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The Global Minimum of Energy Is Not Always a Sum of Local Minima—A Note on Frustration

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A classical lattice gas model with translation-invariant, finite-range competing interactions, for which there does not exist an equivalent translation-invariant, finite-range nonfrustrated potential, is constructed. The construction uses the structure of nonperiodic ground-state configurations of the model. In fact, the model does not have any periodic ground-state configurations. However, its ground-state—a translation-invariant probability measure supported by ground-state configurations—is unique.

KEY WORDS: Frustration; m-potential; nonperiodic ground states; tilings.

1. INTRODUCTION

The low-temperature behavior of systems of many interacting particles results from the competition between energy and entropy, i.e., the minimization of the free energy. At zero temperature this reduces to the minimization of the energy density. Configurations of a system which minimize its energy density are called ground-state configurations. One of the important problems of statistical mechanics is to find ground-state configurations for given interactions between particles. If we can find a configuration such that potential energies of all interactions between particles are minimal, then we can conclude that it is a ground-state configuration. It is then said that such a model is not frustrated. Otherwise, we may rearrange potentials and construct an equivalent Hamiltonian which may not be frustrated and which will enable us to find ground-state configurations. Here we present a classical lattice gas model with translation-invariant, finite-range competing interactions for which there does not exist an equivalent translation-

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invariant, finite-range nonfrustrated potential. In other words: the global minimum of energy is not the sum of its minima attained locally in space. More precisely, one cannot minimize the energy density of interacting particles by minimizing their energy in a finite box and all its translates, no matter how large is the box.

2. CLASSICAL LATTICE GAS MODELS, FRUSTRATION, AND *M*-POTENTIALS

A classical lattice gas model is a system in which every site of a lattice Z^d can be occupied by one of n different particles. An infinite lattice configuration is an assignment of particles to lattice sites, that is, an element of $\Omega = \{1,..., n\}^{Z^d}$. Particles can interact through many-body potentials. A *potential* Φ is a collection of real-valued functions Φ_Λ on configuration spaces $\Omega_\Lambda = \{1,..., n\}^\Lambda$ for all finite $\Lambda \subset Z^d$. Here we assume Φ to have finite range, that is, $\Phi_\Lambda = 0$ if the diameter of Λ is large enough, and to be translation-invariant. The formal Hamiltonian can then be written as

$$H = \sum_\Lambda \Phi_\Lambda$$

Two configurations $X, Y \in \Omega$ are said to be *equal at infinity*, $X \sim Y$, if there exists a finite $\Lambda \subset Z^d$ such that $X = Y$ outside Λ. The relative Hamiltonian is defined by

$$H(X, Y) = \sum_\Lambda [\Phi_\Lambda(X) - \Phi_\Lambda(Y)] \qquad \text{for} \quad X \sim Y$$

$X \in \Omega$ is a *ground-state configuration* of H if

$$H(Y, X) \geqslant 0 \qquad \text{for any} \quad Y \sim X$$

For any potential the set of ground-state configurations is nonempty, but it may not contain any periodic configurations.[1–3] We will be concerned here with nonperiodic ground-state configurations which have uniformly defined frequencies for all finite patterns. By definition the orbit closure of such a ground-state configuration supports a unique strictly ergodic translation-invariant measure called a ground state which is a zero-temperature limit of a low-temperature Gibbs state (an infinite-volume grand canonical probability distribution). If we can find a configuration that minimizes all Φ_Λ, then it is necessarily a ground-state configuration and we call such potential nonfrustrated or an m-potential.[4, 5] Formally, a potential Φ is an *m-potential* if there exists a configuration X such that

$$\Phi_\Lambda(X) = \min_Y \Phi_\Lambda(Y) \qquad \text{for any finite } \Lambda$$

