PHYSICAL REVIEW E **83**, 022101 (2011)

Structures on lattices: Some useful relations

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(Received 11 November 2010; published 23 February 2011)

We consider a lattice and structures on it generated by a set of configurations of a cluster. Using some general considerations, we show that there exist linear relations between fractional contents of these configurations in the structures. Such relations can be useful for the determination of the ground states of lattice-gas models (or equivalent spin models). As an illustration we consider a set of configurations of a seven-site cluster on the triangular lattice.

DOI: 10.1103/PhysRevE.83.022101 PACS number(s): 05.50.+q, 75.10.Hk, 68.43.Fg, 89.75.Kd

In many methods for determination of the ground states of lattice-gas models (or equivalent spin models), the global ground-state structures are constructed with local configurations of some subset of the lattice [1–3]. We show here that there exist some linear relations between the fractional contents of these configurations in any structure that they generate. To avoid equivocacies we first give some simple definitions.

Let us consider a lattice without any restriction on its spatial dimension and topology, for instance, a triangular lattice on an infinite plane, or a three-dimensional face-centered cubic lattice, or a triangular lattice on the surface of an infinite cylinder. As an example we consider the infinite planar triangular lattice.

Let us consider a finite set of sites on the lattice. We will call it a "cluster." In the case of the triangular lattice it can be, for instance, a site with six neighboring sites  (such a cluster is called a "flower"). Two clusters on the lattice are equivalent if each of them can be transformed into the other by a symmetry transformation of the lattice. We assume that all clusters, equivalent to the chosen one, cover the lattice (certainly, with overlaps). For instance, the triangular lattice can be covered with overlapping flowers: each site is the center of a flower. Due to the symmetry of the isotropic triangular lattice, every flower on the lattice is equivalent to every other flower and the orientation of a flower does not matter. We consider equivalent clusters as the same cluster in different positions on the lattice, and we simply say that the lattice can be covered with the cluster.

Each site of the lattice can be in one state from a finite number of states. In the simplest case this number is equal to 2. For instance, a site can be occupied by a particle (we depict such a site as a filled circle) or vacate (an open circle). If the state of each site is determined, then we say that there is a structure on the lattice. Similarly, if the state of every site of a cluster is determined, then we have a configuration of the cluster. For a given structure the configuration of a cluster depends on its position on the lattice.

Consider cluster **K**, which covers the lattice with overlaps and a set of its configurations $\{\mathbf{K}_l\}$ ($l = 1,2,...,L$). Consider subcluster **Q** of this cluster. Let the subcluster occupy M *nonequivalent* positions in the cluster. We enumerate them with subscript m ($m = 1,2,\ldots,M$). Let each cluster **Q** on the lattice be contained in c_m clusters **K** as subcluster **Q** in position number m. Here is an example: the central and lateral positions of the one-site subcluster in the flower ($M = 2$). $c_1 = 1$, because each site is contained in the one flower in central position, and $c_2 = 6$, because each site is contained in six flowers in the lateral position.

Consider a structure **S** on the lattice generated by the set of cluster configurations $\{\mathbf{K}_l\}$. This means that each cluster **K** on the lattice has one of the configurations of the set. We denote the fractional content of configuration $\mathbf{K}_l$ in structure **S** by k_l. The following trivial relation holds true:

$$\sum_l k_l = 1. \tag{1}$$

Now let us consider a subcluster configuration $\mathbf{Q}_t$ from the set of all possible subcluster configurations $\{\mathbf{Q}_t\}$ and let us calculate its content in structure **S**. This can be done in different ways, depending on the position of the subcluster in the cluster. Let it be position m. Then the number of configurations $\mathbf{Q}_t$ per one cluster **K** is equal to

$$\sum_l \frac{k_l n_{ml}}{c_m}, \tag{2}$$

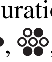
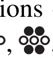
where n_{ml} is the number of configurations $\mathbf{Q}_t$ occupying position m in configuration $\mathbf{K}_l$ of the cluster.

The number of configurations $\mathbf{Q}_t$ should not depend on m. Therefore the following relation holds:

$$\sum_l \frac{k_l n_{m_1 l}}{c_{m_1}} = \sum_l \frac{k_l n_{m_2 l}}{c_{m_2}}, \tag{3}$$

where m_1 and m_2 are arbitrary *nonequivalent* positions of subcluster **Q** in cluster **K**. This equality gives a relation between fractional contents k_l. Considering different pairs of positions of the subcluster in the cluster, we obtain other relations. We can also consider another subcluster of cluster **K**. An important point is that the subcluster should have at least two nonequivalent positions in the cluster.

Let us consider an example. The cluster "flower" on the triangular lattice has only three subclusters of this type: (1) one-site subcluster, (2) a pair of nearest neighbors, and (3) three sites that create a 120° angle. Each of these subclusters has two nonequivalent positions in the cluster flower.

