topology, the suff. cond. (5) can be improved leading also to the agreement with the nec. cond. The threshold conditions thus obtained are presented in Table I, which also contains those of the corresponding Ising model.⁶

III. NECESSARY AND SUFFICIENT CONDITIONS FOR FGS OF THE (J_1, \ldots, J_r, h) MODEL

In this section we study the more general Hamiltonian:

$$H = \sum_{l=1}^{r} \frac{J_l}{2} \sum_{n, \delta_l} \vec{\mathbf{S}}_n \cdot \vec{\mathbf{S}}_{n+\delta_l} - h \sum_n S_n^z \quad . \tag{6}$$

 $\vec{\delta}_I$ are the vectors to the /th NN and J_I the /th NN coupling constants.

A. Necessary condition

For r arbitrary, the discussion of the SWSC is too laborious. But using a lower bound for the SWSC we get for a nec. cond.:

$$\frac{h}{s} > J(0) = \sum_{l=1}^{r} z_l J_l \quad , \tag{7}$$

where z_l is the number of *l*th NN.

B. Sufficient condition

To apply the results of the last section, we decompose the Hamiltonian (9) as follows:

$$H = \sum_{l}' H_{l}(\lambda_{l}) + \sum_{l}'' H_{l}(0) , \qquad (8)$$

where

$$H_{l}(\lambda_{l}) = \frac{J_{l}}{2} \sum_{n, \delta_{l}} \vec{S}_{n} \cdot \vec{S}_{n+\delta_{l}} - \lambda_{l} h \sum_{n} S_{n}^{z}$$

and $\sum_{l=1}^{\prime} \lambda_{l} = 1$. $\sum_{l=1}^{\prime} \lambda_{l} = 1$. Testrict the sum to all l with $J_{l} > 0$ and $J_{l} < 0$, respectively. Taking into account that the ground state of $\sum_{l=1}^{\prime\prime} H_{l}(0)$ is always ferromagnetic, we get for a suff. cond.

$$\frac{h}{s} > \sum_{l=1}^{r} J_l \alpha_l^{(\text{Heis})} , \qquad (9)$$

where $\alpha_l^{(\text{Heis})}$ is the threshold condition of the (J_l, h) model. Using (5) we get an upper bound of condition (9):

$$\frac{h}{s} > 2 \sum_{l=1}^{r} J_l z_l \quad . \tag{10}$$

Thus the suff. cond. is different from the necessary one (7). Whether condition (10) or the lower bound (7) is rough, depends on the lattice and the interactions. For some cases, e.g., the linear chain with Neven, $J_l = 0$ for l even and $J_l > 0$ for l odd, condition (10) is also necessary (SWSC!). In contrast, for the linear chain with $J_l = J/l$, J > 0 (see below) condition (7) is a good approximation to the threshold condition. Conditions (7) and (10) allow us to determine nec. and suff. cond. for (6) with

$$J_l = J/l^{\beta}, J > 0, \beta > 0$$

e.g., for the simple-cubic lattice we get for $r \approx N^{1/3}$ >> 1

$$\frac{h}{s} > 4\pi J \times \begin{cases} \frac{1}{3} \ln(N) \operatorname{nec.} \\ \frac{2}{3} \ln(N) \operatorname{suff.} \text{ for } \beta = 3 \\ \frac{1}{\beta - 3} \operatorname{nec.} \\ \frac{2}{\beta - 3} \operatorname{suff.} \text{ for } \beta > 3 \end{cases}$$

If some J_l are negative, condition (10) is in general too rough, because it does not depend on the ferromagnetic couplings. Therefore in the next section we will improve the sufficient condition for the simplest nontrivial model, the $(-|J_1|, J_2, h)$ model.

IV. NECESSARY AND SUFFICIENT CONDITIONS FOR FGS OF THE $(-|J_1|, J_2, h)$ MODEL

In this section we study the simplest case of a model with both ferromagnetic and antiferromagnetic interactions, the $(-|J_1|, J_2, h)$ model, described by the Hamiltonian:

$$H = -|J_1| \sum_{n, \text{NN}} \vec{S}_n \cdot \vec{S}_{n+\delta_1} + J_2 \sum_{n, \text{NNN}} \vec{S}_n \cdot \vec{S}_{n+\delta_2} - h \sum_n S_n^z \quad .$$
(11)

A discussion of the function $J(\vec{k})$ for this model leads to the nec. cond. for FGS presented in Table

TABLE II. Quantum and Ising thresholds for the "m," A, B, and C cell.