Otherwise, we may try to rearrange interactions to obtain an equivalent m-potential. Two potentials are defined to be *equivalent* if they yield the same relative Hamiltonian and therefore have the same ground-state configurations and the same Gibbs states. It follows that for any periodic configuration its energy density is the same (up to a trivial additive constant which can be chosen to be zero) for all equivalent potentials. It is best illustrated by an example of the antiferromagnetic nearest-neighbor spin-1/2 model on the triangular lattice. The formal Hamiltonian can be written as follows:

$$H = \sum_{i,j} \sigma_i \sigma_j$$

where σ_i, $\sigma_j = \pm 1$ and i and j are nearest-neighbor sites on the triangular lattice. When one looks at an elementary triangle it is easy to see that at least one pair of spins does not minimize its interaction. Two spins align themselves in opposite directions and then the third one can minimize only one of the two remaining interactions. This choice is a source of frustration[6] (see also another approach to frustration[7, 8]). However, we may construct the following equivalent potential:

$$\phi_{\triangle} = \tfrac{1}{2}(\sigma_i \sigma_j + \sigma_j \sigma_k + \sigma_k \sigma_i)$$

where i, j, and k are vertices of an elementary triangle $\triangle$ and $\Phi_A = 0$ otherwise. Now, there are ground-state configurations minimizing every Φ_A. Three spins on every elementary triangle still face choices, but they act collectively and therefore are not frustrated.

In the following section we construct an example of a lattice gas model with nearest-neighbor, translation-invariant frustrated interactions for which there does not exist an equivalent finite-range, translation-invariant m-potential. The main problem of proving the impossibility of an m-potential is that a grouping of interactions in big plaquettes, as in the above example, is not the only way of constructing an equivalent m-potential. To construct it, one may also use information about a global structure of excitations. In some models just grouping is clearly impossible because energy can be lower locally than that of a ground-state configuration and one can pay for it arbitrarily far away, yet one can still construct an equivalent m-potential. One of the easiest examples is a one-dimensional Ising model with the following interactions: the energy of $+-$ neighbors is equal to -1, the energy of $-+$ neighbors is 2, and otherwise the energy is zero. There are arbitrarily long line segments with the energy equal to -1. Nevertheless, the above potential is equivalent to an m-potential with the energy of $-+$ neighbors equal to 1 and zero otherwise, or $-\frac{1}{4}(\sigma_i \sigma_{i+1} - 1)$ using spin variables.

3. AN INTRINSICALLY FRUSTRATED MODEL

The model is based on Robinson's tiles.[9, 10] There is a family of 56 squarelike tiles such that using an infinite number of copies of each of them one can tile the plane only in a nonperiodic fashion. This can be translated into a lattice gas model in the following way, first introduced by Radin.[1-3] Every site of the square lattice can be occupied by one of the 56 different particles–tiles. Two nearest-neighbor particles which do not "match" contribute positive energy, which we choose to be 24 for our purposes; otherwise, the energy is zero. Such a model obviously does not have periodic ground-state configurations. There are uncountably many ground-state configurations, but only one translation-invariant ground-state measure supported by them. There is a one-to-one correspondence between ground-state configurations in the support of this measure and Robinson's nonperiodic tilings. The low-temperature behavior of this model was investigated in refs. 11–13.

We describe now slightly modified Robinson tiles (with a different number of tiles); we follow ref. 9 closely. There are seven basic tiles represented symbolically in Fig. 1. The rest of them can be obtained by rotations and reflections. The first tile on the left is called a cross; the rest are called arms. All tiles are furnished with one of the four parity markings shown in Fig. 2. The crosses can be combined with the parity marking at the lower left in Fig. 2. Vertical arms (the direction of long arrows) can be combined with the marking at the lower right and horizontal arms with the marking at the upper left. All tiles may be combined with the remaining

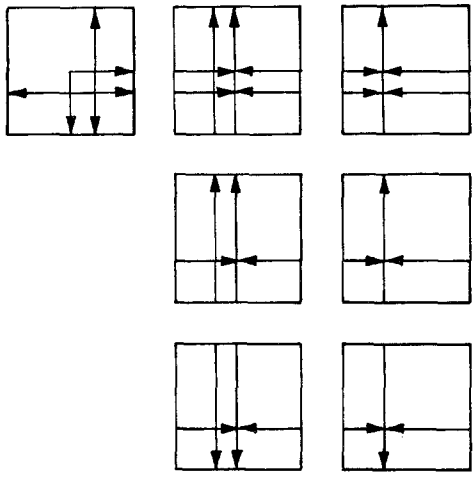

Fig. 1. Crosses and arms.

