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The magnetization process of an Ising-type frustrated $S = 1$ spin chain

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Abstract
The magnetization process of an Ising-type $S = 1$ spin chain with nearest-neighbour interaction (J_1), next-nearest-neighbour interaction (J_2) and single-ion anisotropy (D) is investigated on the basis of the ground state phase diagram of the chain in a magnetic field ($H \geqslant 0$). The 49 possible spin structures for the ground state are obtained using Morita's theorem. The magnetization process is obtained from the ground state phase diagram, giving J_2/J_1 versus H/J_1, determined by comparing the energies of the 49 spin structures. It is shown that (1) among the 49 spin structures, 14 structures with unit cells of $\langle+\rangle$, $\langle 0\rangle$, $\langle+-\rangle$, $\langle+0\rangle$, $\langle++-\rangle$, $\langle++0\rangle$, $\langle+-0\rangle$, $\langle+00\rangle$, $\langle++--\rangle$, $\langle++0-\rangle$, $\langle++00\rangle$, $\langle++-0\rangle$, $\langle+-+00\rangle$ and $\langle++-0+0-\rangle$ appear in the phase diagram; (2) the magnetization process is equivalent to that of the usual Ising model for $D \leqslant 0$; (3) a long period spin structure, $\langle++-0+0-\rangle$, is realized for the intermediate ranges of J_2/J_1 and D/J_1 due to the frustration of the system.

1. Introduction

A great deal of attention has been paid to the spin-1 Ising model with bilinear, biquadratic and single-ion anisotropy interactions, the Blume–Emery–Griffiths (BEG) model, because it exhibits a wide variety of phases. It has been used to describe not only the magnetic properties of the spin-1 magnets but also the properties of many systems ranging across helium mixtures [1], multicomponent fluids [2, 3], microemulsions [5], semiconductor alloys [4], liquid crystals [6] and adsorbate systems [7, 8]. The Hamiltonian of the model in a magnetic field is given as

$$\mathcal{H} = \sum_{i<j}\{J_{ij}\sigma_i\sigma_j + K_{ij}\sigma_i^2\sigma_j^2\} + D\sum_i \sigma_i^2 - H\sum_i \sigma_i, \tag{1}$$

where σ_i $(=\pm 1, 0)$ is a spin variable at the i site; J_{ij} and K_{ij} are respectively the exchange and biquadratic interactions between i and j sites; D and H represent respectively the single-ion anisotropy and the magnetic field. It should be noted that when the interactions satisfy the condition $K_{ij} = 3J_{ij}$, the Hamiltonian (1) is equivalent to the three-state Potts model [9, 10].

As regards the ground state analysis of the model in one dimension, the works done so far are, however, mostly concerned with models either without single-ion anisotropy [11] or in the absence of a magnetic field [8]. It is, therefore, most desirable to extend the ground state analysis to the case with single-ion anisotropy in a magnetic field. Another fascinating subject related to the present model may be the problem of fractional magnetization plateaus, because the $1/3$ plateau state appearing in the magnetization process in the spin-$1/2$ quantum spin model with next-nearest-neighbour interaction has recently been proved to remain at the Ising limit [12], suggesting importance of the analysis of the magnetization process of the present model at the Ising limit.

The purpose of the present study is to analyse the magnetization process by constructing the ground state phase diagram of the one-dimensional frustrated model in a magnetic field given by

$$\mathcal{H}_{1D} = \sum_{\ell=1}^{N} \left\{ \sum_{k=1}^{2} (J_k \sigma_\ell \sigma_{\ell+k} + K_k \sigma_\ell^2 \sigma_{\ell+k}^2) + D\sigma_\ell^2 - H\sigma_\ell \right\} \tag{2}$$

where N is the total number of lattice sites.

