Ground states of the lattice-gas model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with three-particle interaction: Full-dimensional ground states

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In this paper, we completely solve the problem of the ground states of the lattice-gas model on the infinite plane triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with additional interaction between three particles at the vertices of a nearest-neighbor triangle. We use this model to illustrate how the complete solution of the ground-state problem of a lattice-gas model (or equivalent spin model) should look.

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I. INTRODUCTION

Lattice-gas models or equivalent spin models, owing to their numerous applications, still remain a subject of intensive studies. It is natural to start the investigation of such models by determining their ground states. These latter give an idea about the low-temperature behavior of these models and are often the only exact solutions that can be obtained. Although the methods for determining the ground states of lattice-gas models have been developed for more than 50 years [1], no general algorithm existed until now. Moreover, there is no clear understanding as to when this problem can be considered completely solved. The researchers mostly restrict their studies to the ground states in full-dimensional regions of the space of the Hamiltonian parameters including the chemical potential (or the external field for spin Hamiltonians). We will call such ground states full dimensional. But the knowledge of full-dimensional ground states only is not sufficient to answer the question about ground states in the case of a fixed density of particles. In this case, one should also know the ground states at the boundaries of full-dimensional regions.

In Ref. [2], we developed a method for determining ground states of lattice-gas models or equivalent spin models and, using this method, the complete solution for the ground-state problem of the lattice-gas model on the triangular lattice with nearest- and next-nearest-neighbor interactions was found. Here, we refine our method and demonstrate that it is also applicable to the lattice-gas models with many-particle interactions. Lattice-gas models of this kind are interesting not only from a pure theoretical point of view, but are also widely applied to the description of adsorption [3] and intercalation [4] processes. In these cases simple models with pairwise interactions often do not provide an adequate description. For instance, lattice-gas models with pairwise interactions of particles lead to the symmetrical voltage curve (dependence of the chemical potential on the particle density) due to the particle-hole symmetry of the Hamiltonian. In contrast, the voltage curves of real intercalated compounds are asymmetrical [5]. To reproduce this asymmetry, many-particle effective interactions should be introduced into the Hamiltonian. Lattice-gas models with many-particle interactions are also used in the studies of the ground states of the quantum Falicov-Kimball model [6].

Here we consider one of the simplest lattice-gas models with many-particle interaction, namely the lattice-gas model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with interaction between three particles at the vertices of a nearest-neighbor triangle. Ground states of this model were investigated earlier by Brandt and Stolze [7]. They found full-dimensional ground-state structures, however, for two of these structures they did not prove that these really are the ground-state ones. Furthermore, the Brandt and Stolze method does not make it possible to find disordered and ordered-but-aperiodic ground-state structures. This is possible with our approach. Although with the Brandt and Stolze method it is possible to identify the first-order phase transitions, it is not easy, and such an analysis was not performed. It is relatively easy to do this with our method.

This paper represents only a part of our studies of the ground-state problem, but it is the essential part. It contains the description of the method, the complete solution of the ground-state problem, and construction of the full-dimensional ground-state structures. So as not to overburden the paper, construction and analysis of the ground-state structures at the boundaries of the full-dimensional regions are reserved for future publications. The paper is organized as follows. In Sec. II, we explain the principles of our method for the determination of the ground states of lattice-gas models by applying them to the lattice-gas model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with three-particle interaction. In Sec. III, we give the solution of the ground-state problem in the form of a set of the so-called "basic rays" and the corresponding sets of cluster configurations. In Sec. IV, we determine the full-dimensional ground-state structures and prove the completeness of the set of basic rays. Section V contains some concluding remarks.

Our results can be applied, in particular, to the description of some kinds of particles adsorbed on the surface of graphite or sheets of graphene. This is increasingly important from the point of view of possible applications.

II. METHOD FOR CONSTRUCTION OF GROUND-STATE STRUCTURES OF LATTICE-GAS MODELS

A. Lattice-gas Hamiltonian and the family of equivalent Hamiltonians

Let us consider the lattice-gas model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with three-particle interaction between particles at the

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vertices of a nearest-neighbor triangle. The Hamiltonian of this model reads

$$H_{lg} = I_1 \sum_{NN} c_i c_j + I_2 \sum_{NNN} c_i c_j + I_\triangle \sum_{\triangle} c_i c_j c_k - \mu_{lg} \sum_i c_i. \quad (1)$$

Here c_i are the lattice-gas occupation variables ($c_i = 1$ if the ith site is occupied by a particle and $c_i = 0$ otherwise), I_1, I_2 are the nearest- and next-nearest-neighbor couplings, respectively, $I_\triangle$ is the three-particle interaction, and μ_{lg} denotes the chemical potential of particles. NN, NNN, and $\triangle$ denote the summation over the nearest neighbors, the next-nearest neighbors, and the nearest-neighbor triangles, respectively.

It is easy to show that this model is mathematically equivalent to the spin model

$$H_I = J_1 \sum_{NN} \sigma_i \sigma_j + J_2 \sum_{NNN} \sigma_i \sigma_j + J_\triangle \sum_{\triangle} \sigma_i \sigma_j \sigma_k - h \sum_i \sigma_i, \quad (2)$$

with the coupling constants and external field

$$J_1 = \frac{I_1 + I_\triangle}{4}, \quad J_2 = \frac{I_2}{4}, \quad J_\triangle = \frac{I_\triangle}{8}, \quad h = \frac{\mu_{lg}}{2} - 6(J_1 + J_2 - J_\triangle). \quad (3)$$

Here $\sigma_i = 2c_i - 1 = \pm 1$ are spin variables.

Both Hamiltonians (1) and (2) have the same ground states. This is also true for the whole family of Hamiltonians

$$H = V_1 \sum_{NN} (a_1\sigma_i + b_1)(a_1\sigma_j + b_1) + V_2 \sum_{NNN} (a_2\sigma_i + b_2)(a_2\sigma_j + b_2) + V_\triangle \sum_{\triangle} (a_\triangle\sigma_i + b_\triangle)(a_\triangle\sigma_j + b_\triangle)(a_\triangle\sigma_k + b_\triangle) - \mu \sum_i (a_0\sigma_i + b_0), \quad (4)$$

where the couplings V_1, V_2, and $V_\triangle$ and the "chemical potential" μ are related to the parameters of model (2) as

$$J_1 = a_1^2 V_1 + 2a_\triangle^2 b_\triangle V_\triangle, \quad J_2 = a_2^2 V_2, \quad J_\triangle = a_\triangle^3 V_\triangle, \quad h = a_0\mu - 6\left(a_1 b_1 V_1 + a_2 b_2 V_2 + a_\triangle b_\triangle^2 V_\triangle\right). \quad (5)$$

The values a_i, b_i ($i = 0,1,2$), and $a_\triangle$, $b_\triangle$, which are independent of spin variables, can be arbitrary; the only restrictions are $a_i \neq 0$ and $a_\triangle \neq 0$. We will see later that the values b_i and $b_\triangle$ are very important for the determination of the ground states.