Let us consider the following set of configurations of the cluster flower on the triangular lattice: {, , , , }.

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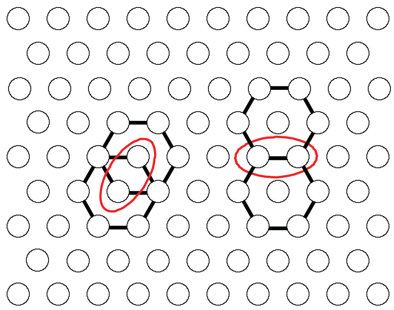

FIG. 1. (Color online) Two-site subcluster [in (red) oval] on the triangular lattice contained in two flowers in the radial position (left) and in two flowers in the lateral position (right).

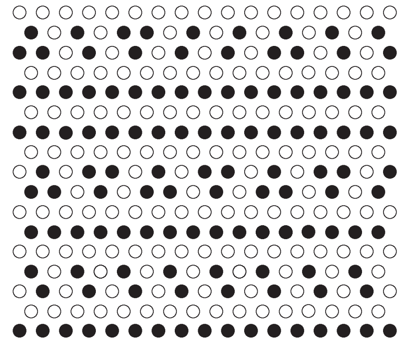

FIG. 2. Example of a structure generated by the set of flower configurations described in the text.

Their fractional contents in a structure are k_1, k_2, k_3, k_4, and k_5, respectively. Let the subcluster be two neighboring sites. This subcluster can occupy two positions in the cluster (Fig. 1): a radial one ($m = 1$) and a lateral one ($m = 2$). Consider the configuration of the subcluster in which both sites are filled. Then we have, for this configuration,

$$\begin{aligned} &c_1 = 2,\ n_{11} = 1,\ n_{12} = 2,\ n_{13} = 0,\ n_{14} = 0,\ n_{15} = 2; \\ &c_2 = 2,\ n_{21} = 0,\ n_{22} = 0,\ n_{23} = 1,\ n_{24} = 2,\ n_{25} = 1. \end{aligned} \tag{4}$$

$c_1 = c_2 = 2$ because the subcluster belongs to two flowers in both radial and lateral positions.

Substituting these numbers in Eq. (3), we obtain a relation between fractional contents of flower configurations in every structure generated by these configurations (an example of such a structure is shown in Fig. 2):

$$k_1 + 2k_2 - k_3 - 2k_4 + k_5 = 0. \tag{5}$$

Consider now the subcluster configuration in which both sites are unoccupied. Numbers n_{ml} for this configuration are as follows:

$$\begin{aligned} &n_{11} = 0, \quad n_{12} = 0, \quad n_{13} = 3, \quad n_{14} = 2, \quad n_{15} = 0; \\ &n_{21} = 4, \quad n_{22} = 2, \quad n_{23} = 1, \quad n_{24} = 0, \quad n_{25} = 3. \end{aligned} \tag{6}$$

Substituting these numbers in Eq. (3), we obtain one more relation:

$$4k_1 + 2k_2 - 2k_3 - 2k_4 + 3k_5 = 0. \tag{7}$$

Hence, besides trivial relation (1), there are two additional relations between fractional contents of configurations , , , ,  in the structures that they generate. It can be shown that other relations (generated by other subclusters) will be linear combinations of these three relations. If we have a set of only three flower configurations, then, in general, three relations completely determine their fractional contents in any structure generated by these configurations. If a structure is generated by a set of four flower configurations, then only one of four fractional contents can be independent.

The knowledge of fractional contents k_l of cluster configurations in a structure makes it possible to find the density $p_{\mathbf{Q}_t}$ (number per cluster $\mathbf{K}$) of any configuration $\mathbf{Q}_t$ of any subcluster $\mathbf{Q}$ in the structure:

$$p_{\mathbf{Q}_t} = \frac{\sum_l k_l n_{\mathbf{Q}_t l}}{c_{\mathbf{Q}}}, \tag{8}$$

where $n_{\mathbf{Q}_t l}$ is the number of configurations $\mathbf{Q}_t$ in the lth configuration of cluster $\mathbf{K}$, and $c_{\mathbf{Q}}$ is the total number of clusters $\mathbf{K}$ containing a subcluster $\mathbf{Q}$ on the lattice. For the same purpose, expression (2) can be used.

Everything stated above is not applicable for a cluster in which there are no subclusters with at least two different positions in the cluster. Ring  is an example of such a cluster on the triangular lattice.

Relations (3) between fractional contents of configurations of a cluster in a structure are interesting by themselves. Moreover, they are very useful and sometimes even necessary in the analysis of ground states of lattice-gas models (or equivalent spin models). This will be shown in our next publication.

Some questions arise that we are not able to answer at the moment. Is there a simple way to determine the number of lineally independent relations for a given cluster? Is there always a subcluster that generates all lineally independent relations as in the example considered?

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