There are several methods of determining the ground state of the present model, which is equivalent to the three-component lattice gas model [8]. One is the method of geometrical inequalities employed in case of the one-dimensional Potts model [10]. Another method is energy comparison among the available structures obtained via the theorem (Morita's theorem) that for the one-dimensional classical lattice system, the ground state is proved to be a regular chain of blocks (unit cells) with maximum length determined by the range of interactions r and the number of states s_M on a lattice site [13]. In this paper, we employ the energy comparison method, focusing our attention on the case of antiferromagnetic nearest-neighbour (NN) interaction ($J_1 > 0$) without biquadratic interactions ($K_1 = K_2 = 0$), namely an Ising-type chain.

For the Ising-type chain without single-ion anisotropy ($D = 0$), the ground state phase diagram [11] is shown to be equivalent to that of the usual ($S = 1/2$) Ising chain with NN and next-nearest-neighbour (NNN) interactions [14] and no phase containing $\sigma_\ell = 0$ sites is realized. On the other hand, a system with positive single-ion anisotropy ($D > 0$) has a tendency to prefer the $\sigma_\ell = 0$ state; it is expected that the introduction of positive single-ion anisotropy may lead to the appearance of phases containing $\sigma_\ell = 0$ sites in the ground state phase diagram.

Using Morita's theorem, we shall obtain 49 spin structures as candidate ground state structures[4]. Taking J_1 as the unit of energy ($J_1 = 1$), we determine the ground state phase diagram in the J_2 versus H plane by comparing the energy of the 49 available spin structures. The phase diagram obtained exhibits a wide variety of phases including the phases containing $\sigma_\ell = 0$ sites. On the basis of the ground state phase diagram, the magnetization process of the system will be discussed.

The organization of this paper is as follows. In the next section (section 2), after reviewing Morita's theorem, we make a list of the candidate ground state spin structures using the theorem. Section 3 deals with the magnetization process obtained from the ground state phase diagram in the J_2 versus H plane constructed by comparison of the energies of the candidates. Finally, a summary and concluding remarks are given in section 4.

2. Candidate spin structures for the ground state

The simplest way of determining the ground state of a classical lattice system is to get the ground state as the state which has the lowest energy among various simple regular orderings.

[4] In [13], the author missed several spin structures satisfying the conditions of the theorem for $s_\mathrm{M} = 3$ and $r = 2$.

Table 1. The spin structure of the unit cell.

