Journal of Statistical Physics, Vol. 58, Nos. 5/6, 1990

A Microscopic Model with Quasicrystalline Properties

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Received June 5, 1989; revision received September 29, 1989

A classical lattice gas model with two-body nearest neighbor interactions and without periodic ground-state configurations is presented. The main result is the existence of a decreasing sequence of temperatures for which the Gibbs states have arbitrarily long periods. It is possible that the sequence accumulates at nonzero temperature, giving rise to a quasiperiodic equilibrium state.

KEY WORDS: Aperiodic tilings; classical lattice gas models; phase transitions; quasicrystals.

1. INTRODUCTION

I would like to address the problem of low-temperature stability of nonperiodic structures. I will discuss a system of many interacting particles such that the configurations with minimal energy density, the so-called ground states, are nonperiodic. Low-temperature behavior of the system results from the competition between energy and entropy, i.e., the minimization of the free energy. Is the entropy contribution big enough to destroy nonperiodic structures or are there equilibrium phases which are small perturbations of nonperiodic ground states? This question is especially interesting in connection with the recently discovered quasicrystals.[1-3]

The model is a classical lattice gas. More precisely, every site of the simple cubic lattice can be occupied by one of several different particles. The particles interact through two-body nearest neighbor potentials. The model does not have periodic ground-state configurations. Although nonperiodic, they are not, however, completely chaotic. They exhibit long-

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range positional order in the sense that states at distant regions are correlated. In fact, ground-state configurations possess highly ordered structures. If a certain fraction of particles is ignored, the rest of a ground-state configuration is periodic: the smaller the fraction, the larger the period.

One would like to see how much of this structure survives at low temperatures. The main result is the following:

Theorem 1. There is a decreasing sequence of temperatures T_n such that if $T < T_n$, then there exists a Gibbs state with period at least $2 \cdot 6^n$ in both directions.

The equilibrium state in Theorem 1 is a small perturbation of a periodic configuration present in a ground-state configuration in the form described above. The translational symmetry is broken. The sequence of temperatures can accumulate at zero or at some positive temperature. The first possibility means that every time T_n decreases to T_{n+1} the period of the equilibrium state increases by a factor of 6. In the second case we have an example of an equilibrium quasicrystal. We are unable to determine which possibility actually happens. An analogous theorem was already proven for an exponentially decaying interaction.[4] Here it holds in the case of the nearest neighbor interaction. The result was already announced in a letter.[5] Here I give the complete proof.

In Section 2 I describe the main features of Robinson's nonperiodic tilings of the plane, construct a classical lattice gas model out of it, and outline the modified Peierls argument. In Section 3 the model is described in full detail. The proof of Theorem 1 follows in Section 4. Section 5 contains a short discussion.

2. TILINGS AND THE PEIERLS ARGUMENT

The present example of a classical lattice gas model is based on Robinson's tiles,[6–8] which is a family of 56 squarelike tiles which 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.[4,9–14] 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; otherwise, the energy is zero. Such a model obviously does not have periodic ground-state configurations. To obtain a three-dimensional model, add the nearest neighbor interaction along the third axis which favors the pairs of identical particles. The ground-state configurations are the previous ones repeated in the third direction.

I now describe the main features of Robinson's nonperiodic tilings. I will concentrate on the lattice positions of four particular tiles denoted by └, ┌, ┘, and ┐ and referred to as crosses. Every odd–odd position on the Z^2 lattice is occupied by these tiles in relative orientations as in Fig. 1. They form a periodic configuration with 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 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. 2.

Using the Peierls argument,[15–17] one would like to construct an equilibrium phase which is a small perturbation of a periodic configuration with period 2^n if the temperature is small enough: $T < T_n$. Imagine a finite-volume Λ excitation X from G, one of the nonperiodic ground-state configurations. Let a be a lattice site belonging to the sublattice L_n of Z^2 associated with the period 2^n of G. Let a be occupied by a different particle in the excited configuration X than in G. Now every walk on L_n which connects any site outsite Λ with a has at least one pair of adjacent sites with particles which are not both crosses or they are both crosses with the relative orientation different from these in Fig. 1. This means that at a distance at most 2^n from this pair there is a broken bond—a nearest neighbor pair of mismatched particles. This leads to the following useful definitions. By a contour of a configuration I mean a connected component of a union of irregular squares. A square of size 2^{n+1} is irregular if it contains a broken bond. Now it follows that a belongs to a contour or one of its interiors. By the very definition of the contour the energy of a contour is proportional to its area—the Peierls condition is satisfied. The number of all possible contours enclosing any given site grows polynomially with their