Cell	Quantum threshold	Ising threshold
m	$\frac{h/s}{J} > m$	$\frac{h/s}{J} > m - 1$
A	$\frac{ J_1 }{J_2} + \frac{h/s}{J_2} > 2$	$\frac{ J_1 }{J_2} + \frac{h/s}{J_2} > 1$
B	$\frac{ J_1 }{J_2} \left(2 - \frac{1}{2s} \right) + \frac{h/s}{J_2} > 2 , \frac{ J_1 }{J_2} \le 1$ $\frac{ J_1 }{J_2} + \frac{h/s}{J_2} > 1 + \frac{1}{2s} , \frac{ J_1 }{J_2} \ge 1$	$\frac{ J_1 }{J_2} + \frac{h/s}{J_2} > 1$
С	$\frac{ J_1 }{J_2} + \frac{h/s}{J_2} > 3$	$\frac{ J_1 }{J_2} + \frac{h/s}{J_2} > 2$

TABLE III. and hexagonal	Necessary and suffic lattice, where $N_i \rightarrow \circ$	ient conditions for FGS and ∞ and for the cubic <i>I</i> , where	the Ising thresholds for the $(- J_1 , J_2, n)$ mo N_i is a multiple of 4). For other N_i the nece	del. The necessary conditions hold essary conditions differ from the a	for N even (except for the linear bove values in order $(1/N^2)$.
Qimension	Lattice	Necessary	Sufficient method A	Sufficient method B	Ising threshold
-	Linear	$\frac{ J_1 }{J_2} + 2\left(\frac{h/s}{J_2}\right)^{1/2} > 4$	$\frac{ J_1 }{J_2} + \frac{2}{3} \frac{h/s}{J_2} > 4$	$\frac{ J_1 }{J_2} + \frac{h/s}{J_2} > 4$	$\frac{ J_1 }{J_2} + \frac{h/s}{J_2} > 2$
2	Square	$\frac{ J_1 }{J_2} + \frac{1}{4} \frac{h/s}{J_2} > 2$	$\frac{ J_1 }{J_2} \left\{ 1 - \frac{1}{4s} \right\} + \frac{1}{4} \frac{h/s}{J_2} > 2, \frac{ J_1 }{J_2} \le 2$ $\frac{ J_1 }{J_2} + \frac{1}{2} \frac{h/s}{J_2} > 2 \left\{ 1 + \frac{1}{2s} \right\}, \frac{ J_1 }{J_2} \ge 2$	$\frac{ J_1 }{J_2} + \frac{1 + \frac{1}{2s}}{4} \frac{h/s}{J_2} > 2\left[1 + \frac{1}{2s}\right]$	$\frac{ J_1 }{J_2} + \frac{1}{2} \frac{h/s}{J_2} > 2$
7	Hexagonal	$\frac{ J_1 }{J_2} + \left(\frac{h/s}{J_2}\right)^{1/2} > 3$	$\frac{ J_1 }{J_2} + \frac{1}{4} \frac{h/s}{J_2} > 3$	$\frac{ J_1 }{J_2} + \frac{1}{3}\frac{h/s}{J_2} > 3$	$\frac{ J_1 }{J_2} + \frac{1}{4} \frac{h/s}{J_2} > \frac{3}{2}, \frac{ J_1 }{J_2} \le 1$ $\frac{ J_1 }{J_2} + \frac{1}{2} \frac{h/s}{J_2} > 2, \frac{ J_1 }{J_2} \ge 1$
m	Cubic P	$\frac{ J_1 }{J_2} + \frac{1}{4} \frac{h/s}{J_2} > 4$	$\frac{ J_1 }{J_2} \left\{ 1 - \frac{1}{4s} \right\} + \frac{1}{6} \frac{h/s}{J_2} > 4, \frac{ J_1 }{J_2} \leqslant 4$ $\frac{ J_1 }{J_2} + \frac{1}{3} \frac{h/s}{J_2} > 4 \left\{ 1 + \frac{1}{2s} \right\}, \frac{ J_1 }{J_2} \geqslant 4$	$\frac{ J_1 }{J_2} + \frac{1 + \frac{1}{2s}}{4} \frac{h/s}{J_2} > 4\left[1 + \frac{1}{2s}\right]$	$\frac{ J_1 }{J_2} + \frac{1}{4} \frac{h/s}{J_2} > 3, \frac{ J_1 }{J_2} \leqslant 2$ $\frac{ J_1 }{J_2} + \frac{1}{2} \frac{h/s}{J_2} > 4, \frac{ J_1 }{J_2} \geqslant 2$
Ω	Cubic I	$\frac{ J_1 }{J_2} + \frac{1}{8} \frac{h/s}{J_2} > \frac{3}{2}$	$\frac{ J_1 }{J_2} \left[1 - \frac{1}{4s} \right] + \frac{1}{8} \frac{h/s}{J_2} > \frac{3}{2}, \frac{ J_1 }{J_2} \le \frac{3}{2} \\ \frac{ J_1 }{J_2} + \frac{1}{4} \frac{h/s}{J_2} > \frac{3}{2} \left[1 + \frac{1}{2s} \right], \frac{ J_1 }{J_2} \ge \frac{3}{2} $	$\frac{ J_1 }{J_2} + \frac{1 + \frac{1}{2s}}{8} \frac{h/s}{J_2} > \frac{3}{2} \left[1 + \frac{1}{2s} \right]$	$\frac{ J_1 }{J_2} + \frac{1}{4} \frac{h/s}{J_2} > \frac{3}{2}$
ŝ	Cubic F	$\frac{ J_1 }{J_2} + \frac{1}{12} \frac{h/s}{J_2} > 1$	$\frac{ J_1 }{J_2} \left[1 - \frac{1}{4s} \right] + \frac{1}{12} \frac{h/s}{J_2} > 1, \frac{ J_1 }{J_2} \leqslant 1$ $\frac{ J_1 }{J_2} + \frac{1}{6} \frac{h/s}{J_2} > 1 + \frac{1}{2s}, \frac{ J_1 }{J_2} \geqslant 1$	$\frac{ J_1 }{J_2} + \frac{1 + \frac{1}{2s}}{12} \frac{h/s}{J_2} > 1 + \frac{1}{2s}$	$\frac{ J_1 }{J_2} + \frac{1}{6} \frac{h/s}{J_2} > 1$