Equations (5) can be reversed as

$$V_1 = \frac{J_1}{a_1^2} - \frac{2b_\triangle J_\triangle}{a_1^2 a_\triangle}, \quad V_2 = \frac{J_2}{a_2^2}, \quad V_\triangle = \frac{J_\triangle}{a_\triangle^3}, \quad \mu = \frac{1}{a_0}\left[h + 6\left(\frac{b_1}{a_1}J_1 + \frac{b_2}{a_2}J_2 + \frac{a_1 b_\triangle^2 - 2b_1 a_\triangle b_\triangle}{a_1 a_\triangle^2} J_\triangle\right)\right]. \quad (6)$$

Let us note that Hamiltonian (2) is invariant with respect to the flip of all spins with simultaneous inversion of the signs of $J_\triangle$ and h. To exploit this symmetry, we consider ground states of Hamiltonian (2), but for the sake of clarity we use the "language of the lattice-gas model." It is easy to switch from spin Hamiltonian (2) to lattice-gas Hamiltonian (1) using the transformations that are inverse to transformations (3)

$$I_1 = 4J_1 - 8J_\triangle, \quad I_2 = 4J_2, \quad I_\triangle = 8J_\triangle, \quad \mu_{lg} = 2h + 12(J_1 + J_2 - J_\triangle). \quad (7)$$

B. Hamiltonian in the form of the sum over flowers

We will build the global ground-state structures with configurations of a cluster. (The terms "structure," "cluster," and "configuration of a cluster" are clearly defined in Ref. [8].) To build a structure with a set of configurations of a cluster means to construct such a structure on the lattice that every cluster of this type in the structure will have one of the configurations belonging to the set. This structure will be a ground-state one (in a region of the space of the Hamiltonian parameters) if the configurations of the set have equal energy and this energy is the smallest one among the energies of all other configurations. Which cluster should be chosen? There is no *a priori* answer for this. Of course, the cluster should be big enough to contain all interactions included into the Hamiltonian; this is a necessary condition. It turns out that the seven-site cluster in the form of a "flower" (hexagon with the central site) is sufficient for construction of all ground-state structures of the model under consideration.

Hence, let us rewrite Hamiltonian (4) in the form of a single sum over all possible flowers on the lattice

$$H = \sum_{\text{flowers}\ i} H_i = \sum_{\text{flowers}\ i} \left\{ \frac{V_1}{2(\beta_1+\beta_2)} \left[\beta_1 \sigma_{i0}^1 \left(\sigma_{i1}^1 + \sigma_{i2}^1 + \sigma_{i3}^1 + \sigma_{i4}^1 + \sigma_{i5}^1 + \sigma_{i6}^1\right) + \beta_2 \left(\sigma_{i1}^1\sigma_{i2}^1 + \sigma_{i2}^1\sigma_{i3}^1 + \sigma_{i3}^1\sigma_{i4}^1 + \sigma_{i4}^1\sigma_{i5}^1 + \sigma_{i5}^1\sigma_{i6}^1\right)\right] + \frac{V_2}{2}\left(\sigma_{i1}^2\sigma_{i3}^2 + \sigma_{i3}^2\sigma_{i5}^2 + \sigma_{i5}^2\sigma_{i1}^2 + \sigma_{i2}^2\sigma_{i4}^2 + \sigma_{i4}^2\sigma_{i6}^2 + \sigma_{i6}^2\sigma_{i2}^2\right) + \frac{V_\triangle}{3}\sigma_{i0}^\triangle\left(\sigma_{i1}^\triangle\sigma_{i2}^\triangle + \sigma_{i2}^\triangle\sigma_{i3}^\triangle + \sigma_{i3}^\triangle\sigma_{i4}^\triangle + \sigma_{i4}^\triangle\sigma_{i5}^\triangle + \sigma_{i5}^\triangle\sigma_{i6}^\triangle + \sigma_{i6}^\triangle\sigma_{i1}^\triangle\right) - \frac{\mu}{\alpha_1 + 6\alpha_2}\left[\alpha_1\sigma_{i0}^0 + \alpha_2\left(\sigma_{i1}^0 + \sigma_{i2}^0 + \sigma_{i3}^0 + \sigma_{i4}^0 + \sigma_{i5}^0 + \sigma_{i6}^0\right)\right]\right\}. \quad (8)$$

Here the following notations are introduced:

$$\sigma_{ij}^{1} = a_1\sigma_{ij} + b_1, \quad \sigma_{ij}^{2} = a_2\sigma_{ij} + b_2,$$
$$\sigma_{ij}^{0} = a_0\sigma_{ij} + b_0, \quad \sigma_{ij}^{\triangle} = a_\triangle\sigma_{ij} + b_\triangle. \tag{9}$$

The first index at spin variables σ_{ij} denotes the host flower, and the second one counts the sites within the flower (the central site is marked as zero). Every bond between a pair of next-nearest neighbors belongs to two different flowers and is counted twice, therefore the factor $\frac{1}{2}$ is introduced in the second term. Every triangle of nearest neighbors belongs to three different flowers, thus we have the factor $\frac{1}{3}$ in the respective term of the Hamiltonian. Arbitrary factors α_1 and α_2 ($\alpha_1 \neq -6\alpha_2$) account for the fact that every site belongs to one flower as the central site and also to six flowers as a lateral site. Similarly, the presence of arbitrary factors β_1 and β_2 ($\beta_2 \neq -\beta_1$) reflects the fact that every bond between nearest-neighbor sites belongs to two flowers as a radial bond and to two other flowers as a lateral bond. One should notice that the Hamiltonian H does not depend on $\alpha_1, \alpha_2, \beta_1$, and β_2, although the local Hamiltonian H_i does depend on them.

Why do we need to introduce "free" coefficients a_k, $a_\triangle$, b_k, $b_\triangle$, α_k, and β_k? The point is that there are only two structures which can be built with a single flower configuration: the empty one (no particles) and the filled one (every site contains a particle). Therefore, we need to minimize the energy H_i of several flower configurations simultaneously. "Free" coefficients are introduced to provide this possibility.

Let us assume that for a certain point in the space of the Hamiltonian parameters $(V_1, V_2, V_\triangle, \mu)$, one can choose such a set of values of a_k, $a_\triangle$, b_k, $b_\triangle$, α_k, and β_k, that some flower configurations (one or more) have equal energy H_i and that this energy is the smallest one among the energies of all other configurations. If at least one structure can be constructed with these configurations, then they generate all ground-state structures at this point. Let us note that, without loss of generality, the coefficients a_k and $a_\triangle$ may be chosen equal, for instance, to $\frac{1}{2}$.

C. Characteristics of a structure and expression for density of energy

To denote and characterize particular structures we will use the notations of Kanamori and Kaburagi [9]: $S(p_0; p_1, p_2, p_3, \ldots; p_\triangle)$, where p_0 is the number of particles per site, p_i ($i = 1,2,3,\ldots$) provides the number of pairs of particles (per particle) that are ith neighbors, and $p_\triangle$ is the number of triplets of particles that are nearest neighbors. The energy per site of a structure can be expressed in terms of p_0, p_1, p_2, …, $p_\triangle$ as

$$E = \sum_i p_0 p_i I_i + p_0 p_\triangle I_\triangle - p_0\mu_{lg}, \quad i = 1,2,\ldots. \tag{10}$$

One can switch from the parameters of lattice-gas Hamiltonian to the parameters of spin Hamiltonian using the following relations [compare to Eqs. (7)]:

$$I_1 = 4J_1 - 8J_\triangle, \quad I_i = 4J_i\ (i = 2,3,\ldots),$$
$$I_\triangle = 8J_\triangle, \quad \mu_{lg} = 2h + 2\sum_k z_k J_k - 12J_\triangle. \tag{11}$$

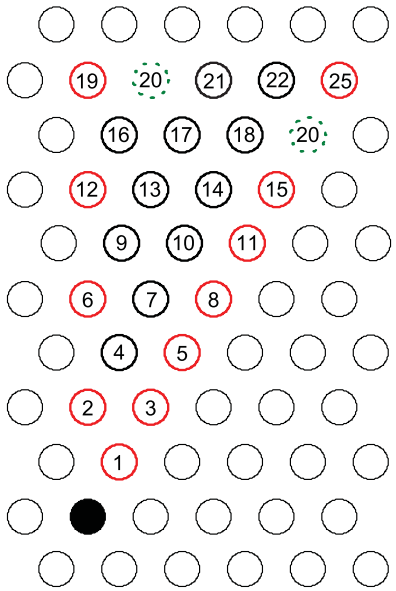


FIG. 1. (Color online) Neighbors on the triangular lattice (with respect to the solid circle at the bottom). Neighbors with coordination numbers 6, 12, and 18 are represented by red (light gray), black, and dotted olive circles, respectively.

Here z_k is the coordination number of kth neighbors. One can see from Fig. 1 that for $k \leqslant 25$, the coordination number z_k can be equal to 6 (red circles), 12 (black circles), or 18 (for 20th neighbors, olive dotted circles).