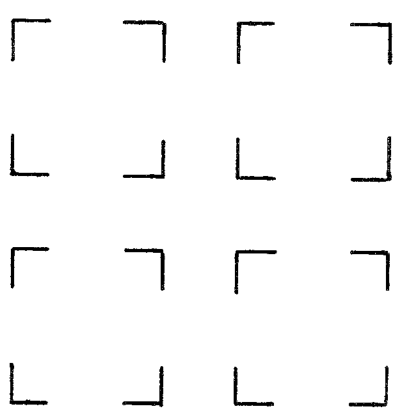

Fig. 1. Relative orientation of crosses.

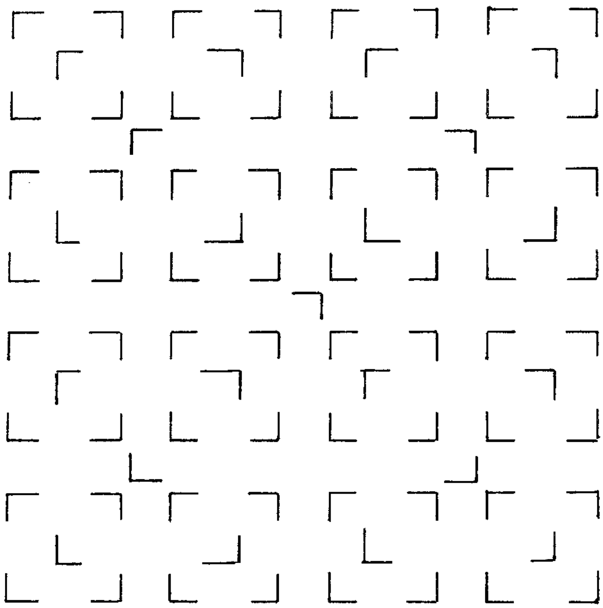

Fig. 2. Robinson's nonperiodic ground state configuration.

areas. If one could prove that the probability of any contour is bounded by $\exp[-\beta A(n)]$—the Peierls bound—where β is the inverse temperature and $A(n)$ is the area of the contour, then the standard Peierls argument, showing that the probability of the site a being occupied by a different particle than in G is very small for large enough β, would finish the proof of Theorem 1. Unfortunately, in order to prove the Peierls exponential bound, one has to modify Robinson's tiles a little bit.

3. DESCRIPTION OF THE MODEL

I describe here the modification of Robinson's tiles.[6–8] Every tile is a square with several levels of markings. Two adjacent tiles match if markings at every level match. In the case of colorings, the colors should match in the prescribed manner. If the markings consist of lines, we cannot break them throughout any tiling. The markings of the first level are presented in Fig. 3. The first tile on the left is called a cross; the remaining ones are called arms. Allowing rotations, we have four crosses, four horizontal arms, and four vertical arms.

All tiles are furnished with one of the four parity markings shown in Fig. 4. The crosses are combined with the parity marking at the lower left

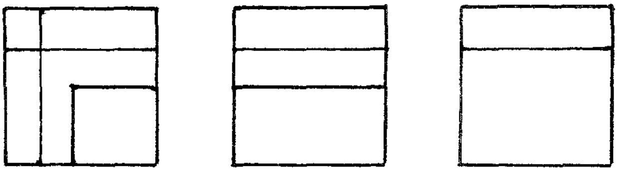

Fig. 3. Crosses and arms.

in Fig. 4. Vertical arms can be combined with the marking at the upper left and horizontal arms with the marking at the lower right. All tiles may be combined with the remaining marking. Two parity markings match if arrow head meets arrow tail. Observe that if the plane is tiled with tiles with such markings, then these must alternate both horizontally and vertically in the manner shown in Fig. 4. The markings described so far force any tiling to have the pattern of crosses shown in Fig. 1.