<u>24</u>

CONDITIONS FOR A FERROMAGNETIC GROUND STATE OF . . .

2573

III. Suff. cond. can be derived with the following two methods:

A. Cell method

The Hamiltonian (11) is decomposed into the same cells as in II, of course with a magnetic field. The threshold conditions for these cells are presented in Table II and lead to the sufficient conditions shown in Table III.

B. (λ_1, λ_2) method

To use the known results we decompose the Hamiltonian (11) as follows:

$$H = H_1(\lambda_1) + H(\lambda_2) \quad , \tag{12}$$

$$H_{1}(\lambda_{1}) = -|J_{1}| \sum_{n, \text{NN}} \vec{S}_{n} \cdot \vec{S}_{n+\delta_{1}} + \lambda_{1}J_{2} \sum_{n, \text{NNN}} \vec{S}_{n} \cdot \vec{S}_{n+\delta_{2}} , \qquad (12a)$$

$$H_2(\lambda_2) = \lambda_2 J_2 \sum_{n,\text{NNN}} \vec{S}_n \cdot \vec{S}_{n+\delta_2} - h \sum_n S_n^z , \quad (12b)$$

with

$$\lambda_1 + \lambda_2 = 1 \quad . \tag{13}$$

This decomposition leads to the suff. cond.:

$$\alpha_{J_{2},\hbar} \frac{|J_{1}|}{J_{2}} + \alpha_{J_{1}J_{2}} \frac{h/s}{J_{2}} > \alpha_{J_{1}J_{2}} \alpha_{J_{2},\hbar} \quad , \tag{14}$$

where $\alpha_{J_1J_2}$ and $\alpha_{J_2,h}$ are the thresholds of the (J_1, J_2) model and (J_2, h) model, respectively. Taking $\alpha_{J_1J_2}$ or if not known exactly the upper bounds given in Table III of paper (II) and $\alpha_{J_2,h}$ of Table I of this paper we obtain the suff. cond. presented in Table III.

