Exact ground-state diagrams for the generalized Blume-Emery-Griffiths model

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A simple way for constructing exact ground-state diagrams of classical spin models with nearest- or (in certain cases) also with next-to-nearest-neighbor interactions is proposed for a large class of lattices. Such diagrams are constructed for the most general spin-1 Ising model on the unfrustrated lattices with nearest-neighbor interaction. Nine topologically different diagrams are found. The same model is considered on the triangular lattice and on the square lattice with nearest- and next-to-nearest-neighbor interactions. Intermediate nonuniform phases are revealed and the conditions of their nonexistence are obtained.

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In 1971 in Ref. 1, Blume, Emery, and Griffiths considered an incomplete spin-1 Ising model in the mean field approximation and applied it to a concrete physical object, namely, to the ^{3}He-^{4}He mixture. Since then this model has been studied intensively and used to describe different physical objects such as gas-liquid-solid systems,[2] multicomponent fluids and liquid crystal mixtures,[2] semiconductor alloys,[3] microemulsions,[4] adsorbate systems,[5] and intercalated crystals,[6] etc. To our surprise, we have nowhere found an *exact* description of the ground states of this model on different two- and three-dimensional lattices. It seems that only the ground states of the one-dimensional Blume-Emery-Griffiths (BEG) model with nearest-neighbor (NN) and next-to-nearest-neighbor (NNN) interactions have been analyzed.[7] We propose a simple method of constructing the ground-state diagrams for classical spin models with arbitrary value of spin and investigate the ground states of the spin-1 Ising model on unfrustrated lattices with NN interaction. We also consider an example of a frustrated lattice (triangular one), and the square lattice with NN and NNN interactions.

So, let us find the exact ground states of the most general spin-1 Ising model:

$$H^* = -J^*\sum_{\langle ij\rangle} s_i s_j - K^*\sum_{\langle ij\rangle} s_i^2 s_j^2 - C^*\sum_{\langle ij\rangle}\left(s_i^2 s_j + s_i s_j^2\right) + \sum_i\left(-hs_i + \Delta s_i^2\right), \qquad (1)$$

where s_i, the spin variable on the i site, takes on the values $-1, 0, +1$, $\Sigma_{\langle ij\rangle}$ means the sum over the nearest-neighbor pairs, and J^*, K^*, and C^* characterize, respectively, the bilinear, biquadratic, and mixed interactions between the nearest neighbors; h and Δ are the "fields."

Let us rewrite the Hamiltonian (1) replacing the sum over the sites by the sum over the bonds. We will consider only lattices with the same number z of bonds around each site. The "site energy" $-hs_i+\Delta s_i^2$ will be distributed uniformly over z bonds which surround the i site. Instead of the Hamiltonian H^* we will consider the Hamiltonian $H=zH^*$ which reads

$$H = -J\sum_{\langle ij\rangle} s_i s_j - K\sum_{\langle ij\rangle} s_i^2 s_j^2 - C\sum_{\langle ij\rangle}\left(s_i^2 s_j + s_i s_j^2\right) + \sum_{\langle ij\rangle}\left[-h\left(s_i + s_j\right) + \Delta\left(s_i^2 + s_j^2\right)\right], \qquad (2)$$

where the notations $J=zJ^*$, $K=zK^*$, and $C=zC^*$ were introduced. The ground-state diagrams are the same for both Hamiltonians.

Consider all possible bonds or two-site blocks and the respective energies. They are shown in Table I. We will construct the ground-state diagrams for unfrustrated lattices in the (Δ, h) plane. The region in this plane which corresponds to a particular two-site block is determined by the system of inequalities obtained from the condition of the minimum of the energy of the block (in comparison with the energies of the other blocks). It is easy to find the conditions when the regions exist. The uniform regions $\langle 00\rangle$, $\langle --\rangle$, and $\langle ++\rangle$ exist always, the antiferromagnetic region $\langle +-\rangle$ exists at the condition $J<0$ and its width is equal to $-2J$, the region $\langle 0+\rangle$ exists at the condition $C<-\frac{1}{2}(J+K)$ and its width is equal to $-(\sqrt{2}/2)(J+K+2C)$, and the region $\langle 0-\rangle$ exists at the condition $C>\frac{1}{2}(J+K)$ and its width is equal to $-(\sqrt{2}/2)(J+K-2C)$. If $J+K<0$ and $|C|<-\frac{1}{2}(J+K)$, the regions $\langle 0+\rangle$ and $\langle 0-\rangle$ exist simultaneously, otherwise only one of them exists. It follows from the above considerations that in the case $J\geqslant 0$, $K\geqslant -J$, and $|C|\leqslant \frac{1}{2}(J+K)$ there are no nonuniform phases (i.e., $\langle 0+\rangle$, $\langle 0-\rangle$, $\langle +-\rangle$) at all. Let us note that this is also true for frustrated lattices. Hence, the condition of positivity of J and K, which is usually imposed,[6,8] is