Now are would like crosses of higher scale to appear not in every square as in Fig. 2, but in the center of every third square as in Fig. 5. The reason is that in order to get the Peierls exponential bound on the probability of the occurrence of a contour connected with one scale, the higher scales should be sparser so as not to interfere energetically. This will be evident in the proof of Proposition 3. To achieve that, let us color the edges of crosses. Both horizontal and both vertical edges should be colored in the same way: either green, red, or blue. We have therefore nine different colored crosses. One would like colors of crosses to alternate both horizontally and vertically in the above order and then to have a cross in the red-blue square only as in Fig. 6. To force the desired sequence of colored

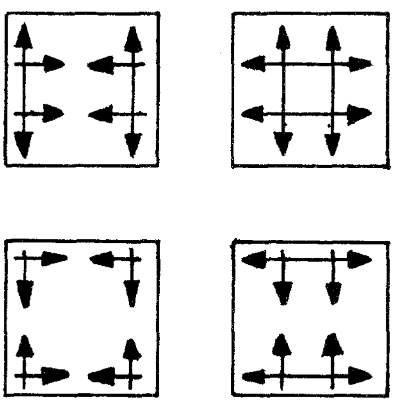

Fig. 4. Parity markings.

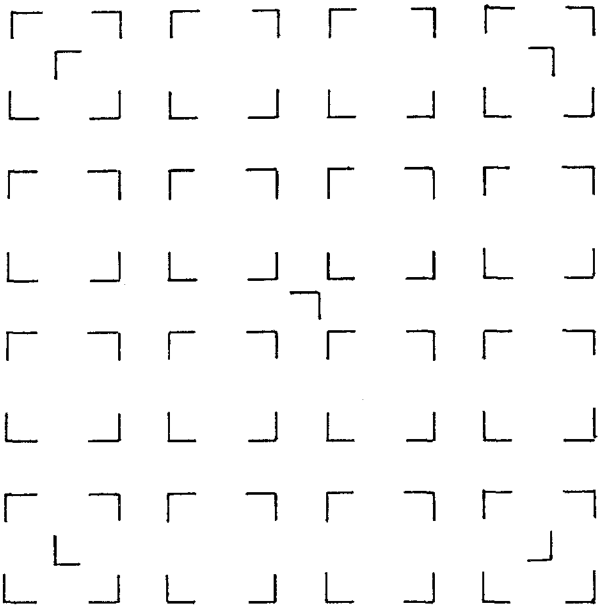

Fig. 5. Modified nonperiodic ground state configuration.

crosses, color the edges of the arms tiles as well. In distinction to crosses, only two edges perpendicular to the markings of the first level are colored. To enforce blue–green sequence, one has yellow arms; yellow matches itself and matches blue to the left or bottom and green to the right or top as in Fig. 7. Similarly, for green–red sequence one has orange arms; orange matches itself and matches green to the left or bottom and red to the right or top. Finally, for red–blue sequence one has red arms, blue arms, and two special arms: a horizontal arm with the red left edge and blue right one and a vertical arm with the red bottom edge and blue top one; all colors match themselves in a natural way. These special arms will play an important role in forcing crosses to appear in the center of every red–blue square. To have the horizontal green–red–blue sequence repeating vertically and the green–red–blue vertical sequence repeating horizontally, I introduce a second level of colorings matching themselves in a natural way. First-level marking lines of a cross get colors of edges parallel to them. First-level arms marking lines can get green, red, or blue color in an arbitrary way. This finally forces a pattern of crosses shown in Fig. 6. To force crosses to appear in the center of every red–blue square, I introduce the last level of markings. A horizontal, second-level red, lower double arm and a horizontal, second-level blue, upper double arm with the red left edge and the blue