Label	Unit cell	p_1	p_2	q_1	q_2	n	m
$[1] = [\bar{2}]$	$\langle + \rangle$	1	1	1	1	1	1
[3]	$\langle 0 \rangle$	0	0	0	0	0	0
[4]	$\langle +- \rangle$	−1	1	1	1	1	0
$[5] = [\bar{6}]$	$\langle +0 \rangle$	0	1/2	0	1/2	1/2	1/2
$[7] = [\bar{9}]$	$\langle ++- \rangle$	−1/3	−1/3	1	1	1	1/3
$[8] = [\overline{12}]$	$\langle ++0 \rangle$	1/3	1/3	1/3	1/3	2/3	2/3
[10]	$\langle +0- \rangle$	−1/3	−1/3	1/3	1/3	2/3	0
$[11] = [\overline{13}]$	$\langle +00 \rangle$	0	0	0	0	1/3	1/3
[14]	$\langle ++-- \rangle$	0	−1	1	1	1	0
$[15] = [\overline{18}]$	$\langle ++0- \rangle$	0	−1/2	1/2	1/2	3/4	1/4
$[16] = [\overline{22}]$	$\langle ++00 \rangle$	1/4	0	1/4	0	1/2	1/2
$[17] = [\overline{19}]$	$\langle +-+0 \rangle$	−1/2	1/2	1/2	1/2	3/4	1/4
[20]	$\langle +00- \rangle$	−1/4	0	1/4	0	1/2	0
[21]	$\langle +0-0 \rangle$	0	−1/2	0	1/2	1/2	0
[23]	$\langle ++-0- \rangle$	−1/5	−1/5	3/5	3/5	4/5	0
$[24] = [\overline{28}]$	$\langle ++0-0 \rangle$	1/5	−2/5	1/5	2/5	3/5	1/5
$[25] = [\overline{27}]$	$\langle +-+00 \rangle$	−2/5	1/5	2/5	1/5	3/5	1/5
[26]	$\langle +--+0 \rangle$	−1/5	−1/5	3/5	3/5	4/5	0
[29]	$\langle ++-00- \rangle$	−1/6	−1/3	1/2	1/3	2/3	0
[30]	$\langle ++0--0 \rangle$	1/3	−1/3	1/3	1/3	2/3	0
[31]	$\langle +-+0-0 \rangle$	−1/3	−1/6	1/3	1/2	2/3	0
[32]	$\langle +--+00 \rangle$	−1/6	−1/3	1/2	1/3	2/3	0
[33]	$\langle +-0+0- \rangle$	−1/3	−1/6	1/3	1/2	2/3	0
[34]	$\langle +-0-+0 \rangle$	−1/3	1/3	1/3	1/3	2/3	0
$[35] = [\overline{40}]$	$\langle ++0-+0- \rangle$	−1/7	−3/7	3/7	3/7	5/7	1/7
$[36] = [\overline{39}]$	$\langle ++-0+0- \rangle$	−1/7	−4/7	3/7	4/7	5/7	1/7
$[37] = [\overline{38}]$	$\langle ++0-+-0 \rangle$	−1/7	−1/7	3/7	3/7	5/7	1/7
[41]	$\langle +0-+00- \rangle$	−2/7	−1/7	2/7	1/7	4/7	0
[42]	$\langle +-0-+00 \rangle$	−2/7	1/7	2/7	1/7	4/7	0
[43]	$\langle +-00-+0 \rangle$	−2/7	1/7	2/7	1/7	4/7	0
$[44] = [\overline{46}]$	$\langle ++-0++0- \rangle$	0	−1/2	1/2	1/2	3/4	1/4
[45]	$\langle +-+0-+-0 \rangle$	−1/2	0	1/2	1/2	3/4	0
$[47] = [\overline{48}]$	$\langle +-0+0-+0 \rangle$	−1/4	−1/8	1/4	3/8	5/8	1/8
[49]	$\langle +-00-+00 \rangle$	−1/4	0	1/4	0	1/2	0

Such an attempt has not always been justified. However, in the case of the one-dimensional classical lattice system with inversion symmetry, Morita proved the theorem that

(1) *the ground state energy can be produced by a regular chain of irreducible blocks with two or fewer symmetry points*;
(2) *the blocks consist of* $s_{\mathrm{M}}^{r} - s_{\mathrm{M}}^{[(r+1)/2]} + 2$ *or fewer sites*.

Here, s_{M} and r are the number of states (configurations) on a lattice site and the range of the interactions, respectively. In the present case of $s_{\mathrm{M}} = 3$ and $r = 2$, the maximum length of the unit cell equals 8. Applying the theorem, we obtain 49 spin structures listed in table 1 as candidate ground states. In the table, we show only the structures with non-negative magnetization, introducing notation which indicates the repeating unit of σ_ℓ as $\langle \sigma_1 \sigma_2 \cdots \sigma_n \rangle$; for example, $\langle +-0 \rangle$ represents the spin structure with the repeating unit $(\sigma_1 \sigma_2 \sigma_3) = (+1\, -1\, 0)$. Table 1 also lists the label [i] of the phase for the spin structures together with p_1, p_2, q_1, q_2,