Structures can be characterized also by the fractional content of configurations of a cluster that includes all interactions which are considered. We will numerate the cluster configurations of a structure by index l and denote the fraction of the lth configuration in the structure by k_l. Values p_0, p_i ($i = 1,2,3,\ldots$), $p_\triangle$ can be expressed in terms of k_l,

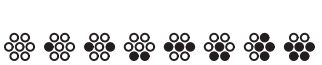
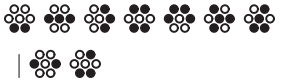
$$p_0 = \sum_l k_l p_{0l}, \quad p_i = \frac{\sum_l k_l p_{il}}{c_i p_0}, \quad p_\triangle = \frac{\sum_l k_l p_{\triangle l}}{c_\triangle p_0}, \tag{12}$$

where p_{0l} is the density of particles in lth configuration, p_{il} is the number of ith-neighbor pairs in the lth configuration, $p_{\triangle l}$ is the number of triplets of particles that are nearest neighbors in the lth configuration, and c_i and $c_\triangle$ are the numbers of clusters on the lattice which include a bond between ith neighbors and a nearest-neighbor triangle, respectively. (All bonds between ith neighbors as well as all nearest-neighbor triangles are supposed to be equivalent.) The calculation of p_0, p_i ($i = 1,2,3,\ldots$), and $p_\triangle$ using Eqs. (12) is simpler than direct calculations of these values.

Sometimes, to simplify calculations of p_0, p_i ($i = 1,2,3,\ldots$), and $p_\triangle$, the following statement will be useful (it is easy to prove it): If structures $S\left(p_0; p_1, p_2, p_3, \ldots; p_\triangle\right)$ and $S\left(\bar{p}_0; \bar{p}_1, \bar{p}_2, \bar{p}_3, \ldots; \bar{p}_\triangle\right)$ are mutually symmetrical with respect to the particle-vacancy symmetry, then

$$\bar{p}_0 = 1 - p_0, \quad \bar{p}_i = z_i + \frac{2p_0 p_i - z_i}{2(1 - p_0)},$$
$$\bar{p}_\triangle = \frac{2 - p_0(6 - 2p_1 + p_\triangle)}{1 - p_0}. \tag{13}$$

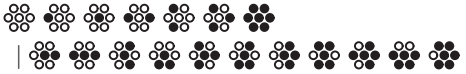
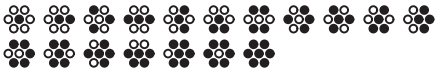
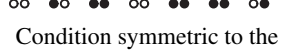
TABLE I. Basic rays and basic sets of flower configurations for the spin model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with three-spin nearest-neighbor interaction. $J_\triangle \geqslant 0$.

Basic ray		Basic set of flower	Full-dimensional	"Free"
$\mathbf{r}_i$	$(h, J_1, J_2, J_\triangle)$	configurations $\mathbf{R}_i$	structures	coefficients
$\mathbf{r}_1$	(0,0, − 1,0)		1, $\bar{1}$, 3, $\bar{3}$	$\beta_2 = 0$
$\mathbf{r}_2$	(0,0,1,0)		$4a$, $\overline{4a}$, $4b$, $\overline{4b}$, 5, 6, 9, $\bar{9}$	$\beta_2 = 0$
$\mathbf{r}_3$	(6,0,1,0)		1, 2, $4a$, $4b$	$\beta_2 = 0$
$\mathbf{r}_4$	(0,0,1,3)		$\bar{1}$, 2, 3, $\overline{4a}$, 9, 10, 11, 12	$\beta_2 = 0, b_\triangle = 0$
$\mathbf{r}_5$	(6, − 2,0,3)		1, $\bar{1}$, 2, 3	$\alpha_2 = 0, \beta_2 = 0,$ $b_\triangle = -a_\triangle$
$\mathbf{r}_6$	(2, − 2,2,3)		$\bar{1}$, 2, $\overline{4a}$, $4b$, 5, 9	$\alpha_2 = \frac{2b_\triangle}{a_\triangle + b_\triangle}\alpha_1, \beta_2 = 0,$ $b_1 = \frac{a_\triangle^2 + 3b_\triangle^2}{6a_\triangle b_\triangle}a_1$
$\mathbf{r}_7$	(6, − 4,2,3)		1, $\bar{1}$, 2, $4b$, 5	$\alpha_2 = \frac{a_\triangle + 2b_\triangle}{a_\triangle + b_\triangle}\alpha_1, \beta_2 = 0,$ $b_1 = \frac{b_\triangle^2}{a_\triangle(a_\triangle + 2b_\triangle)}a_1$
$\mathbf{r}_8$	(−2, − 1,1,0)		$\bar{1}$, $\overline{4a}$, $\overline{4b}$, 5	$\alpha_1 = 0, \beta_2 = 0, a_1 = 3b_1$
$\mathbf{r}_9$	(4,1,1,0)		2, $4a$, $4b$, 6, 9	$\alpha_1 = 0, a_1 = -3b_1$
$\mathbf{r}_{10}$	(−6,2,0,1)		$\bar{1}$, $\bar{2}$, 3, $\bar{3}$, $\overline{4a}$, 6, 10, 11	$\alpha_2 = 2\alpha_1, b_1 = \frac{(a_\triangle + b_\triangle)}{2a_\triangle}a_1$
$\mathbf{r}_{11}$	(6,4,2,3)		2, 3, 6, 9, 11, 12	$\alpha_2 = -\frac{a_\triangle - 2b_\triangle}{a_\triangle - b_\triangle}\alpha_1, \beta_2 = 0,$ $b_1 = -\frac{b_\triangle^2}{a_\triangle(a_\triangle - 2b_\triangle)}a_1$
$\mathbf{r}_{12}$	(−2,2,2,3)		$\overline{4a}$, 6, 9, 10, 12	$\alpha_2 = -\frac{2b_\triangle}{a_\triangle - b_\triangle}\alpha_1, \beta_2 = 0,$ $b_1 = -\frac{a_\triangle^2 - 3b_\triangle^2}{6a_\triangle b_\triangle}a_1$
$\mathbf{r}_{13}$	(−10,14,8,15)	 [ ,  , enter in structures with the neighborhoods shown in Fig. 2(b)]	6, 10, 11, 12	$\alpha_2 = \frac{2(a_\triangle - 5b_\triangle)}{5(a_\triangle - b_\triangle)}\alpha_1, \beta_2 = 0,$ $b_1 = \frac{5(a_\triangle^2 - 3b_\triangle^2)}{6a_\triangle(a_\triangle - 5b_\triangle)}a_1$

III. BASIC RAYS (VECTORS) AND BASIC SETS OF FLOWER CONFIGURATIONS

In the Hamiltonian parameter space, the region that corresponds to a ground state is a convex polyhedral cone with the vertex at the origin of the coordinates. Convexity allows one to find ground-state structures in any point of the Hamiltonian parameter space if all edges of full-dimensional polyhedral cones, as well as ground-state structures on these edges, are known. We will call such edges "basic rays." In mathematical usage, they are 1-faces of multidimensional polyhedral cones that correspond to full-dimensional ground states. If the complete set of basic rays is known (it will be shown later what the term "complete" means and how the completeness can be proven), as well as all ground-state structures in them, then, in principle, the problem can be considered solved. The construction of ground states in any point of Hamiltonian parameter space reduces then to a "purely technical" problem. However, the determination of the complete set of basic rays is difficult and tedious. We did not manage to elaborate the universal algorithm for it, so we do not provide the details of our calculations. We give only the final output that can be easily verified

TABLE II. Basic rays and basic sets of flower configurations for the spin model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with three-spin nearest-neighbor interaction. $J_\triangle \leqslant 0$.