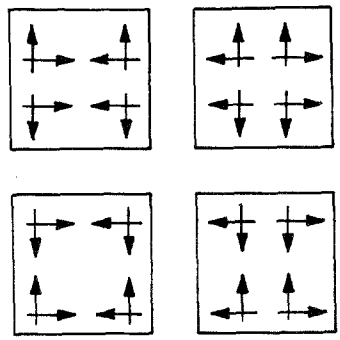

Fig. 2. Parity markings.

marking. Two nearest-neighbor tiles "match" if arrowheads meet arrow tails separately for the parity markings and the markings of crosses and arms.

Let us now describe the mean features of Robinson's nonperiodic tilings. We will concentrate on the lattice positions of crosses denoted by ⌊, ⌈, ⌋, and ⌉, where directions of line segments correspond to double arrows in Fig. 1. Every odd–odd position on the Z^2 lattice (if columns and rows are suitably numbered) is occupied by these tiles in relative orientations as in Fig. 3. They form the periodic configuration with the period 4. Then in the center of each "square" one has to put again a cross such that the previous pattern reproduces, but this time with the period 8. Continuing this procedure infinitely many times, we obtain a nonperiodic configuration. It has built in periodic configurations of period 2^n, $n \geqslant 2$, on sublattices of Z^2 as shown in Fig. 4.

Now we will modify the above model, introducing another level of markings which are optional, that is, they can be present (one at a time) or absent in appropriate tiles. Every cross can be equipped with one of the

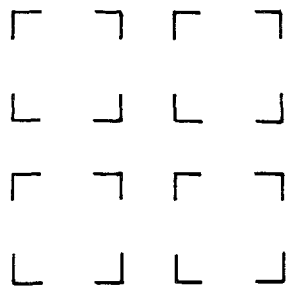

Fig. 3. Relative orientation of crosses.

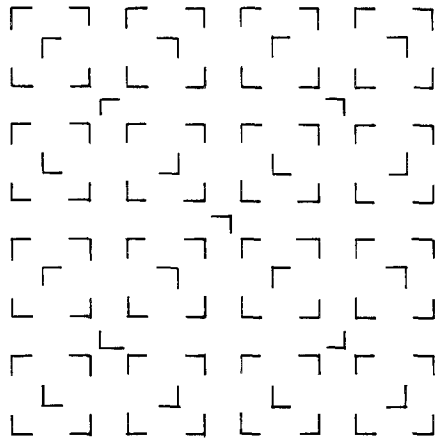

Fig. 4. Robinson's nonperiodic ground-state configuration.

two markings shown at the left in Fig. 5. The orientation of a marking at the top should be the same as the orientation of its cross and it comes in either red or yellow color; the second marking is red. Arms can be furnished with red or yellow lines shown in the middle column in Fig. 5 (colored lines should be parallel to long arrows). Arms at the top in Fig. 1 can be equipped with a marking at the upper right in Fig. 5 with yellow–red, red–yellow, or yellow–yellow (but not red–red) segments perpendicular to long arrows and closer to their tails than to their heads, or a red marking at the lower right in Fig. 5 with a short segment parallel to long arrows and pointing in the other direction. Finally, arms in the middle row and at the bottom in Fig. 1 can be equipped with a marking at the upper right in Fig. 5 with yellow–red, red–yellow, yellow–yellow, and

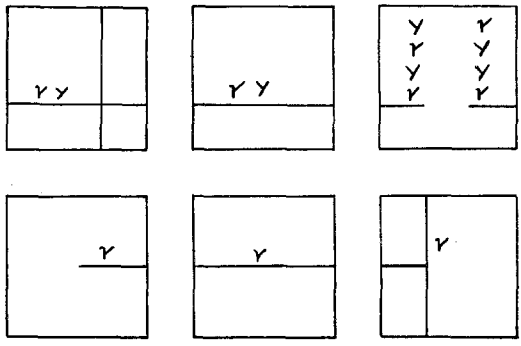

Fig. 5. Additional markings.