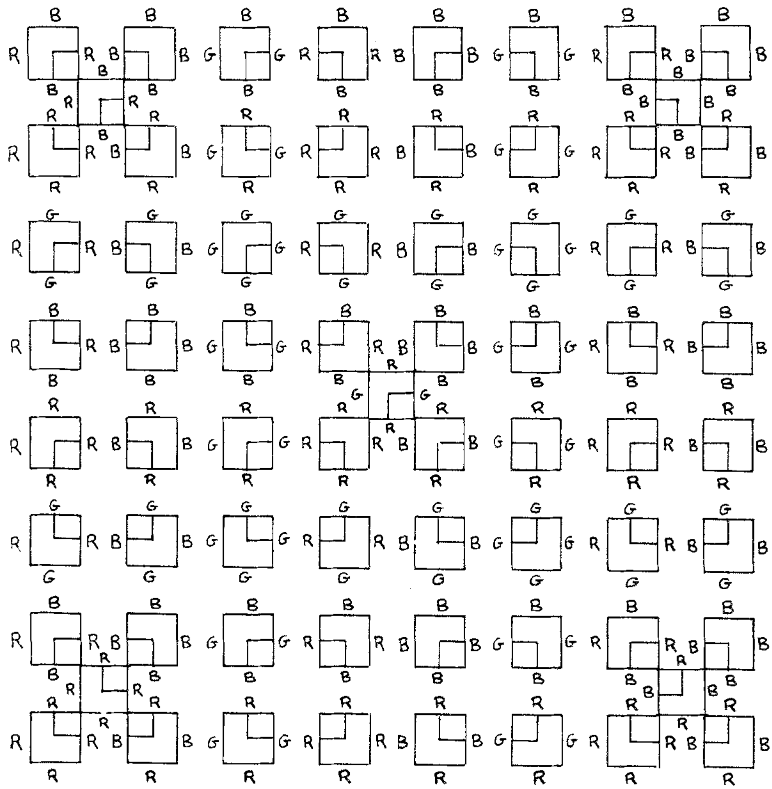

Fig. 6. Colorings of crosses.

right edge are equipped with a half line as in Fig. 8 and have in addition all the markings of a vertical arm. A vertical second-level red, left double arm and a vertical, second-level blue, right double arm with the red bottom edge and the blue top edge are marked similarly. Every other horizontal/vertical arm can be equipped with the optional middle horizontal/vertical line and every cross with the upper right parity with two crossed lines as shown in Fig. 8. This will force a cross to appear in the center of a red–blue square to form a structure shown in Fig. 9. The remaining special horizontal/vertical red–blue arms either have all the markings of a vertical/horizontal arm or the other sides are left plain as in all remaining arms. Finally, I introduce a plain square tile with the upper right parity marking.

Counting all combinations of markings, there are 72 crosses, 384 special arms forcing crosses in the middle of chosen squares, 3880 other special arms, 192 remaining arms, and one plain tile; altogether, 4529 tiles–

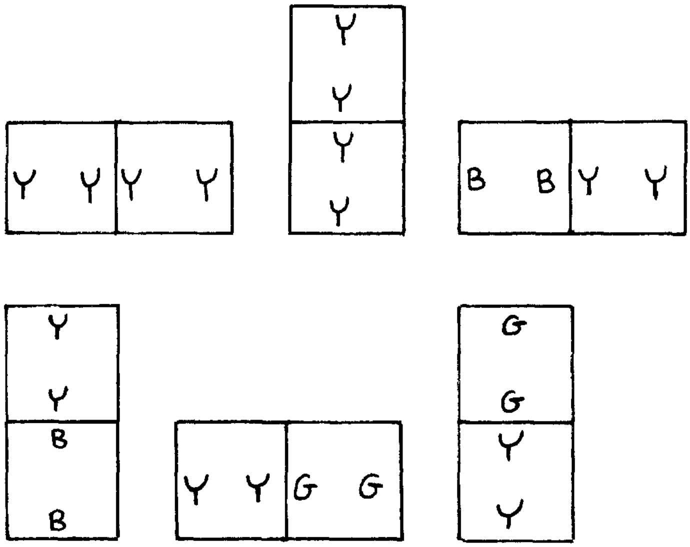

Fig. 7. Colorings of arms.

particles. I made no effort to minimize the number of particles. The most important fact is that there are finitely many of them.

Once the crosses are forced to appear, they are arranged in a fixed pattern. It repeats infinitely many times, producing a nonperiodic tiling G of the plane. This defines in a natural way an infinite sequence of square lattices $L_n \subset Z^2$ with lattice spacing $2 \cdot 6^{n-1}$, $n=1,\ldots$, such that if $a \in L_n$, then $G(a)$ is a cross and the crosses form a periodic configuration with period 6 on L_n, hence $2 \cdot 6^n$ true period.