TABLE I. Two-site blocks and their energies.

Block	Energy
○—○	0
○—⊕	$-h+\Delta$
○—⊖	$h+\Delta$
⊕—⊖	$J-K+2\Delta$
⊕—⊕	$-J-K-2C-2h+2\Delta$
⊖—⊖	$-J-K+2C+2h+2\Delta$

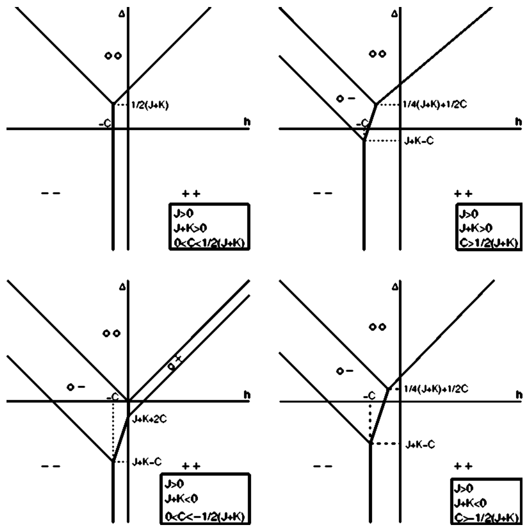


FIG. 1. Ground-state diagrams of the spin-1 Ising model in the case $J>0$, $C>0$ (unfrustrated lattice).

too strong. Reference 9, where an uncomplete BEG model was considered in the mean field approximation, proves it.

The exact ground-state diagrams of the spin-1 Ising model for unfrustrated lattices are shown in Figs. 1 and 2. The coefficient C is chosen nonnegative because the diagrams with values of C equal in magnitude but opposite in sign are symmetric with respect to the axis $O\Delta$, only the signs in the phase notations are replaced by the opposite ones. As one can see, nine topologically nonequivalent diagrams are

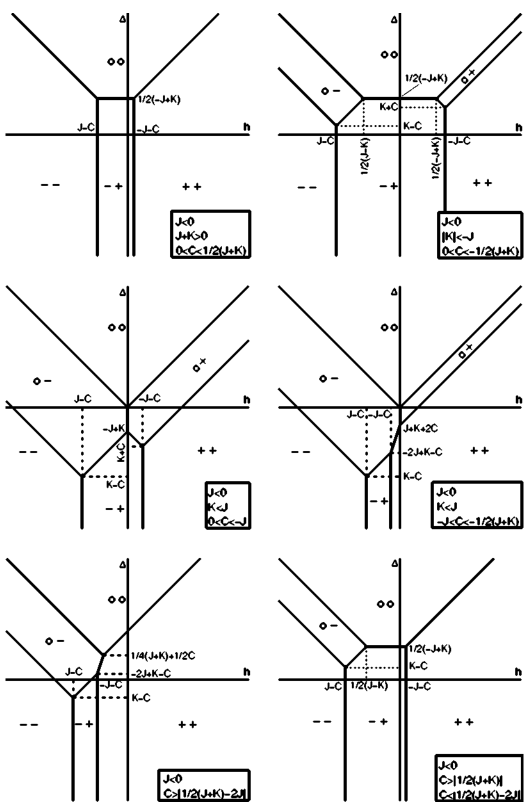


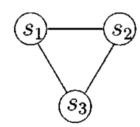
FIG. 2. Ground-state diagrams of the spin-1 Ising model in the case $J<0$, $C>0$ (unfrustrated lattice).