red–red segments perpendicular to long arrows. Now, two tiles match if in addition to previous requirements there are no broken lines of new markings and adjacent colors are the same. In the corresponding classical lattice gas model in addition to two-body nearest-neighbor interactions we introduce a chemical potential equal to 1 for yellow crosses and having a negative value $\tau > -1$ for red crosses with the marking at the upper left in Fig. 5 (called simply red crosses from now on) and zero value for the remaining particles–tiles. Let us notice that in the absence of broken bonds our matching rules force the number of yellow crosses to be at least equal to the number of red crosses.

Proposition. For $\tau > -1$ the unique ground-state measure of the modified model is the same as that of the original Robinson model.

Proof. Let a broken bond be a unit segment on the dual lattice separating two nearest-neighbor particles with a positive interaction energy (a common side of two nearest-neighbor tiles which do not match). Let us divide the lattice into connected components without broken bonds (two lattice sites are connected if they are nearest neighbors) such that, on every component, crosses having a relative orientation shown in Fig. 3 form a $2Z^2$ sublattice. This can be achieved by paths on the lattice dual to Z^2 with lengths smaller than 8 and joining broken bonds. For any such component either all crosses on its $2Z^2$ sublattice are colored and then no other cross can be colored, or no cross on this sublattice is colored. This follows from the fact that there are four lines of colored arms emanating from each cross and such lines cannot intersect each other. We call a cross on a $2Z^2$ (2^nZ^2, $n \geqslant 1$, in general) sublattice a boundary cross if its distance from the boundary of its connected component is smaller than 2 (2^n, $n \geqslant 1$, in general). Now, we decompose further every connected component without colored crosses on its $2Z^2$ sublattice into connected components such that crosses form there a $4Z^2$ sublattice. This time it is achieved by paths on the dual lattice with lengths smaller than 16 and again joining broken bonds. Again, for any such component either all crosses on its $4Z^2$ sublattice are colored and then no other cross is colored, or no cross on this sublattice is colored. In the latter case we have to decompose further this component. We repeat this procedure for all 2^nZ^2 sublattices for every $n \geqslant 1$. Now, the total number of all paths and every n in every finite region is bounded above by three times the number of broken bonds (broken bonds and paths can be regarded as vertices and edges of a planar graph and our bound follows from Euler's formula). This shows that the density of red boundary crosses is bounded above by 24 times the density of broken bonds. The negative chemical potential of red boundary crosses is then

compensated by the positive energy of broken bonds. On the other hand, the density of yellow crosses is at least equal to the density of red crosses which are not boundary ones, so the negative chemical potential of these red crosses is compensated by the positive chemical potential of yellow crosses ($\tau > -1$). It follows that the energy of a configuration is at least proportional to the total length of broken bonds (a Peierls condition is satisfied). Hence in any ground-state configuration in the support of a ground-state measure broken bonds are absent. Among configurations without broken bonds, configurations without any colored particles (Robinson's original configurations) have the minimal energy density (equal to zero) and are therefore the only ground-state configurations. This follows again from the fact that $\tau > -1$ and the number of yellow crosses is greater than or equal to the number of red crosses. ▮

Obviously, our interactions do not constitute an m-potential. Moreover, it is impossible to construct a translation-invariant, finite-range m-potential by grouping interactions in big plaquettes as was done in the antiferromagnetic example. One may locate colored crosses on the sublattice $2^n Z^2$, therefore decreasing energy locally and paying for it arbitrarily far away (see Fig. 6). Now we will prove that for some τ an equivalent translation-invariant, finite-range m-potential does not actually exist.

Theorem. The above-described model for $-1 < \tau < -6/10$ does not have an equivalent translation-invariant, finite-range m-potential.