V. MAGNETIZATION AT 0 K

The zero-temperature magnetization for some Ising systems were already discussed.⁵⁻¹² For the NN-antiferromagnetic chain with $s = \frac{1}{2}$ the magnetization is presented in Fig. 1. For more than NN interaction there can be more than one step. The magnetization for the classical⁴ and the $s = \frac{1}{2}$ quantum (NN) antiferromagnet¹³ are also presented in Fig. 1.



FIG. 1. Magnetization for the quantum (----), classical (---), and Ising (---) NN antiferromagnetic linear chain with $s = \frac{1}{2}$.

For more than (NN) interactions there are to our knowledge no results for the magnetization for the quantum case. We have solved the eigenvalue problem for the A cell (linear chain, N = 3, open boundary) and the B cell (square lattice, N = 4, open or periodic boundaries). For notation see Paper II. The ground-state magnetization is presented in Figs. 2 and 3, respectively. For an illustration, the ferromagnetic region G_F for the B cell, defined in the next section, is presented in Fig. 4. The B cell shows the interesting feature that the behavior of the magnetization depends strongly on $|J_1|/J_2$.



FIG. 2. Magnetization for the quantum and classical (---) open linear chain (N=3). The reason for $\sigma^{z}(0) \neq 0$ is the odd number of spins.

2574



FIG. 3. Magnetization for the quantum square lattice (N = 4) for the cases: (a): $|J_1|/J_2 < 1$ and (b): $|J_1|/J_2 > 1$.

VI. THRESHOLD INEQUALITIES

Let $G_F = \{(J_1, \ldots, J_r, h)/(J_1, \ldots, J_r, h) \text{ model}$ has only FGS}, then the inequalities in III are replaced for h = 0 by^{14, 15}

(i) $G_F^{(1s)} \supset G_F^{(\text{Heis})}_{qm}$, (ii) $G_F^{(1s)} \supseteq G_F^{(\text{Heis})}_{cl}$, (iii) $G_F^{(\text{Heis})}_{cl} \supseteq G_F^{(\text{Heis})}_{qm}$.

For $h \neq 0$ (i) and (iii) remain true. However inequality (ii) must be replaced by

 $(\mathrm{ii}') \, G_F^{(\mathrm{ls})} \supset G_{F_{\mathrm{cl}}}^{(\mathrm{Heis})} \quad .$

The equality is excluded because a nonferromagnetic ground-state spin configuration of the Ising model is



FIG. 4. Ferromagnetic region G_F for the square lattice with 4 sites (*B* cell).

never a ground-state spin configuration of the corresponding classical Heisenberg model for $h \neq 0.4$ The exclusion of the equality sign in (ii') makes a prediction of a nontrivial *s* dependence as described in III impossible. However, because of the continuity of the threshold¹⁵ $G_{f_{qm}}^{(\text{Heis})}$ has a nontrivial *s* dependence for *h* small compared to J_i 's if it possesses such a one for h = 0.

VII. DISCUSSION

Generalizing the ideas of papers I and II, nec. and suff. cond. for FGS of the (J,h), (J_1, \ldots, J_r, h) and $(-|J_1|, J_2, h)$ model were derived for some lattices. Using the SWSC we obtained nec. cond. which are also sufficient for the corresponding classical model. Let us make some comments on the results.

(i) For deriving suff. cond., besides the cell method, the (λ_i) method was used, leading to suff. cond. which, because of the linearity in the couplings, are the convex hull of the known sufficient sectors in the two-dimensional 2D subspaces $(J_i, J_j) i \neq j$ and (J_i, h) , respectively. In fact the convex hull of some regions, each contained in G_F , is itself contained in G_F because G_F is always(!) a convex (simple connected) cone in the (J_1, \ldots, J_r, h) space^{14, 15} (see, e.g., Fig. 4).