Basic ray		Basic set of flower	Full-dimensional
$\mathbf{r}_i^-$	$(h, J_1, J_2, J_\triangle)$	configurations $\mathbf{R}_i^-$	structures
$\mathbf{r}_3^-$	(−6,0,1,0)		$\bar{1}$, $\bar{2}$, $\overline{4a}$, $\overline{4b}$
$\mathbf{r}_4^-$	(0,0,1, − 3)		1, $\bar{2}$, $\bar{3}$, $4a$, $\bar{9}$, $\overline{10}$, $\overline{11}$, $\overline{12}$
$\mathbf{r}_5^-$	(−6, − 2,0, − 3)		1, $\bar{1}$, $\bar{2}$, $\bar{3}$
$\mathbf{r}_6^-$	(−2, − 2,2, − 3)		1, $\bar{2}$, $4a$, $\overline{4b}$, 5, $\bar{9}$
$\mathbf{r}_7^-$	(−6, − 4,2, − 3)		1, $\bar{1}$, $\bar{2}$, $\overline{4b}$, 5
$\mathbf{r}_8^-$	(2, − 1,1,0)		1, $4a$, $4b$, 5
$\mathbf{r}_9^-$	(−4,1,1,0)		$\bar{2}$, $\overline{4a}$, $\overline{4b}$, 6, $\bar{9}$
$\mathbf{r}_{10}^-$	(6,2,0, − 1)		1, 2, 3, $\bar{3}$, $4a$,6,$\overline{10}$,$\overline{11}$
$\mathbf{r}_{11}^-$	(−6,4,2, − 3)		$\bar{2}$, $\bar{3}$, 6, $\bar{9}$, $\overline{11}$, $\overline{12}$
$\mathbf{r}_{12}^-$	(2,2,2, − 3)		$4a$, 6, $\bar{9}$, $\overline{10}$, $\overline{12}$
$\mathbf{r}_{13}^-$	(10,14,8, − 15)		6,$\overline{10}$,
		Condition symmetric to the condition for $\mathbf{r}_{13}$.	$\overline{11}$, $\overline{12}$

even without a computer. Let us note that the results obtained previously by Brandt and Stolze [7] facilitated our task.

A complete set of basic rays for a spin model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with three-spin nearest-neighbor interaction is given in Tables I and II. In the first, second, third, fourth, and fifth columns of Table I, the notations of basic rays, their direction vectors (we will also call these vectors "basic" and the notations for them will be the same as for corresponding basic rays), the sets $\mathbf{R}_i$ of flower configurations generating the ground-state structures in the corresponding basic rays, the full-dimensional ground-state structures in these rays (see Sec. IV), and the "free" coefficients in Hamiltonian (8) are given, respectively.

Let us explain, for instance, the eighth row of Table I. Its meaning is the following: If in Hamiltonian H_i [see Eqs. (8) and (6)] $\alpha_1 = 0$, $\beta_2 = 0$, and $a_1 = 3b_1$, then at $h = -2g$, $J_1 = -g$, $J_2 = g$, and $J_3 = 0$, where g is arbitrary positive number, the following flower configurations have the minimal (and equal for all) energy:  , and  . (Here and thereafter, open circles represent vacancies, solid circles, except for gray ones, represent particles, and gray circles are undefined.) The last and next to last configurations (separated from the others by the symbol |) cannot be realized in such a set, though they have the minimal energy, also. These configurations are incompatible with the others and with themselves and can be rejected. Ground-state structures without defects in this ray are only such structures in which every flower has one of the enumerated configurations. Among these structures, there are four full-dimensional ones: $\bar{1}$, $\overline{4a}$, $\overline{4b}$, and 5 (see Sec. IV).

Basic rays $\mathbf{r}_i^-$ (see Table II) have been obtained from basic rays $\mathbf{r}_i$ by the inversions $h \to -h$ and $J_\triangle \to -J_\triangle$. The respective sets of flower configurations $\mathbf{R}_i^-$ have been obtained from sets $\mathbf{R}_i$ by the inversion $\sigma = -1 \leftrightarrow \sigma = +1$ (or particle $\leftrightarrow$ vacancy) that reflects the symmetry of Hamiltonian (2). Basic rays $\mathbf{r}_1$ and $\mathbf{r}_2$ and the corresponding sets of flower configurations are self-symmetric.

The most complicated problem that we managed to solve is the determination of the basic ray $\mathbf{r}_{13}$ and the corresponding set of flower configurations $\mathbf{R}_{13}$. The principle for construction of ground states in this basic ray is a little different than in other basic rays. One should not simply fill the triangular lattice with flower configurations of basic set $\mathbf{R}_{13}$, but fill it in such a way that three configurations of this set, namely  ,  , and  , enter in structures only with the neighborhoods depicted in Fig. 2(b). Let us prove that structures constructed in such a manner exhaust all ground states without defects in this ray.

If $\beta_2 = 0$, $\alpha_2 = \frac{2(a_\triangle - 5b_\triangle)}{5(a_\triangle - b_\triangle)}\alpha_1$, $b_1 = \frac{5(a_\triangle^2 - 3b_\triangle^2)}{6a_\triangle(a_\triangle - 5b_\triangle)}a_1$ (without loss of generality $b_\triangle$ can be set equal to zero), then in ray $h = -\frac{5}{7}J_1$, $J_2 = \frac{4}{7}J_1$, $J_\triangle = \frac{15}{14}J_1$, $J_1 > 0$ (basic ray $\mathbf{r}_{13}$), configurations  ,  , and have equal energy which is less than the energy of any other configuration, except configuration  ; the latter has the smallest energy. Let us take the energy of configurations  ,  , and  as zero. Then the energy of configuration is negative and equal to

$-\frac{2}{7}J_1$, and the energies of other configurations are positive. Now we will prove that the energy per one flower for any structure in ray $\mathbf{r}_{13}$ cannot be less than zero, and we will find all structures for which it is equal to zero.

Let us call flower configurations which have positive (zero, negative) energy "positive" ("zero," "negative") flowers. All flowers in a structure can be grouped in the following way: Every positive flower is grouped with such negative flowers, the central sites of which are lateral sites of this positive flower. The energy of the flower which enters in two or more groups is shared equally between these groups. It is easy to see that every negative flower enters in a group with at least one positive flower. Among all positive flowers only the following ones are compatible and can be grouped with a negative flower (the corresponding energies are indicated in parentheses): ($\frac{26}{7}J_1$), ($\frac{2}{7}J_1$), ($\frac{8}{7}J_1$), ($\frac{8}{7}J_1$), ($\frac{2}{7}J_1$), ($\frac{6}{7}J_1$), ($\frac{12}{7}J_1$), and ($\frac{12}{7}J_1$). These groups are depicted in Fig. 2(a).

As one can see, there are no groups with negative energy. Four groups can have zero energy. These are groups with flowers, , , and . But they have zero energy only if every flower contained in such a group belongs only to this group. Therefore the group with flower cannot enter in ground-state structures and three other groups enter only with the neighborhoods depicted in Fig. 2(b).

Therefore, we have proven that the ground-state structures in ray $\mathbf{r}_{13}$ are constructed with flowers , , , , , , and in such a way that flowers , , and enter in these structures only with the neighborhoods depicted in Fig. 2(b). Notice that in this ray, flower can be combined only with flower .

To conclude, we have found ground states in ray $\mathbf{r}_{13}$ by grouping the terms of Hamiltonian (8) in two ways: (1) grouping them accordingly to the flowers and (2) grouping the flowers themselves. This simple but nontrivial way enabled us to use only seven-site cluster in the form of a flower. If we searched ground states in this ray in the same way as in all other basic rays, we would have to consider a much larger cluster (ten or maybe even more sites) and the problem would become very complicated.

To facilitate the understanding of the concept of basic rays and basic sets of configurations, the $J_\triangle = 0$ case is considered in the Appendix. The space of Hamiltonian parameters can be visualized in this case.

