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

Jacek Miękisz
Institut de Physique Théorique
Université Catholique de Louvain
Chemin du Cyclotron, 2
B-1348 Louvain-la-Neuve, Belgium.

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Abstract. 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

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 I present 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. 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 latice 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 be translation-invariant. The formal Hamiltonian can be then 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

$$H(X,Y) = \sum_\Lambda (\Phi_\Lambda(X) - \Phi_\Lambda(Y)) \ \ for \ \ X \sim Y.$$

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

$$H(Y,X) \geq 0 \ \ for \ \ any \ \ Y \sim X.$$

For any potential the set of ground state configurations is nonempty but it may not contain any periodic configurations [1, 2, 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

$$\Phi_{\Lambda}(X) = min_{Y} \Phi_{\Lambda}(Y) \;\; for \;\; any \;\; finite \;\; \Lambda.$$

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 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 $\sigma_i, \sigma_j = \pm 1$ and i and j are nearest neighbor sites on the triangular lattice. When you look at an elementary triangle it is easy to see that at least one pair of spins does not minimize its interaction. Two spins allign 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:

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

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

In the following section I 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, like in the above example, is not the only way of constructing an equivalent m-potential. To construct it one may also use an 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 you 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 $-1/4(\sigma_i \sigma_{i+1} - 1)$ using spin variables.

3 An Intrinsically Frustrated Model

The model is based on Robinson's tiles [9, 10]. There is a family of 56 square-like 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, 2, 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, say 2; 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. Low temperature behavior of this model was investigated in [11, 12, 13].

I describe now slightly modified Robinson tiles [14]. 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 left and horizontal arms with the marking at the upper left. All tiles may be combined with the remaining marking. Two tiles "match" if arrow head meets arrow tail. Let us observe

that if the plane is tiled with tiles with such markings then these parity markings must alternate both horizontally and vertically in the manner shown in Fig.2.

Let me now describe the main features of the Robinson's nonperiodic tilings. I will concentrate on the lattice positions of crosses denoted by $\lfloor, \lceil, \rfloor, \rceil$, where directions of line segments correspond to double arrows in Fig.1. Every odd-odd position on the Z^2 lattice 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, $n \geq 2$ on sublattices of Z^2 as shown in Fig.4.

Now I will modify the above model a little bit introducing another level of markings which are optional, that it is to say they can be present or absent in appropriate tiles. Every cross can be equipped with one of the 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 double arrrows of its cross and it comes in either red or green color. The second marking comes only in red color. Arms at the left in Fig.1 can be furnished with red or green lines shown in the middle column in Fig.5. Finally, arms at the top of Fig.1 can be equipped with either a red marking at the upper right in Fig.5 or a marking at the lower right in Fig.5 with green-red, red-green, or green-green sides. Now, two tiles match if there are no broken lines and adjacent colors are the same. In the corresponding classical lattice gas model in addition to two-body nearest neighbor interactions I will introduce a chemical potential equal to 1 for green crosses and having a negative value τ for red crosses and zero value for uncolored crosses and all arms.

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

Proof: Let a broken bond be a segment on the dual lattice separating two nearest neighbor particles with a positive interaction energy. I will prove that in any ground state configuration broken bonds are absent. Let us observe that the matching rules are such that on any $2^n Z^2$ sublattice, $n \geq 1$, in any region without broken bonds, crosses should be oriented like in Fig. 3 except possibly on a sublattice boundary. The lower bound of the energy of interacting particles in any such region is obtained if crosses on the boundary of every sublattice are red and all other crosses are not colored and we take into account only the negative energy of chemical potentials of red crosses. For any broken bond there can be at most two red crosses hence the energy of a configuration is at least proportional to the total length of broken bonds (a variation of a Peierls condition is satisfied). This shows that in any ground state configuration broken bonds are absent. Among configurations without broken bonds, configurations without any colored particles (Robinsons's original configurations) have the minimal energy density (equal to zero) and are therefore the only ground state configurations.□

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 like it was done in the antiferromagnetic example. One may locate colored crosses on vertices of a square with a size 2^n therefore decreasing energy locally and paying for it arbitrarily far away [see Fig.6]. Now I will prove that for some τ an equivalent translation-invariant finite range m-potential does not actually exist.

Theorem 1 *The above described model for $-1 < \tau < 4/5$ 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 local excitations from a Robinson ground state configuration shown in Fig.6, where squares have size 2^{n+1}. Equating relative Hamiltonians for the original interaction and a hypothetical equivalent m-potential we obtain:

$$\tau + 3 = a_r + b_{rg} + c_g + d_g + e_g + f_g + g_g + h_{gr}, \tag{1}$$

$$2\tau + 2 = a_r + b_{rg} + c_g + d_g + e_g + f_{gr} + g_r + h_r + i_r, \tag{2}$$

$$2\tau + 2 = a_r + b_r + c_r + d_{rg} + e_g + f_g + g_g + h_{gr} + i_r, \tag{3}$$

where on the right hand sides we have nonnegative contributions to energy due to a hypothetical m-potential and coming from regions labelled in the upper left corners of the squares in Fig.6; subscripts correspond to configurations of optional markings with r denoting red and g denoting green.

Now, set $\tau = -1+\delta/2$. From (2) we obtain $a_r \leq \delta$ and $b_{rg}+c_g+d_g+e_g \leq \delta$, and from (3) $f_g + g_g + h_{gr} \leq \delta$. Then it follows from (1) that $a_r \geq 2 - 3/2\delta$ which contradicts $a_r \leq \delta$ if $\delta < 4/5$. This contradiction rules out the existence of an equivalent translation-invariant finite range m-potential. $\Box$

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, like 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. Its both choices can be present in a ground state configuration making therefore 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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