TABLE II. Three-site blocks for the triangular lattice and the corresponding energies.

Block	Energy
$\langle 000\rangle$	0
$\langle 00+\rangle$	$-h+\Delta$
$\langle 00-\rangle$	$h+\Delta$
$\langle 0++\rangle$	$-J-K-2C-2h+2\Delta$
$\langle 0+-\rangle$	$J-K+2\Delta$
$\langle 0--\rangle$	$-J-K+2C+2h+2\Delta$
$\langle +++\rangle$	$-3J-3K-6C-3h+3\Delta$
$\langle ++-\rangle$	$J-3K-2C-h+3\Delta$
$\langle +--\rangle$	$J-3K-2C+h+3\Delta$
$\langle ---\rangle$	$-3J-3K+6C+3h+3\Delta$

possible: three for $J\geqslant 0$ and six for $J<0$. In the case of existence of nonuniform phases $\langle 0+\rangle$ or $\langle 0-\rangle$ the model is equivalent to the usual spin-$\frac{1}{2}$ Ising model when $J\geqslant 0$, $\Delta<J+K-|C|$ or $J<0$, $\Delta<K-|C|$. For the case when these nonuniform phases do not exist the model is equivalent to the spin-$\frac{1}{2}$ Ising model when $\Delta<\frac{1}{2}(|J|+K)$.

Now let us pass to the Hamiltonian (1) on the triangular lattice. For constructing the ground-state diagrams we need to consider not two- but three-site blocks,



Adding one additional zero-spin site to the two-site blocks, we obtain three-site blocks with at least one zero spin. The expressions for their energies are the same as for the energies of corresponding two-site blocks, only $J=3J^*$ not $J=6J^*$, etc., i.e., z is equal to 3 not 6 as for the two-site blocks on the triangular lattice. There are also four three-site blocks without any zero spin. The three-site blocks and their energies are given in Table II, where the following notations are introduced: $J=3J^*$, $K=3K^*$, and $C=3C^*$. The region corresponding to a particular three-site block is determined by the minimum energy condition, as before.

If in a certain region the energy of one of three uniform two-site blocks has a minimum, then in this region the energy of the corresponding uniform three-site block also has a minimum. Thus, only those two-site regions will change where the energy of nonuniform two-site blocks was minimal. The uniform phase regions can expand at the cost of nonuniform ones.

Ground-state diagrams for the triangular lattice in the case $J>0$ are shown in Fig. 3. As one can see, there can be two intermediate regions between the uniform regions $\langle 000\rangle$ and $\langle +++\rangle$ (or $\langle ---\rangle$). If $J<0$ there are also intermediate regions ($\langle +--\rangle$ and $\langle ++-\rangle$) between the uniform regions $\langle +++\rangle$ and $\langle ---\rangle$ (see Fig. 4).

In the case of unfrustrated lattices all regions were unbounded. For the triangular lattice there can be one

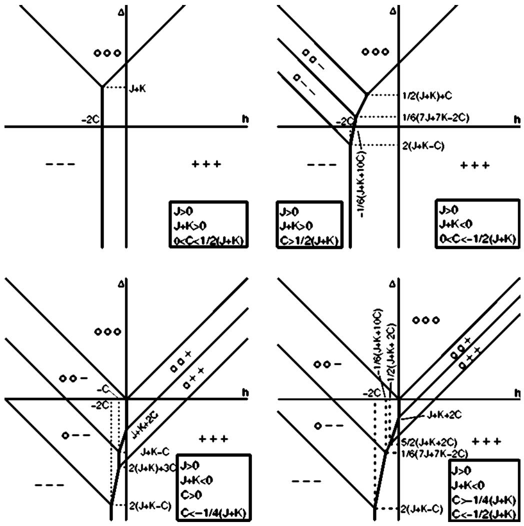
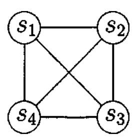


FIG. 3. Ground-state diagrams of the spin-1 Ising model on the triangular lattice in the case $J>0$, $C>0$.

bounded region ($\langle 0+-\rangle$). The condition of its existence is $J<0$, $J<-3K$, $|C|<-\frac{1}{2}(J+K)$, and $|C|<-\frac{1}{4}(7J+K)$.

