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Nonperiodic Long-Range Order for Fast-Decaying Interactions at Positive Temperatures

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We present the first example of an exponentially decaying interaction which gives rise to nonperiodic long-range order at positive temperatures.

KEY WORDS: Classical lattice-gas models; nonperiodic ground and Gibbs states; long-range order; Thue–Morse sequences; stratified Gibbs states; quasicrystals.

1. INTRODUCTION

Since the discovery of quasicrystals,[29] there has been an interest in understanding their occurrence in statistical mechanics models of interacting particles, see for example refs. 2, 18, 25, and 30. One would like to show that a quasicrystalline phase occurs in appropriate models at sufficiently low temperatures. We interpret this as the occurrence of ground states or Gibbs states which possess a quasi-periodic, or more generally, a nonperiodic long-range order[1, 9, 24, 28].

Up till now there only exist some partial results going in this direction. Most of them have been obtained for lattice models, and here again we will get a result of this type.

In classical lattice-gas models, every site of a regular lattice, Z^d, is occupied by one of n different types of particles (equivalently, by $+1$ or -1 in spin 1/2 models). Configurations of such models are therefore

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elements of $\Omega = \{1,..., n\}^{Z^d}$. Particles interact through possibly many-body potentials which are represented by functions $\Phi_\Lambda : \Omega_\Lambda \to R$ for all finite $\Lambda \subset Z^d$, where $\Omega_\Lambda = \{1,..., n\}^\Lambda$. We assume that the Φ_Λ are translation invariant and decay exponentially in $N(\Lambda)$, the number of sites in Λ, and in fact in what we need for the next section, even in $diam(\Lambda)$. The formal Hamiltonian can be therefore written as $H_\Phi = \sum_\Lambda \Phi_\Lambda$. By ground states of H_Φ, we mean translation-invariant probability measures supported by configurations with minimal energy density. Ground states are zero-temperature limits of translation-invariant Gibbs states (equilibrium states).

Following are the main results which are known to us, concerning non-periodic order of ground states and Gibbs states of lattice models:

(1) For finite-range interactions, non-periodic long-range order in the ground state can occur in dimension 2 and higher, but not in dimension 1.[19, 25, 26]

(2) In dimension 1, non-periodic long-range order in the ground state can occur for infinite-range, but arbitrarily fast decaying interactions.[1, 13, 24]

(3) In dimension 2, non-periodic long-range order in the ground state can occur for nearest-neighbor interactions.[18, 20, 22, 23, 25, 27] At positive temperatures in such models, the best result proven so far is the existence of an infinite sequence of temperatures with the period doubling of periodic Gibbs states.[21]

(4) At positive temperatures, non-periodic long-range order can occur for slowly decaying (summable) interactions (in arbitrary dimensions). These interactions can be finite-body, or even pair interactions.[8, 10]

In this note we want to present an example and a general construction where non-periodic long-range order occurs at positive temperatures for fast (exponentially) decaying interactions in 3 dimensions. Before entering into details of the argument, which is based on ref. 14, and is indeed more or less a corollary of that paper, we want to make a few comments.

(1) Although at zero temperature there exists an important qualitative difference between strictly finite-range interactions and interactions which are of infinite range but have a fast decaying tail, this qualitative difference is not expected to persist at positive temperatures.

(2) There is a conjecture that two-dimensional lattice gas models with short-range interactions always have at most finitely many (periodic) Gibbs states, which rules out the possibility of non-periodic long-range order. For some arguments and results supporting this conjecture, see refs. 7, 31, and 32. It would mean that our results could not be true in 2 dimensions.

(3) A limitation of our result is that we prove the existence of non-periodic structures in only one direction. We conjecture that this limitation is not really necessary, but our method does not give the stronger result (non-periodic order in three directions at the same time).

2. THE EXAMPLE

Let us recall a definition of the Thue–Morse state. We begin by constructing a one-sided Thue–Morse sequence. We put $+$ at the origin and perform successively a substitution: $+ \to + -$, $- \to - +$, obtaining $+$, $+ -$, $+ - - +$, $+ - - + - + + -$,... We get a one-sided sequence $\{X_{TM}(i)\}$, $i \geqslant 0$. We define $X_{TM} \in \Omega = \{+, -\}^Z$ by setting $X_{TM}(i) = X_{TM}(-i-1)$ for $i < 0$.