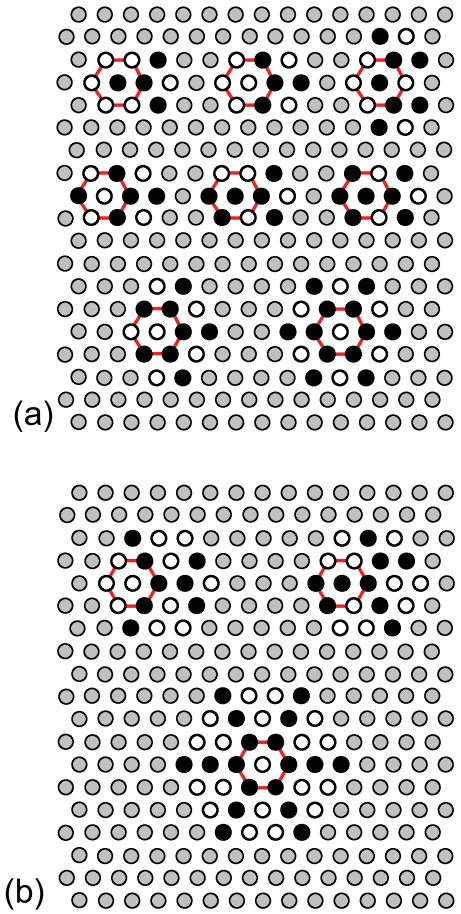


FIG. 2. (Color online) (a) Groups of positive flowers with the negative flower. (b) Neighborhoods of the zero-energy groups.

IV. FULL-DIMENSIONAL STRUCTURES AND COMPLETENESS OF THE SET OF BASIC RAYS

A. Construction of the ground-state structures using the basic set of configurations

The 24 basic rays given in Tables I and II constitute a complete set of basic rays, that is, knowing all ground states in these rays, one can easily find ground states in every point of the Hamiltonian parameter space. But before proving the completeness of the set of basic rays, one should show how to construct ground-state structures using basic sets of configurations. It should be mentioned that a basic set cannot be a subset of any other basic set. To find the region in the Hamiltonian parameter space where a structure (or a set of structures) is a ground-state structure, one needs to determine all basic sets for which the generating set of the structure (that is, the set of flower configurations of this structure) is a subset. The region to be found will be the linear hull with non-negative coefficients of the corresponding basic vectors. In mathematical usage this type of hull is called a conical hull. Hence, a structure is the ground-state one if and only if its generating set of configurations is a subset of at least one basic set. If such a basic set is unique then this structure is a ground state only in the respective basic ray. We call such a structure one dimensional. If a structure is generated by a set of configurations which is a subset of two basic sets only, then such a structure is a ground state in a two-dimensional region (two-dimensional angle). Radius vectors of points of this region are linear combinations with non-negative coefficients (conical combinations) of two basic vectors. We call such a structure two dimensional.

A structure which is a ground-state one in an m-dimensional region (an m-dimensional convex polyhedral cone with the vertex at the origin of coordinates) is called an m-dimensional structure. It is generated by a set of configurations that is a subset of at least m basic sets given the condition that among the corresponding basic vectors there are m linearly independent ones (and not more). We call the structures which

are ground-state ones in regions with the dimensionality equal to that of the Hamiltonian parameter space (the Hamiltonian should include the chemical potential or the external field) the full-dimensional structures.

Researchers usually found only full-dimensional structures (see, e.g., Ref. [7]). But it is not the complete solution of a ground-state problem. Knowing only full-dimensional ground states does not make it possible to find the ground states at a fixed density of particles (not the chemical potential). Moreover, in this case, one cannot determine the order of phase transition between two neighboring full-dimensional structures (phases).

A ground-state problem can be considered as completely solved only if the complete set of basic rays and all ground states in them or the corresponding basic sets of configurations are found (how to prove the completeness will be shown later). The rest is a "technical" problem of simple combinatorics and multidimensional analytical geometry. True, the knowledge of all full-dimensional structures enables one to find the complete set of basic rays, but it is not sufficient; one should also know all ground states in these rays.

B. Full-dimensional ground-state regions and structures

Let us find full-dimensional structures for our set of basic rays and corresponding basic sets of configurations. To do so, we should find all sets of basic rays with the following properties: (1) The set contains at least four basic rays and between corresponding basic vectors there are four linearly independent ones; (2) at least one structure on the triangular lattice can be constructed with flower configurations belonging to the intersection of corresponding basic sets of configurations; and (3) this intersection is not a subset of any other basic set except the basic sets corresponding to the considered set of basic rays. Such an intersection of basic sets generates full-dimensional structure(s) in the region which is the conical hull of the corresponding basic vectors. If the set of rays contains the ray $\mathbf{r}_{13}$ or $\mathbf{r}_{13}^{-}$, then the additional condition (restriction) should be taken into account when constructing ground-state structures.

We numerate full-dimensional structures and corresponding regions in the same manner as in Ref. [7] and we write their characteristics in the form used by Kaburagi and Kanamori [9] and also in the form that we introduced here. All full-dimensional structures are described in Tables III and IV. The bar over the number of a region (structure) indicates that this region (structure) is symmetric to the region (structure) with the same number but without the bar. We mean the symmetry $h \leftrightarrow -h$ and $J_\triangle \leftrightarrow -J_\triangle$ in regards to regions and the symmetry $\sigma = -1 \leftrightarrow \sigma = +1$ (or particle $\leftrightarrow$ vacancy) in regards to structures. Regions 5 and 6 and corresponding structures are self-symmetric.

In the first, second, third, and fourth columns of Tables III and IV are given, respectively: (1) the notation of the region, (2) the set of flower configurations generating ground-state structures in this region, (3) the characteristics of the structures $S(p_0; p_1, p_2; p_\triangle)$ and also (in square brackets) the fractional contents of the corresponding flower configurations in the structures, and (4) the dimensions of the unit cell of the structure. In the fourth column, "Disorder" specifies regions where there is an infinite number of ground-state structures, including disordered ones. In column five, there are numbers of hyperfaces of full-dimensional regions (i.e., of full-dimensional polyhedral cones). In the last column of Tables III and IV, the conditions for existence of full-dimensional regions in the plane (h, J_2) are given.

The full-dimensional structures with numbers without bars, except for the completely filled one, are depicted in Figs. 3–5. There are 20 full-dimensional structures (phases) in total. Notice that the flowers ❀, ❀, and ❀ generate an infinite number of structures with equal density of energy. Among these structures there are ordered ones as well as disordered ones. The ordered structure with the smallest unit cell is shown in Fig. 4(a). We denote it $9a$. From the infinite number of structures 9, Brandt and Stolze [7] found only this one. Starting from structure $9a$, one can obtain all structures 9, shifting the rows of this structure either along smaller (structures of type A) or larger sides of the unit cell (structures of type B) [see Figs. 4(b) and 4(c)]. A part of these structures will be periodic and another part will be aperiodic (i.e., with an infinite period). One can say that phase 9 is chaotic, meaning this infinite number of structures. It is easy to see that none of structures 9 can be transformed into another of these structures using only local changes. Therefore, this degeneracy does not lead to the residual density of entropy and this disorder can be called one dimensional.

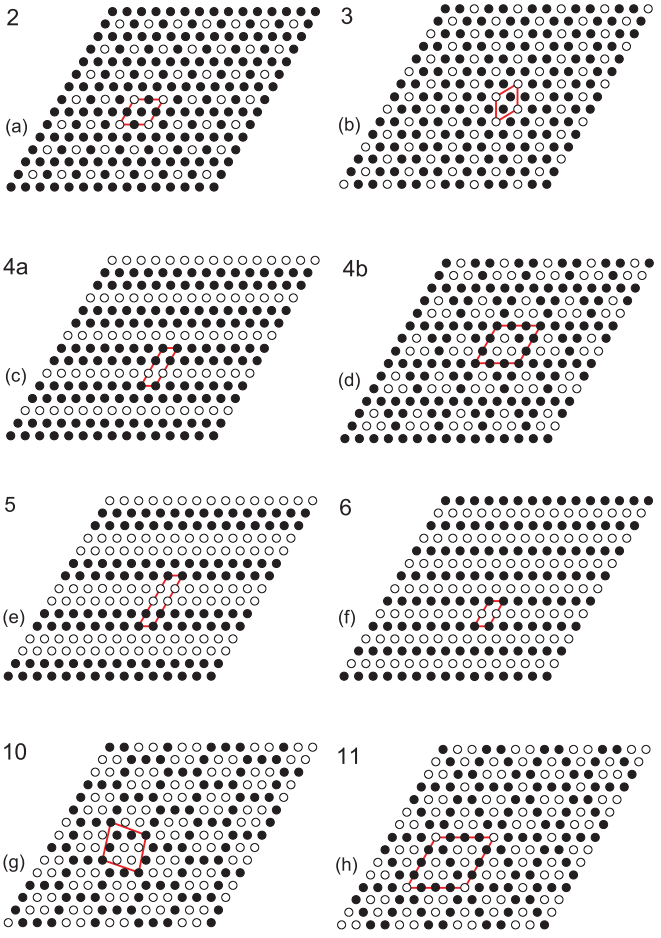


FIG. 3. (Color online) Full-dimensional structures (a) 2, (b) 3, (c) $4a$, (d) $4b$, (e) 5, (f) 6, (g) 10, and (h) 11. Unit cells are indicated.