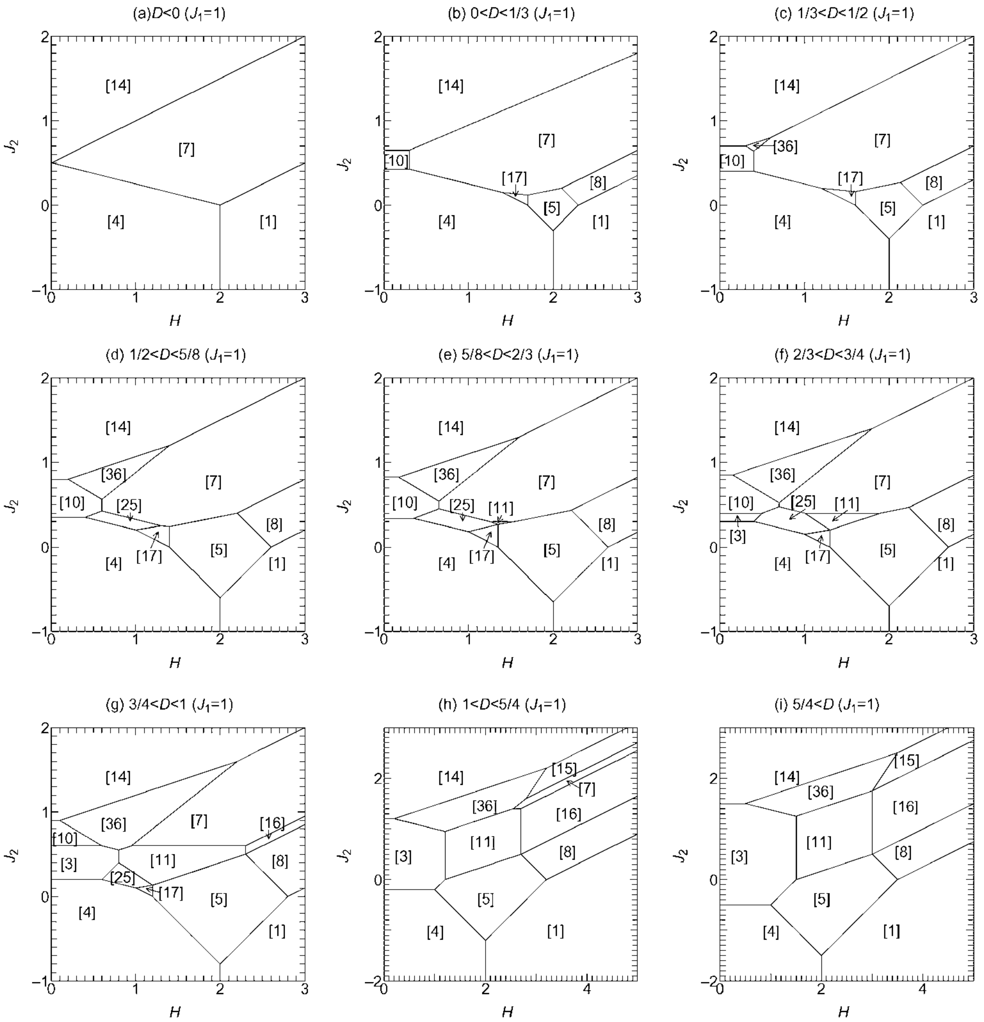

Figure 1. The ground state phase diagram in the J_2 versus H plane for the cases of (a) $D \leqslant 0$; (b) $0 < D \leqslant 1/3$; (c) $1/3 < D \leqslant 1/2$; (d) $1/2 < D \leqslant 5/8$; (e) $5/8 < D \leqslant 2/3$; (f) $2/3 < D \leqslant 3/4$; (g) $3/4 < D \leqslant 1$; (h) $1 < D \leqslant 5/4$; (i) $5/4 < D$.

n and m defined by

$$p_k = \frac{1}{N} \sum_{\ell} \sigma_\ell \sigma_{\ell+k} \qquad (k = 1, 2), \tag{3}$$

$$q_k = \frac{1}{N} \sum_{\ell} \sigma_\ell^2 \sigma_{\ell+k}^2 \qquad (k = 1, 2), \tag{4}$$

$$n = \frac{1}{N} \sum_{\ell} \sigma_\ell^2, \tag{5}$$

$$m = \frac{1}{N} \sum_{\ell} \sigma_\ell. \tag{6}$$

Table 2. Coefficients for the phase boundary line.