Let T be a translation operator, i.e., $T: \Omega \to \Omega$, $T(X)(i) = X(i-1)$, $X \in \Omega$. Let G_{TM} be the closure (in the product topology of the discrete topology on $\{+, -\}$) of the orbit of X_{TM} by translations, i.e., $G_{TM} = \{T^n(X_{TM}), n \geqslant 0\}^{cl}$. It can be shown that G_{TM} supports exactly one translation-invariant probability measure μ_{TM} on Ω.[15,16] μ_{TM} is the only ground state of a certain fast decaying four-spin interaction[13] (see (1) below).

We will combine this construction of ref. 13 with the result of ref. 14 on "stratified" Gibbs measures. Thus in one of the directions we start by choosing the interaction of ref. 13, while in the other two directions we have the nearest-neighbor ferromagnetic interaction. This model has as ground-state configurations the "stratified" (or stacked) Thue–Morse sequences, that is they are Thue–Morse sequences (i.e., elements of G_{TM}) in one direction, and translation-invariant in the other two directions. Thus in the terminology of ref. 14 we are in a stratified situation: even though the interaction is translation invariant, ground-state configurations building up the single translation-invariant ground-state measure are nonperiodic (Thue–Morse) layered structures.

Let us mention some other works considering low-temperature behavior of models with periodic stratified ground states. The phase diagram of the ANNNI model was investigated in refs. 4, 5 and 11. General three-dimensional stratified models were discussed in ref. 12 and some related results were recently obtained in a model with a layered magnetic field.[17]

It has been known for some time that ground-state configurations which have no energy barrier between them in one dimension (example: the kink states in the one-dimensional Ising model) can give rise to corresponding Gibbs states in three dimensions. These Gibbs states have the same structure in one direction and are ferromagnetically ordered in the other two directions (example: the Dobrushin states in the three-dimensional Ising model[6]). The ideas of Dobrushin have been extended to more general situations in ref. 14, and here we observe that these recent results can be applied to the non-periodic Thue–Morse ground-state configurations studied in ref. 13. In one dimension, we will consider the sequences supporting the translation-invariant Thue–Morse measure μ_{TM} (which is the only translation-invariant ground-state measure). The energy barriers between them may be arbitrarily small, but this does not need to matter; in fact, as we have just remarked, even for ground states with zero-energy barriers, it is the case that adding ferromagnetic nearest-neighbor terms in two extra dimensions can stabilize them. In the general approach of ref. 14, the result is that the stratified structures appear, not necessarily for the original interaction, but for a small (weak and exponentially decaying) perturbation thereof. In our case it is to be expected that in fact such a perturbation will be needed. We will start with the Hamiltonian $H_{TM}+H_F$, where

$$H_{TM}=\sum_{i\in Z^3}\sum_{r=0}^{\infty}\sum_{p=0}^{\infty}J(r,p)(\sigma_i+\sigma_{i+(2^p)e_1})^2 \times(\sigma_{i+(2r+1)2^pe_1}+\sigma_{i+(2r+2)2^pe_1})^2 \tag{1}$$

$$H_F=\sum_{i\in Z^3}J(\sigma_i\sigma_{i+e_2}+\sigma_i\sigma_{i+e_3}) \tag{2}$$

where e_n is the unit vector in the nth direction, $\sigma_i=\pm 1$ is a spin variable and $J(r,p)>0$ and decays to zero exponentially fast when distances between interacting particles increase.

The Thue–Morse layers are ground-state configurations of $H_{TM}+H_F$. We need to take care against the possibility that there are periodically layered structures which have more low-energy excitations and therefore compensate for having a higher energy at zero temperature. To illustrate the phenomenon we need to control, assume for the moment that in the first sum, only the term $J(0,0)$ in the above expression is non-zero. That is, one excludes local configurations with three successive pluses or minuses. Then, in the horizontal direction, next to the Thue–Morse sequences, there are many more ground states, and it is easy to see that, for example, the 3-periodic structures $--+$ or $++-$ have more lowest energy excitations ($8J$ which is the energy of overturning one spin without creating three successive pluses or minuses) than (and hence in the terminology of ref. 3 dominate) the Thue–Morse ones. This effect explains the necessity of having an extra interaction term in our theorem, to make low-temperature Gibbs measures "Thue–Morse-like" in the first direction.