TABLE III. Full-dimensional grounds-state regions and structures for the spin model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with three-spin nearest-neighbor interaction.

Region	Generating configurations of the structure	Characteristics of the structure	Dimensions of the unit cell	Basic rays	Number of hyperfaces	Conditions for existence in the plane (h, J_2)
1		$S(1;3,3;2)$	1×1	$\mathbf{r}_1,\mathbf{r}_3,\mathbf{r}_5,\mathbf{r}_7,\mathbf{r}_4^-,\mathbf{r}_5^-,$	8	Always
		$[1]$		$\mathbf{r}_6^-,\mathbf{r}_7^-,\mathbf{r}_8^-,\mathbf{r}_{10}^-$		
2		$S\left(\frac{3}{4};2,2;\frac{2}{3}\right)$	2×2	$\mathbf{r}_3,\mathbf{r}_4,\mathbf{r}_5,\mathbf{r}_6,\mathbf{r}_7,\mathbf{r}_9,$	7	$-3J_1 - 4J_\triangle \leqslant 0,$
		$\left[\frac{3}{4},\frac{1}{4}\right]$		$\mathbf{r}_{11},\mathbf{r}_{10}^-$		$-J_1 - 2J_\triangle \leqslant 0$
3		$S\left(\frac{2}{3};\frac{3}{2},3;0\right)$	$\sqrt{3} \times \sqrt{3}$	$\mathbf{r}_1,\mathbf{r}_4,\mathbf{r}_5,\mathbf{r}_{10},\mathbf{r}_{11},\mathbf{r}_{10}^-$	6	$-3J_1 - 2J_\triangle \leqslant 0,$
		$\left[\frac{2}{3},\frac{1}{3}\right]$				$-J_1 - 2J_\triangle \leqslant 0$
4*a*		$S\left(\frac{2}{3};2,\frac{3}{2};1\right)$	1×3	$\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_9,\mathbf{r}_4^-,\mathbf{r}_6^-,\mathbf{r}_8^-,$	7	$J_\triangle \leqslant 0$
		$\left[\frac{1}{3},\frac{2}{3}\right]$		$\mathbf{r}_{10}^-,\mathbf{r}_{12}^-$		
4*b*		$S\left(\frac{2}{3};2,\frac{3}{2};\frac{5}{6}\right)$	3×3	$\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_6,\mathbf{r}_7,\mathbf{r}_9,\mathbf{r}_8^-$	5	$-J_\triangle \leqslant 0$
		$\left[\frac{1}{3},\frac{1}{3},\frac{1}{3}\right]$				
5		$S\left(\frac{1}{2};2,1;1\right)$	1×4	$\mathbf{r}_2,\mathbf{r}_6,\mathbf{r}_7,\mathbf{r}_8,\mathbf{r}_6^-,\mathbf{r}_7^-,$	6	$3J_1 - 2J_\triangle \leqslant 0,$
		$\left[\frac{1}{2},\frac{1}{2}\right]$		$\mathbf{r}_8^-$		$3J_1 + 2J_\triangle \leqslant 0$
6		$S\left(\frac{1}{2};1,1;0\right)$	1×2	$\mathbf{r}_2,\mathbf{r}_9,\mathbf{r}_{10},\mathbf{r}_{11},\mathbf{r}_{12},\mathbf{r}_{13},$	14	$-3J_1 + 2J_\triangle \leqslant 0,$
		$\left[\frac{1}{2},\frac{1}{2}\right]$		$\mathbf{r}_9^-,\mathbf{r}_{10}^-,\mathbf{r}_{11}^-,\mathbf{r}_{12}^-,\mathbf{r}_{13}^-$		$-3J_1 - 2J_\triangle \leqslant 0$
9		$S\left(\frac{3}{5};\frac{5}{3},\frac{4}{3};\frac{4}{9}\right)$	Disorder	$\mathbf{r}_2,\mathbf{r}_4,\mathbf{r}_6,\mathbf{r}_9,\mathbf{r}_{11},\mathbf{r}_{12}$	5	$-J_\triangle \leqslant 0,$
		$\left[\frac{2}{5},\frac{2}{5},\frac{1}{5}\right]$				$-3J_1 - 2J_\triangle \leqslant 0$
10		$S\left(\frac{1}{2};\frac{5}{4},\frac{3}{2};0\right)$	$\sqrt{7} \times \sqrt{7}$	$\mathbf{r}_4,\mathbf{r}_{10},\mathbf{r}_{12},\mathbf{r}_{13}$	4	$-J_1 \leqslant 0,$
		$\left[\frac{1}{4},\frac{1}{4},\frac{1}{4},\frac{1}{4}\right]$				$J_1 - 2J_\triangle \leqslant 0$
11		$S\left(\frac{9}{16};\frac{4}{3},2;0\right)$	4×4	$\mathbf{r}_4,\mathbf{r}_{10},\mathbf{r}_{11},\mathbf{r}_{13}$	4	$-J_1 \leqslant 0,$
	 forbidden	$\left[\frac{3}{16},\frac{3}{8},\frac{3}{8},\frac{1}{16}\right]$				$J_1 - 2J_\triangle \leqslant 0$
12		$S\left(\frac{5}{9};\frac{7}{5},\frac{8}{5};\frac{2}{15}\right)$	Disorder	$\mathbf{r}_4,\mathbf{r}_{11},\mathbf{r}_{12},\mathbf{r}_{13}$	4	$-J_1 \leqslant 0,$
	 forbidden	$\left[\frac{1}{9},\frac{4}{9},\frac{2}{9},\frac{2}{9}\right]$				$3J_1 - 4J_\triangle \leqslant 0$

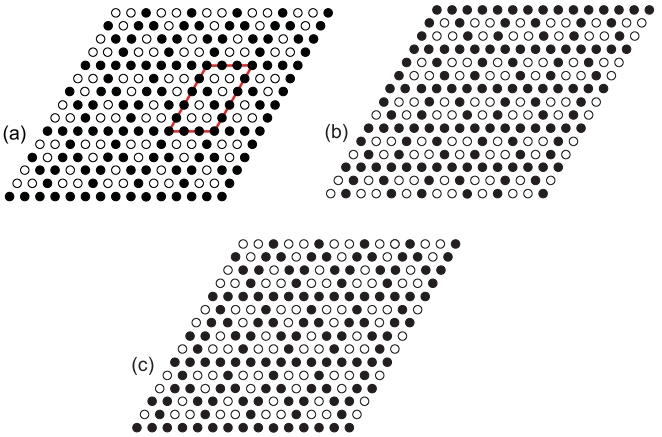


FIG. 4. (Color online) (a) Ordered structure 9 with the smallest unit cell and (b) structures 9 of type *A* and (c) of type *B*.

The set of structures 12 is generated with flower configurations  ,  ,  , and  at the condition that configuration  enters into the structures with its neighborhood depicted in Fig. 2(b). Here this condition is equivalent to the requirement of the absence of configuration  . As seen in Fig. 5(a), full-dimensional phase 12 is also chaotic. One site from each pair of neighboring gray sites should be filled and the other should be vacant. However, if in a pair of gray sites we fill, for instance, the upper site, then in all other pairs of gray sites of this band only the upper sites should be filled. That means that we have the one-dimensional disorder: the order in vertical direction and partial disorder in horizontal direction. Brandt and Stolze [7] found only one structure from the infinite number of structures 12, namely this one which has the smallest unit cell [structure 12*a*, Fig. 5(b)].