Consider now a square lattice with NN and NNN interactions. In this case one needs to find the possible values of the energy of the four-site block,



We will denote the interactions along the sides of the square by J, K, C and along the diagonals by J_1, K_1, C_1. Taking into account that each site belongs to four blocks and each bond along a side to two (we consider a two-dimensional lattice), we can write the energies of all possible four-site blocks (see Table III).

At fixed J, K, C, J_1, K_1, and C_1 in the (Δ,h) plane from 3 to 15 regions can exist: phases corresponding to the blocks that differ only by order of sites (for example, $\langle ++--\rangle$ and $\langle +-+-\rangle$) cannot exist simultaneously.

The change of sign of both coefficients C and C_1 leads to the mapping of the ground-state diagram with respect to the axis $O\Delta$ (with changing signs in the phase notations); hence we need to consider only the case $C\geqslant 0$ (or $C_1\geqslant 0$).

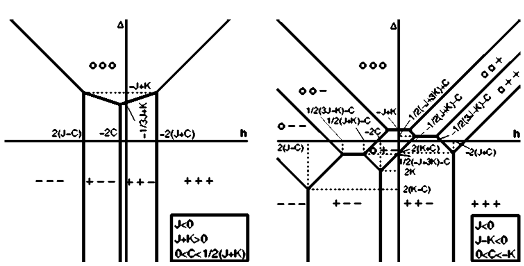


FIG. 4. The poorest (five phases) and one of the richest (ten phases) ground-state diagrams of the spin-1 Ising model on the triangular lattice in the case $J<0$, $C>0$.

TABLE III. Four-site blocks and their energies for a lattice with NN and NNN interactions.

	Block	Energy
1	$\langle 0000\rangle$	0
2	$\langle 000+\rangle$	$-1/4h+1/4\Delta$
3	$\langle 000-\rangle$	$+1/4h+1/4\Delta$
4	$\langle 00++\rangle$	$-1/2J-1/2K-C-1/2h+1/2\Delta$
5	$\langle 0+0+\rangle$	$-J_1-K_1-2C_1-1/2h+1/2\Delta$
6	$\langle 00+-\rangle$	$1/2J-1/2K+1/2\Delta$
7	$\langle 0+0-\rangle$	$J_1-K_1+1/2\Delta$
8	$\langle 00--\rangle$	$-1/2J-1/2K+C+1/2h+1/2\Delta$
9	$\langle 0-0-\rangle$	$-J_1-K_1+2C_1+1/2h+1/2\Delta$
10	$\langle 0+++\rangle$	$-J-K-2C-J_1-K_1-2C_1+3/4h+3/4\Delta$
11	$\langle 0++-\rangle$	$-K-C+J_1-K_1-1/4h+3/4\Delta$
12	$\langle 0+-+\rangle$	$J-K-J_1-K_1-2C_1-1/4h+3/4\Delta$
13	$\langle 0+--\rangle$	$-K+C+J_1-K_1-1/4h+3/4\Delta$
14	$\langle 0-+-\rangle$	$J-K-J_1-K_1+2C_1-1/4h+3/4\Delta$
15	$\langle 0---\rangle$	$-J-K+2C-J_1-K_1-2C_1+3/4h+3/4\Delta$
16	$\langle ++++\rangle$	$-2J-2K-4C+2J_1-2K_1-4C_1-h+\Delta$
17	$\langle +++-\rangle$	$-2K+2C-2K_1-2C_1-1/2h+\Delta$
18	$\langle ++--\rangle$	$-2K+2J_1-2K_1+\Delta$
19	$\langle +-+-\rangle$	$2J-2K-2J_1-2K_1+\Delta$
20	$\langle +---\rangle$	$-2K+2C-2K_1+2C_1+1/2h+\Delta$
21	$\langle ----\rangle$	$-2J-2K+4C-2J_1-2K_1+4C_1+h+\Delta$

Note that the blocks of type *aaab* (six blocks) and *aabc* (three blocks) correspond to infinitely degenerate phases with nonzero entropy per site. It is the so called residual entropy. In the case of only NN interaction there were no regions with residual entropy. In the previous cases, it occurred only at the boundaries of phases. An example of a most reached ground-state diagram (15 phases) is shown in Fig. 5. The phases $\langle 000+\rangle$, $\langle 000-\rangle$, $\langle 0+++\rangle$, $\langle 0---\rangle$, $\langle +---\rangle$, $\langle +++-\rangle$, $\langle 00+-\rangle$, and $\langle 0--+\rangle$ are infinitely degenerate.