(ii) For some lattices the cell method works better than the (λ_i) method and vice versa. This can be understood by the convexity property.

(iii) As for h = 0 the suff. cond. for FGS of the $(-|J_1|, J_2, h)$ model possess a nontrivial s dependence for the square and cubic lattices in agreement with the prediction in Sec. V.

(iv) Rescaling the coupling constants and the field: $J_i \rightarrow J_i/s^2$, $h \rightarrow h/s$ the quantum conditions converge for $s \rightarrow \infty$ to the classical threshold conditions (excluding the linear and hexagonal lattices, which can be understood), in agreement with the classical spin limit.

(v) It is easily checked that the conditions in Tables I–III are consistent with the threshold inequalities in Sec. VI.

(vi) Last but not least the special behavior of the ground-state magnetization of the *B* cell should be mentioned. For $|J_1|/J_2 < \alpha_{cl}^{(\text{Heis})} = 1$ the magnetization shown in Fig. 3 is similar to that of the (NN)-antiferromagnetic chain in Fig. 1, except for the smoothness. However, for $\alpha_{cl}^{(\text{Heis})} < |J_1|/J_2 < \alpha_{qm}^{(\text{Heis})} = 1 + 1/2s$ there exists a critical field $h_c = s(J_2 - |J_1|) + J_2/2$ for which the susceptibility is singular. It may be that this behavior is not an artifact of the finite cell for two reasons. First, finite cells normally behave like the 1D chain (*A*, *C* cell and many others, not considered here) and second it seems plausible that for lattices with s-dependent thresholds for h = 0

the quantum system for $|J_1|/J_2 < \alpha_{cl}^{(\text{Heis})}$ behaves more like a NN antiferromagnet. This means that with variable *h* the ground state runs through all eigenspaces of \vec{S}^2 the square of the total spin.

eigenspaces of \overline{S}^2 the square of the total spin. For $\alpha_{cl}^{(\text{Heis})} < |J_1|/J_2 < \alpha_{qm}^{(\text{Heis})}(s)$ however the system may switch directly from S = 0 (antiferromagnetic) to S = Ns (ferromagnetic) at a critical field h_c . Thus with an external field, the classical threshold value would play an important role also for the quantum system.

The application of the methods is not restrictive to periodic boundaries, but can also be done for open boundaries.^{1,14,16}

ACKNOWLEDGMENT

We would like to thank Professor W. Baltensperger for carefully reading the manuscript.

- ¹H.-P. Bader and R. Schilling, Phys. Rev. B <u>19</u>, 3556 (1979).
- ²H.-P. Bader and R. Schilling, Phys. Rev. B <u>21</u>, 1304 (1980).
- ³R. Schilling and H.-P. Bader, Phys. Rev. B 20, 1977 (1979).
- ⁴H. W. Broughton and W. J. Mullin, Phys. Rev. B <u>6</u>, 277 (1972).
- ⁵T. Morita, J. Phys. A 7, 289 (1974).
- ⁶J. Kanamori, Prog. Theor. Phys. <u>35</u>, 16 (1966).
- ⁷Y. Tanaka and N. Uryû, J. Phys. Soc. Jpn. <u>39</u>, 825 (1975).
- ⁸T. Horiguchi and T. Morita, Phys. Lett. <u>41A</u>, 9 (1972).
- ⁹T. Kudo and S. Katsura, Prog. Theor. Phys. <u>56</u>, 435 (1976).
- ¹⁰S. Katsura and A. Narita, Prog. Theor. Phys. <u>50</u>, 1750 (1973).
- ¹¹T. Morita and T. Horiguchi, Phys. Lett. <u>38A</u>, 223 (1972).
- ¹²S. Katsura and A. Narita, Prog. Theor. Phys. <u>50</u>, 1426 (1973).
- ¹³R. B. Griffiths, Phys. Rev. <u>133</u>, A786 (1964).
- ¹⁴H.-P. Bader, Ph. D. dissertation (Eidgenossische Technische Hochschule, 1980) (unpublished).
- ¹⁵H.-P. Bader (unpublished).
- ¹⁶H.-P. Bader and R. Schilling (unpublished).

2576