The comparison with the case $J_\triangle = 0$ (see Ref. [2]) shows that the three-spin interaction can lead to the appearance of eight full-dimensional phases: 9, 10, 11, 12, $\bar{9}$, $\overline{10}$, $\overline{11}$, and $\overline{12}$.

TABLE IV. Full-dimensional grounds-state regions and structures (numbered with bars) for the spin model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with three-spin nearest-neighbor interaction.

Region	Generating configurations of the structure	Characteristics of the structure	Dimensions of the unit cell	Basic rays	Number of hyperfaces	Conditions for existence in the plane (h, J_2)
$\bar{1}$		$S(0;0,0;0)$ [1]	1×1	$\mathbf{r}_1, \mathbf{r}_4, \mathbf{r}_5, \mathbf{r}_6, \mathbf{r}_7, \mathbf{r}_8, \mathbf{r}_{10}, \mathbf{r}_3^-, \mathbf{r}_5^-, \mathbf{r}_7^-$	8	Always
$\bar{2}$		$S\left(\frac{1}{4};0,0;0\right)$ $\left[\frac{1}{4},\frac{3}{4}\right]$	2×2	$\mathbf{r}_{10}, \mathbf{r}_3^-, \mathbf{r}_4^-, \mathbf{r}_5^-, \mathbf{r}_6^-, \mathbf{r}_7^-, \mathbf{r}_9^-, \mathbf{r}_{11}^-$	7	$-3J_1 + 4J_\triangle \leqslant 0$, $-J_1 + 2J_\triangle \leqslant 0$
$\bar{3}$		$S\left(\frac{1}{3};0,3;0\right)$ $\left[\frac{1}{3},\frac{2}{3}\right]$	$\sqrt{3} \times \sqrt{3}$	$\mathbf{r}_1, \mathbf{r}_{10}, \mathbf{r}_4^-, \mathbf{r}_5^-, \mathbf{r}_{10}^-, \mathbf{r}_{11}^-$	6	$-3J_1 + 2J_\triangle \leqslant 0$, $-J_1 + 2J_\triangle \leqslant 0$
$\overline{4a}$		$S\left(\frac{1}{3};1,0;0\right)$ $\left[\frac{2}{3},\frac{1}{3}\right]$	1×3	$\mathbf{r}_2, \mathbf{r}_4, \mathbf{r}_6, \mathbf{r}_8, \mathbf{r}_{10}, \mathbf{r}_{12}, \mathbf{r}_3^-, \mathbf{r}_9^-$	7	$-J_\triangle \leqslant 0$
$\overline{4b}$		$S\left(\frac{1}{3};1,0;\frac{1}{3}\right)$ $\left[\frac{1}{3},\frac{1}{3},\frac{1}{3}\right]$	3×3	$\mathbf{r}_2, \mathbf{r}_8, \mathbf{r}_3^-, \mathbf{r}_6^-, \mathbf{r}_7^-, \mathbf{r}_9^-$	5	$J_\triangle \leqslant 0$
$\bar{9}$		$S\left(\frac{2}{5};1,\frac{1}{2};\frac{1}{3}\right)$ $\left[\frac{1}{5},\frac{2}{5},\frac{2}{5}\right]$	Disorder	$\mathbf{r}_2, \mathbf{r}_4^-, \mathbf{r}_6^-, \mathbf{r}_9^-, \mathbf{r}_{11}^-, \mathbf{r}_{12}^-$,	5	$J_\triangle \leqslant 0$, $-3J_1 + 2J_\triangle \leqslant 0$
$\overline{10}$		$S\left(\frac{1}{2};\frac{5}{4},\frac{3}{2};\frac{1}{2}\right)$ $\left[\frac{1}{4},\frac{1}{4},\frac{1}{4},\frac{1}{4}\right]$	$\sqrt{7} \times \sqrt{7}$	$\mathbf{r}_4^-, \mathbf{r}_{10}^-, \mathbf{r}_{12}^-, \mathbf{r}_{13}^-$	4	$-J_1 \leqslant 0$, $J_1 + 2J_\triangle \leqslant 0$
$\overline{11}$	 forbidden 	$S\left(\frac{7}{16};\frac{6}{7},\frac{12}{7};\frac{2}{7}\right)$ $\left[\frac{1}{16},\frac{3}{8},\frac{3}{8},\frac{3}{16}\right]$	4×4	$\mathbf{r}_4^-, \mathbf{r}_{10}^-, \mathbf{r}_{11}^-, \mathbf{r}_{13}^-$	4	$-J_1 \leqslant 0$, $J_1 + 2J_\triangle \leqslant 0$
$\overline{12}$	 forbidden 	$S\left(\frac{4}{9};1,\frac{5}{4};\frac{1}{3}\right)$ $\left[\frac{2}{9},\frac{2}{9},\frac{4}{9},\frac{1}{9}\right]$	Disorder	$\mathbf{r}_4^-, \mathbf{r}_{11}^-, \mathbf{r}_{12}^-, \mathbf{r}_{13}^-$	4	$-J_1 \leqslant 0$, $3J_1 + 4J_\triangle \leqslant 0$

C. Proof of the completeness of the set of basic rays

Now we can prove the completeness of the set of basic rays. It means to show that the full-dimensional regions found on the base of these rays fill the space of parameters without gaps. Let us recall that full-dimensional regions in n-dimensional Hamiltonian parameter space are convex polyhedral cones with their vertices at the origin of coordinates. An n-dimensional polyhedral cone is bounded by a zero-dimensional vertex, one-dimensional edges, and two-, three-, . . ., $(n-1)$-dimensional faces. In mathematics, these geometrical objects are called i-faces: 0-face is a vertex, 1-face is an edge, 2-face is a two-dimensional face, etc. The boundary between full-dimensional regions is the conical hull of basic vectors corresponding to those basic rays (1-faces) which are common for these regions. And the ground-state structures on this boundary are generated with those cluster configurations which are common for corresponding basic sets.

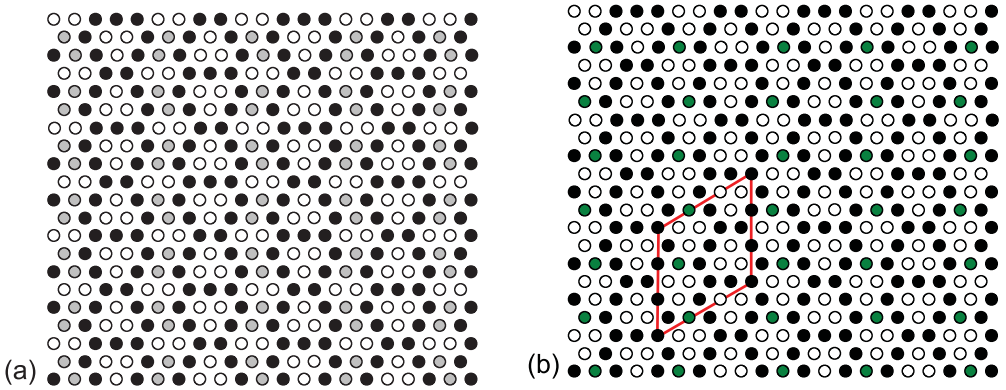
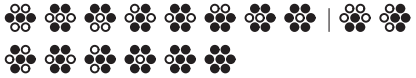
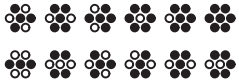
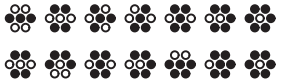
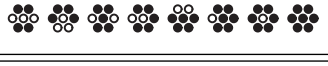


FIG. 5. (Color online) (a) Chaotization of phase 12. In every zigzag, either upper or lower gray circles in each pair should be solid (but identically for each pair of the zigzag). (b) Structure 12a with the smallest unit cell.