As may be seen from the figure, certain regions are bounded; others are not. It is easy to find the necessary

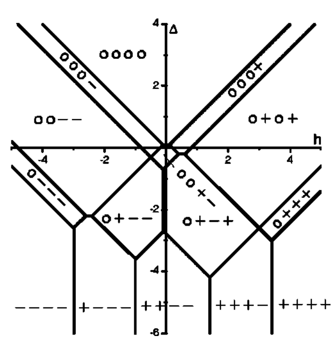


FIG. 5. Ground-state diagram of the spin-1 Ising model on the square lattice with NN and NNN interactions. $J=-0.5$, $K=-0.4$, $C=-0.25$, $J_1=-0.3$, $K_1=-0.3$, and $C_1=0.2$.

TABLE IV. Unbounded four-site regions and conditions of their existence for a square lattice with NN and NNN interactions.

	Region	Condition
1	$\langle 0000 \rangle$	Always
2	$\langle 000+ \rangle$	$a<0,\ a_1<0$
3	$\langle 000- \rangle$	$b<0,\ b_1<0$
4	$\langle 00++ \rangle$	$\lvert a\rvert<-2a_1$
5	$\langle 0+0+ \rangle$	$a<0,\ a<2a_1$
8	$\langle 00-- \rangle$	$\lvert b\rvert<-2b_1$
9	$\langle 0-0- \rangle$	$b<0,\ b<2b_1$
10	$\langle 0+++ \rangle$	$a<0,\ a_1<0$
15	$\langle 0--- \rangle$	$b<0,\ b_1<0$
16	$\langle ++++ \rangle$	Always
17	$\langle +++- \rangle$	$J<0,\ J_1<0$
18	$\langle ++-- \rangle$	$\lvert J\rvert<-2J_1$
19	$\langle +-+- \rangle$	$J<0,\ J<2J_1$
20	$\langle +--- \rangle$	$J<0,\ J_1<0$
21	$\langle ---- \rangle$	Always

and sufficient conditions of existence of the unbounded regions. They are shown in Table IV, where the following notations are introduced: $a=\frac{1}{2}(J+K)+C$, $a_1=\frac{1}{2}(J_1+K_1)+C_1$, $b=\frac{1}{2}(J+K)-C$, and $b_1=\frac{1}{2}(J_1+K_1)-C_1$. As to bounded regions, the conditions of their existence cannot be written in such a simple form as for the unbounded ones, and therefore we will not give them.

Now let us write the condition of nonexistence of regions 2–5, 8–10, and 15:

$$a_1 \geqslant -\frac{a}{2}, \quad a \geqslant 0, \quad b_1 \geqslant -\frac{b}{2}, \quad b \geqslant 0, \tag{3}$$

and also the condition of nonexistence of regions 17–20:

$$J \geqslant 0, \quad J_1 \geqslant -\frac{J}{2}. \tag{4}$$

If both conditions are satisfied there are only uniform phases.

Thus, the simple method that we have proposed gives the possibility to construct exact ground-state diagrams for the spin-1 Ising model on a large class of lattices: two dimensional as well as three dimensional, with NN interaction as well as with, in certain cases, NN and NNN interactions. Using this method, we have obtained nine topologically different ground-state diagrams for the most general spin-1 Ising model on unfrustrated lattices and found the conditions of existence (or nonexistence) of nonuniform phases. We have also obtained the conditions of equivalence of the spin-1 Ising model at zero temperature to the usual spin-$\frac{1}{2}$ Ising model. We have investigated as well the ground states of the spin-1 Isin model on the triangular lattice and on the square lattice with NN and NNN interactions. In a similar way, ground-state diagrams for the Ising models with spin $S>1$ may be constructed.

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