L(i, j)	($a_1, a_2, b_1, b_2, \delta n, \delta m$)	L(i, j)	($a_1, a_2, b_1, b_2, \delta n, \delta m$)
L([1], [4])	(2, 0, 0, 0, 0, 1)	L([1], [5])	(2, 1, 2, 1, 1, 1)
L([1], [7])	(2, 2, 0, 0, 0, 1)	L([1], [8])	(2, 2, 2, 2, 1, 1)
L([3], [4])	(1, −1, −1, −1, −1, 0)	L([3], [5])	(0, 1, 0, 1, 1, 1)
L([3], [10])	(1, 1, −1, −1, −2, 0)	L([3], [25])	(2, −1, −2, −1, −3, −1)
L([3], [36])	(1, 4, −3, −4, −5, −1)		
L([4], [5])	(−2, 1, 2, 1, 1, −1)	L([4], [7])	(−2, 4, 0, 0, 0, −1)
L([4], [10])	(−2, 4, 2, 2, 1, 0)	L([4], [17])	(−2, 2, 2, 2, 1, −1)
L([4], [25])	(−3, 4, 3, 4, 2, −1)		
L([5], [7])	(2, 5, −6, −3, −3, 1)	L([5], [8])	(−2, 1, −2, 1, −1, −1)
L([5], [11])	(0, 3, 0, 3, 1, 1)	L([5], [17])	(2, 0, −2, 0, −1, 1)
L([7], [8])	(−2, −2, 2, 2, 1, −1)	L([7], [10])	(0, 0, 2, 2, 1, 1)
L([7], [11])	(−1, −1, 3, 3, 2, 0)	L([7], [14])	(−1, 2, 0, 0, 0, 1)
L([7], [15])	(−4, 2, 6, 6, 3, 1)	L([7], [16])	(−7, −4, 9, 12, 6, −2)
L([7], [17])	(2, −10, 6, 6, 3, 1)	L([7], [25])	(1, −8, 9, 12, 6, 2)
L([7], [36])	(−4, 5, 12, 9, 6, 4)		
L([8], [16])	(1, 4, 1, 4, 2, 2)		
L([10], [14])	(−1, 2, −2, −2, −1, 0)	L([10], [25])	(1, −8, −1, 2, 1, −3)
L([10], [36])	(−4, 5, −2, −5, −1, −3)		
L([11], [16])	(3, 0, 3, 0, 2, 2)	L([11], [25])	(6, −3, −6, −3, −4, 2)
L([11], [36])	(3, 12, −9, −12, −8, 4)		
L([14], [15])	(0, −2, 2, 2, 1, −1)	L([14], [36])	(1, −3, 4, 3, 2, −1)
L([15], [16])	(−1, −2, 1, 2, 1, −1)	L([15], [36])	(4, 2, 2, −2, 1, 3)
L([17], [25])	(−2, 6, 2, 6, 3, 1)		

A label with a bar, [$\bar{\text{i}}$], denotes a phase obtained by reversing the spin variable σ_ℓ in the phase [i] to $-\sigma_\ell$. Although q_1 and q_2 are not needed for the present analysis, we list them because the information may make it straightforward to analyse the ground state of the case with biquadratic interactions.

3. The ground state phase diagram

The ground state phase diagram of the present system can be obtained by finding the state of lowest energy in each region of the space spanning the phase diagram. Since the energy phase with the spin structure listed in table 1 is given by

$$E(i) = N(J_1 p_1^i + J_2 p_2^i + K_1 q_1^i + K_2 q_2^i + Dn^i - Hm^i), \tag{7}$$

the equation for the phase boundary line L(i, j) between i and j phases is obtained by setting the energy difference

$$E(i) - E(j) = Nc^{ij}(J_1 a_1^{ij} + J_2 a_2^{ij} + K_1 b_1^{ij} + K_2 b_2^{ij} + D\,\delta n^{ij} - H\,\delta m^{ij}), \tag{8}$$

where

$$\begin{aligned} a_k^{ij} &= c^{ij}(p_k^i - p_k^j), \qquad & b_k^{ij} &= c^{ij}(q_k^i - q_k^j), \\ \delta n^{ij} &= c^{ij}(n^i - n^j), \qquad & \delta m^{ij} &= c^{ij}(m^i - m^j), \end{aligned} \tag{9}$$

to zero as

$$\mathrm{L}(i, j); \qquad (J_1 a_1^{ij} + J_2 a_2^{ij} + K_1 b_1^{ij} + K_2 b_2^{ij} + D\,\delta n^{ij} - H\,\delta m^{ij}) = 0. \tag{10}$$

As was stated in the introduction, we focus our attention in this paper on the case of antiferromagnetic NN interaction ($J_1 > 0$) without biquadratic interactions ($K_1 = K_2 = 0$).