Proof. Let us assume otherwise and let its range be smaller than 2^n. Let us consider three configurations with periodic arrangements of colored markings and with their periods shown in Fig. 6, where squares have size 2^{n+1} and only colored markings of the central tile of each square are shown. Equating their energy densities for the original interaction and a hypothetical equivalent m-potential, we obtain

$$\tau + 3 = a_r + b_{ry} + c_y + d_{yr} + e_{ry} + g_y + i_y + j_y + k_y + l_y + m_{yr} + o_y \tag{1}$$

$$2\tau + 2 = a_r + b_{ry} + c_y + d_{yr} + e_r + f_r + g_y + i_r + j_{ry} + k_y + l_{ry} + m_r + o_y \tag{2}$$

$$2\tau + 2 = a_r + b_r + c_r + d_r + e_{ry} + f_r + g_{ry} + i_y + j_y + k_y + l_y + m_{yr} + o_{yr} \tag{3}$$

where on the right-hand sides we have nonnegative contributions to the energy due to a hypothetical m-potential (we know from the Proposition that the energy density of the ground state is zero, so an m-potential cannot be negative) and coming from regions labeled in the upper left corners of the squares in Fig. 6; subscripts correspond to configurations of optional markings, with r denoting red, y denoting yellow, and ry and yr meaning a change of colors along a line of arms.

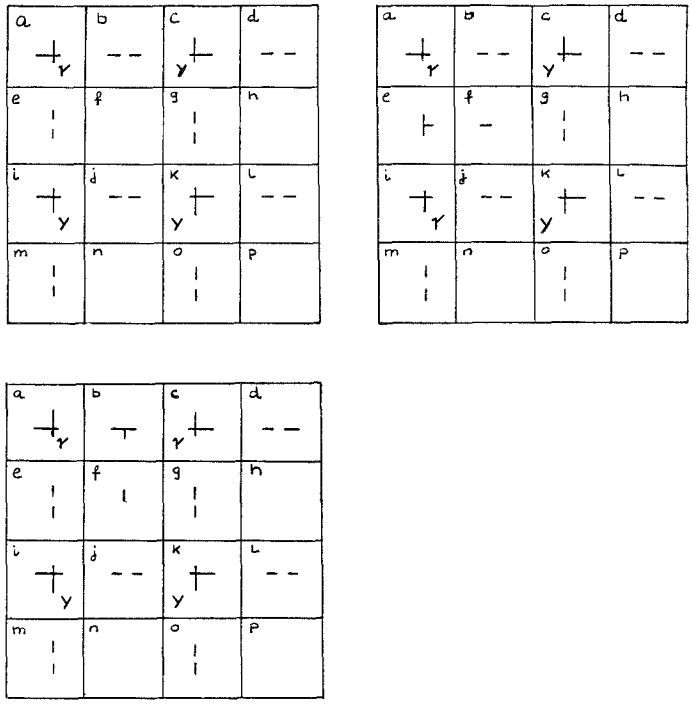

Fig. 6. Periodic configurations of colored markings.

Now, set $\tau = -1 + \delta/2$. From (2) we obtain $a_r \leqslant \delta$ and $b_{ry} + c_y + d_{yr} + g_y + o_y \leqslant \delta$, and from (3), $e_{ry} + i_y + j_y + k_y + l_y + m_{yr} \leqslant \delta$. Then it follows from (1) that $a_r \geqslant 2 - (3/2)\delta$, which contradicts $a_r \leqslant \delta$ if $\delta < 4/5$. This contradiction rules out the existence of an equivalent translation-invariant, finite-range m-potential. ∎

4. CONCLUSIONS

A classical lattice gas model with translation-invariant nearest-neighbor competing interactions is constructed. Its unique translation-invariant ground-state measure is supported by nonperiodic ground-state configurations. There are local excitations in the model such that the energy is locally lower than that of a ground-state configuration and one pays for it arbitrarily far away. This shows that by grouping interactions in big plaquettes, as in the antiferromagnetic model on the triangular lattice, one cannot construct an equivalent finite-range m-potential. More generally it is proved that such a potential actually does not exist. The model is therefore intrinsically frustrated.

Let us note that in the antiferromagnetic model a spin on an elementary triangle is frustrated because it faces a choice of direction. Both of its choices can be present in a ground-state configuration, therefore making a ground state highly degenerate. In our example a particle may choose a local minimum of energy and then it appears that this does not lead to a ground-state configuration.

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