In the following, we will consider one-dimensional interactions $\Phi=\{\Phi_\Lambda:\Omega_\Lambda\to R\}$ such that for every $X\in\Omega_\Lambda$, $|\Phi_\Lambda(X)|\leqslant\varepsilon\omega^{diam(\Lambda)}$ for some ε, $\omega>0$. We denote by $\mathscr{H}^{\varepsilon,\omega}$ the family of such interactions. If X is a ground-state configuration, then by a Gibbs state which is a small perturbation of it we mean a Gibbs state ρ_X such that $\rho_X(P_a^X) < \varepsilon(T)$, where P_a^X is a projection on configurations which are different from X at a lattice site a and $\varepsilon(T) \to 0$, when the temperature $T \to 0$.

The subsequent theorems follow from the Main Theorem of ref. 14. Proofs and more technical details one can find there.

Theorem 1. Fix some $J > 0$ in (2) (e.g., $J = 1$). Then there exist strictly positive constants C, ε_0 and T_0 such that the following is true: For each $\varepsilon < \varepsilon_0$ and $\omega = Ce^{-2J/T}$ with $T < T_0$ there exists a map

$$\begin{aligned} \mathscr{H}^{\varepsilon, \omega} &\to \bigcup_{\varepsilon_1 \in (\varepsilon, \varepsilon + \omega)} \mathscr{H}^{\varepsilon_1, \omega} \\ H_0 &\mapsto H_1 \end{aligned} \tag{3}$$

such that for each ground-state configuration X of $H^* = H_1 + H_F$ there exists a Gibbs state μ_X of $H = H_0 + H_F$, which is a small perturbation of X.

Actually, one can give an explicit formula for the perturbative Hamiltonian $H_1 - H_0$ in terms of quickly converging cluster expansion series, whose (small!) terms change only slowly with H_0 and H_F.

Our aim is to construct a translation-invariant Gibbs state of H such that it has only non-periodic Gibbs states in its extremal decomposition. In order to do so we would like H^* to have a unique ground-state measure supported by non-periodic ground-state configurations (Thue–Morse stratified sequences in our example). The following inverse mapping type theorem assures us of this (the Lipschitz property is rather obvious if one inspects the explicit formulas given in ref. 14 for H_1).

Theorem 2. With the notation of Theorem 1, the map (3) is Lipschitz continuous in the sense that if $H_0 - H'_0 \in \mathscr{H}^{\varepsilon', \omega}$ with $\varepsilon' < \varepsilon_0$, then $H_1 - H'_1 \in \mathscr{H}^{\varepsilon'', \omega}$ with $\varepsilon'' = \varepsilon' \omega$. In particular, if we choose ε_1 such that $\varepsilon_0 - \varepsilon_1 > \omega$, then for every $H_1 \in \mathscr{H}^{\varepsilon_1, \omega}$, there exists a preimage $H_0 \in \mathscr{H}^{\varepsilon_0, \omega}$ such that there is one-to-one correspondence between stratified ground-state configurations of H^* and stratified Gibbs states of H.

Now we put $H^* = H_{TM} + H_F$ and use Theorem 1 and 2 to obtain non-periodic Thue–Morse Gibbs states of H, which are small perturbations of the Thue–Morse stratified ground-state configurations. Therefore, there exists a translation-invariant Thue–Morse Gibbs state, ρ_{TM}, which has only non-periodic (Thue–Morse) Gibbs states in its extremal decomposition.

ρ_{TM} is a Gibbs state which is extremal among the translation-invariant Gibbs states of H. We expect that H does not have any other translation-invariant Gibbs states. However, we cannot exclude at the moment some "exotic" translation-invariant states which do not arise from stratified configurations.

3. GENERALIZATIONS AND OPEN PROBLEMS

It was shown by Aubry and Radin[1, 24] that any strictly ergodic measure on Ω is a unique ground state of a certain one-dimensional, many-body, infinite-range but arbitrarily fast decaying interaction. Our construction shows the existence of another interaction of the same type such that when adding ferromagnetic interactions in two extra dimensions one obtains a model with a low-temperature Gibbs state which is a small perturbation of the original measure.

As we have already discussed, we do not expect the nonperiodic order for the original Thue–Morse interaction. A likely possibility here is the existence of an infinite sequence of temperatures, decreasing to zero, at which the periods of the corresponding extremal Gibbs states grow. It is an open problem to construct a two-body (or even finite-body) interaction (finite range or exponentially decaying) without periodic ground-state configurations and with a nonperiodic Gibbs state.

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