Table 3. Multi-critical points.

P (phases)	(H, J_2)	Related figures
P([1], [4], [5])	$(2, -D)$	(b), (c), (d), (e), (f), (g), (h), (i)
P([1], [4], [7])	$(2, 0)$	(a)
P([1], [5], [8])	$(2 + D, 0)$	(b), (c), (d), (e), (f), (g), (h), (i)
P([3], [4], [5])	$(1, 1 - D)$	(h), (i)
P([3], [4], [25])	$(-1 + 2D, 1 - D)$	(f), (g)
P([3], [5], [11])	$(D, 0)$	(h), (i)
P([3], [10], [25])	$(-3 + 5D, -1 + 2D)$	(f)
P([3], [10], [36])	$(3 - 3D, -1 + 2D)$	(g)
P([3], [11], [25])	$(D, 2(1 - D))$	(g)
P([3], [11], [36])	$(D, (-1 + 4D)/4)$	(g), (h), (i)
P([3], [14], [36])	$(-1 + D, D)$	(h), (i)
P([4], [5], [17])	$(2 - D, 0)$	(b), (c), (d), (e), (f), (g)
P([4], [7], [10])	$(D, (2 - D)/4)$	(b), (c)
P([4], [7], [14])	$(0, 1/2)$	(a)
P([4], [7], [17])	$(2 - 2D, D/2)$	(b), (c)
P([4], [10], [25])	$(1 - D, (2 - D)/4)$	(d), (e)
P([4], [17], [25])	$(1, (1 - D)/2)$	(d), (e), (f), (g)
P([5], [7], [8])	$((6 + D)/3, 2D/3)$	(b), (c), (d), (e), (f)
P([5], [7], [11])	$(-3 + 7D, -1 + 2D)$	(e), (f)
P([5], [7], [17])	$(2 - D, 2D/5)$	(b), (c), (d)
P([5], [8], [11], [16])	$((3 + 2D)/2, 1/2)$	(g), (h), (i)
P([5], [11], [17], [25])	$(2 - D, 2(1 - D)/3)$	(e), (f), (g)
P([7], [10], [14])	$(D, (1 + D)/2)$	(b)
P([7], [10], [25])	$(D, (1 + 4D)/8)$	(d), (e), (f)
P([7], [10], [36])	$(D, 2(2 - D)/5)$	(c), (d), (e), (f)
P([7], [11], [16])	$((3 + 2D)/2, -1 + 2D)$	(g), (h)
P([7], [11], [25])	$((9 - 10D)/2, -1 + 2D)$	(e), (f)
P([7], [11], [36])	$((-9 + 16D)/4, -1 + 2D)$	(g), (h)
P([7], [14], [36])	$(-1 + 4D, 2D)$	(c), (d), (e), (f), (g)
P([7], [15], [36])	$(4 - D, 2(2 - D))$	(h)
P([7], [17], [25])	$((-1 + 6D)/2, 1/4)$	(d)
P([10], [14], [36])	$((1 - D)/2, (1 + D)/2)$	(c), (d), (e), (f), (g)
P([11], [15], [16], [36])	$((3 + 2D)/2, (1 + 4D)/4)$	(i)
P([14], [15], [36])	$(2 + D, 1 + D)$	(h), (i)