TABLE V. Basic rays and basic sets of flower configurations for the spin model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions.

Basic ray		Basic set of flower	Full-dimensional
r	(h, J_1, J_2)	configurations $\mathbf{R}_i$	structures
O	(0,1,0)		$3, \bar{3}, 6$
A	$(-2,-1,1)$		$\bar{1}, \overline{4a}, \overline{4b}, 5$
B	$(0,-2,1)$		$1, \bar{1}, 5$
C	$(-4,1,1)$		$\bar{2}, \overline{4a}, \overline{4b}, 6$
D	$(-6,1,0)$		$\bar{1}, \bar{2}, \bar{3}$
E	$(-12,5,1)$		$\bar{2}, \bar{3}, 6$
F	$(-6,0,1)$		$\bar{1}, \bar{2}, \overline{4a}, \overline{4b}$
G	$(0,0,-1)$		$1, \bar{1}, 3, \bar{3},$
H	(0,0,1)		$4a, 4b, \overline{4a}, \overline{4b}, 5, 6$
$\mathbf{A}^-$	$(2,-1,1)$		$1, 4a, 4b, 5$
$\mathbf{C}^-$	(4,1,1)		$2, 4a, 4b, 6$
$\mathbf{D}^-$	(6,1,0)		$1, 2, 3$
$\mathbf{E}^-$	(12,5,1)		$2, 3, 6$
$\mathbf{F}^-$	(6,0,1)		$1, 2, 4a, 4b$

Two full-dimensional regions can share an i-face if $0 \leqslant i \leqslant n-1$. If two full-dimensional regions share a $(n-1)$-face, then we call them neighboring regions. In our four-dimensional Hamiltonian parameter space, boundaries between two neighboring full-dimensional regions are 3-faces. We call them hyperfaces. 2-faces are called simply "faces." If the set of basic vectors (rays) for a full-dimensional region is known, then one can find its subsets, the elements of which generate hyperfaces of the region. A hyperface is generated by three or more basic vectors (rays). To prove the completeness of the set of basic rays it is necessary (1) to find all hyperfaces of the full-dimensional regions and (2) to show that each hyperface belongs to two different full-dimensional regions. It is easy to do this in the three-dimensional case when $J_\triangle = 0$ (see the Appendix).

Let us show how to find the hyperfaces of the full-dimensional regions. Let $\mathbf{r}_i$, $\mathbf{r}_j$, and $\mathbf{r}_k$ be the three basic vectors (rays) of a hyperface. (Every triplet of basic vectors of a full-dimensional region is linearly independent.) The equation

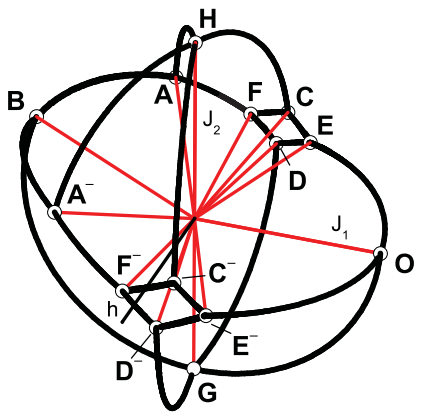


FIG. 6. (Color online) Three-dimensional ground-state phase diagram for the spin model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions (see also Tables V and VI). Basic rays are marked in red (light gray).

TABLE VI. Full-dimensional grounds-state regions and structures for the spin model on the triangular lattice with nearest- and next-nearest-neighbor pairwise interactions.

Region	Generating configurations of the structure(s)	Basic rays
1		A^-, B, G, D^-, F^-
$\bar{1}$		A, B, G, D, F
2		C^-, E^-, D^-, F^-
$\bar{2}$		C, E, D, F
3		O, G, D^-, E^-
$\bar{3}$		O, G, D, E
4		A^-, H, C^-, F^-
$\bar{4}$		A, H, C, F
5		A, B, A^-, H
6		O, E, C, H, C^-, E^-

of the hyperplane that contains the origin of the coordinates and the tips of $\mathbf{r}_i$, $\mathbf{r}_j$, and $\mathbf{r}_k$ vectors reads

$$\det|\mathbf{r}-\mathbf{r}_i,\mathbf{r}_j-\mathbf{r}_i,\mathbf{r}_k-\mathbf{r}_i,\mathbf{r}_i|=0, \tag{14}$$

where $\mathbf{r}=(h,J_1,J_2,J_\triangle)^T$ is the column vector of the spin Hamiltonian's parameters.

Vector $\mathbf{n}$, composed out of the coefficients near the variables h, J_1, J_2, and $J_\triangle$ in this determinant, is orthogonal to the hyperplane. If the scalar products of this vector with all basic vectors of the considered full-dimensional region have the same sign or some of them are equal to zero, then the conical hull of vectors $\mathbf{r}_i$, $\mathbf{r}_j$, $\mathbf{r}_k$, and those vectors of the full-dimensional region which are orthogonal to vector $\mathbf{n}$ will be a hyperface of this region. If every hyperface of every full-dimensional region is at the same time a hyperface of one more full-dimensional region (the neighboring one), then these regions filled the Hamiltonian parameter space with no gaps, and, therefore, the set of basic vectors is complete. In such a way we verified the completeness of the set of basic rays (vectors) that we had found. The total number of hyperfaces is rather large (equal to 60), therefore we will not enumerate them here.

V. CONCLUSIONS

In conclusion, we developed a method for determination of the ground states of lattice-gas models, and by using it, we found a complete solution for the ground-state problem of the lattice-gas model (or the equivalent spin model) on the infinite plane triangular lattice with nearest- and next-nearest-neighbor pairwise interactions and with an additional interaction between triplets of particles at the vertices of nearest-neighbor triangles. The main idea of this method is to construct global configurations of a lattice using the set of configurations of a finite-size cluster. We proved that for finding ground states in any point of the Hamiltonian parameter space it suffices to find all ground states in 24 rays originating from the origin of coordinates, and we showed that in 22 rays the ground states are generated with sets of configurations of a seven-site cluster in the form of a flower (without any restriction). In the remaining two mutually symmetric rays, the ground states are constructed with some flower configurations but also with an additional restriction (three configurations enter into structures only with some neighborhoods). To prove this, we formulated a rule for grouping the flowers of structures and we found the groups with minimal energy. This method can be used also for the determination of the ground states of some other lattice-gas models.

Having found the flower configurations for the ground states in 24 rays, we determined all full-dimensional ground-state structures (some of them turned out to be chaotic), and we proved the completeness of the determined set of basic rays.

In principle, the results presented here can be considered as a complete solution for the ground-state problem. What remains is to construct, using the solution found, the ground-state structures on hyperfaces of full-dimensional regions. It will give, in particular, the possibility to analyze the types of phase transitions between full-dimensional structures and, even more important, to determine all ground-state structures at a fixed density of particles (but not the chemical potential). This is nearly done and will be a subject of future publications.

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APPENDIX: $J_\triangle = 0$ CASE

To further clarify the concept of basic rays and basic sets of configuration, let us consider the simple particular case $J_\triangle = 0$ analyzed in Ref. [2]. The solution of this ground-state problem can be represented in the form of basic rays and basic sets of flower configurations (see Table V). The full-dimensional regions and structures are indicated in Table VI.

Since the space of parameters is three dimensional, one can visualize the polyhedral cones corresponding to the full-dimensional ground states. They are depicted in Fig. 6. The faces of polyhedral cones in the figure are bordered by arcs of the unit sphere.

In Table VI, the basic rays for every full-dimensional region are enumerated in such an order that each pair of neighboring rays (the first and the last ones are also neighboring) generates a two-dimensional face of the three-dimensional region. As one can easily see, each face belongs to two full-dimensional regions. It means that there are no gaps between full-dimensional regions, and, therefore, the set of basic rays is complete.

Let us note that in region 4 ($\bar{4}$) there are two ground-state structures: $4a$ and $4b$ ($\overline{4a}$ and $\overline{4b}$).

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