Hereafter we take J_1 as the unit of energy ($J_1 = 1$); this means that J_2, D and H (>0) should be read as J_2/J_1, D/J_1 and H/J_1, respectively. It is easily shown in this case that the phases appearing with non-negative magnetization are $[1] = \langle + \rangle$, $[3] = \langle 0 \rangle$, $[4] = \langle +- \rangle$, $[5] = \langle +0 \rangle$, $[7] = \langle ++- \rangle$, $[8] = \langle ++0 \rangle$, $[10] = \langle +0- \rangle$, $[11] = \langle +00 \rangle$, $[14] = \langle ++-- \rangle$, $[15] = \langle ++0- \rangle$, $[16] = \langle ++00 \rangle$, $[17] = \langle +-+0 \rangle$, $[25] = \langle +-+00 \rangle$ and $[36] = \langle ++-0+0- \rangle$, and the phases containing the $\sigma_\ell = 0$ site are, as expected, realized.

In figures 1(a)–(i), we show the phase diagram for each case. It should be noted that the phase diagram for case (a) of $D \leqslant 0$ is equivalent to that of the usual Ising chain [14]. We also note that a long period structure [36] ($\langle ++-0+0- \rangle$) is realized for intermediate values of J_2.

The phase boundary lines in the phase diagram can be obtained from table 2 which lists the coefficients a_1^{ij}, a_2^{ij}, b_1^{ij}, b_2^{ij}, δn^{ij} and δm^{ij} for the phases of the present system appearing.

Table 3 gives the coordinates (H, J_2) of the multi-critical points $\mathrm{P}(i_1, \ldots, i_k)$, at which phases $i_1, \ldots, i_k$ ($k = 3$ or 4) meet, in the phase diagram as a function of D.

The magnetization process for each region of D and J_2 is easily obtained from figures 1(a) to (i), combining the results shown in tables 2 and 3. For example, in case (a) of $D \leqslant 0$, the magnetization process with increasing magnetic field H is obtained as

for $J_2 \leqslant 0$: [4] $\rightarrow$ [1];
for $0 < J_2 \leqslant 1/2$: [4] $\rightarrow$ [7] $\rightarrow$ [1];
for $1/2 < J_2$: [14] $\rightarrow$ [7] $\rightarrow$ [1].

The critical field H_c^{ij} at which the transition from the i phase to the j phase takes place can be easily obtained from the values of a_1^{ij}, a_2^{ij}, δn^{ij} and δm^{ij} listed in table 2:

$$H_c^{ij} = (a_1^{ij} + J_2 a_2^{ij} + D\,\delta n^{ij})/\delta m^{ij}. \tag{11}$$

For example, the critical fields for transitions from [4] to [1], from [4] to [7], from [7] to [1] and from [14] to [7] are respectively obtained as $H_c = 2$, $2 - 4J_2$, $2 + 4J_2$ and $2J_2 - 1$.

In the same way, we can construct the magnetization processes for all other cases.

4. Summary

The magnetization process of an Ising-type $S = 1$ spin chain with antiferromagnetic NN interaction ($J_1 = 1$), NNN interaction (J_2) and single-ion anisotropy (D) is investigated on the basis of the ground state phase diagram of the chain in a magnetic field ($H \geqslant 0$). The 49 possible spin structures for the ground state are obtained using Morita's theorem. The magnetization process is obtained from the ground state phase diagram giving J_2 versus H, determined by comparing the energies of the 49 spin structures. It is shown that

(1) among the 49 spin structures, 14 structures with unit cells of $\langle+\rangle$, $\langle 0\rangle$, $\langle+-\rangle$, $\langle+0\rangle$, $\langle++-\rangle$, $\langle++0\rangle$, $\langle+-0\rangle$, $\langle+00\rangle$, $\langle++--\rangle$, $\langle++0-\rangle$, $\langle++00\rangle$, $\langle++-0\rangle$, $\langle+-+00\rangle$, $\langle++-0+0-\rangle$ appear in the phase diagram;
(2) the magnetization process is equivalent to that of the usual Ising model for $D \leqslant 0$;
(3) a long period phase with spin structure $\langle++-0+0-\rangle$ is realized for intermediate ranges of J_2 and D due to the frustration of the system.

The phase diagram obtained in the present study will be a keystone for the analysis of the fractional magnetization plateaus in the quantum version of the present model.

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