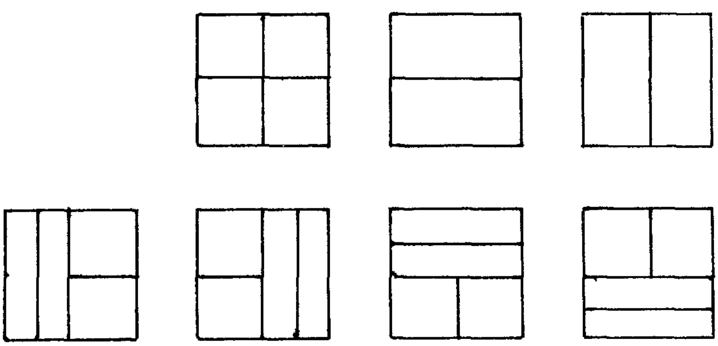

Fig. 8. Additional markings.

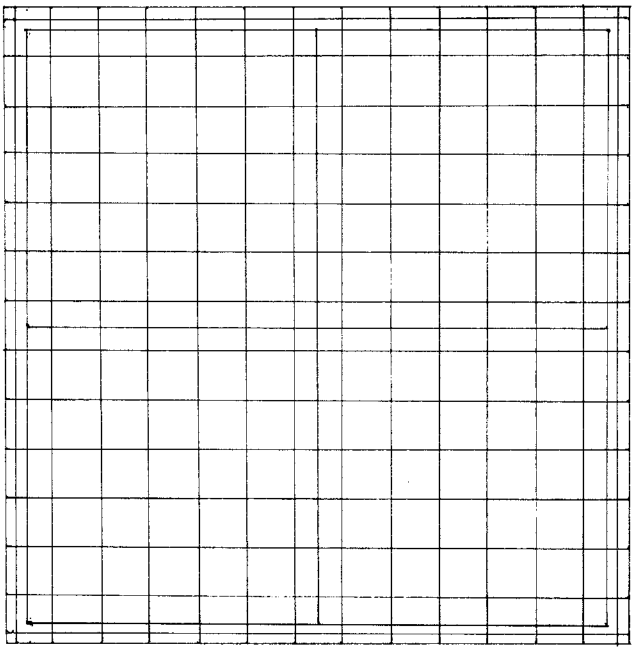

Fig. 9. Forcing a cross in the center of a big square.

In the next section I will prove the existence of Gibbs states which are small perturbations of the above-described periodic configurations.

Now I introduce the nearest neighbor two-body interaction U between particles–tiles. If a and b are nearest neighbors on the square lattice and $X(a)$ and $X(b)$ are particles at a and b, respectively, then

$$U_{ab} \equiv U(X(a), X(b)) = \begin{cases} 0 & \text{if } X(a) \text{ and } X(b) \text{ match} \\ 1 & \text{otherwise} \end{cases}$$

The Hamiltonian in the finite volume Λ can be written as follows:

$$H_\Lambda = \sum_{\langle a,b \rangle} U_{ab}$$

and the relative Hamiltonian

$$H(X \mid Y) = \sum_{\langle a,b \rangle} (U_{ab}(X) - U_{ab}(Y))$$

where X and Y are two infinite-volume configurations which differ only on a finite subset of the lattice. All ground-state configurations of this lattice gas model correspond to the nonperiodic tilings.

Observe that the nearest neighbor interaction based on the tiles just described is not isotropic. Increasing the number of tiles, one can construct an isotropic interaction with the same structure of ground-state configurations.

4. THE PROOF

Let G be one of the nonperiodic ground-state configurations of the model, Λ be a finite subset of the square lattice, and $\langle \cdot \rangle_\Lambda^G$ be a finite-volume Gibbs state with G boundary conditions. Let $\langle \cdot \rangle^G$ be a cluster point of $\langle \cdot \rangle_\Lambda^G$ when $\Lambda \to Z^2$, $a \in L_n$, and Pr_a^G be the projection on all configurations which are different from $G(a)$ at a, where L_n is a sublattice described in the end of the previous section. I will prove the following theorem.

Theorem 2. There is an increasing sequence of inverse temperatures β_n such that if $\beta > \beta_n$, then $\langle \mathrm{Pr}_a^G \rangle^G < \varepsilon(\beta) \to 0$ when $\beta \to \infty$.

The theorem says that if $\beta > \beta_n$, then the infinite-volume limit Gibbs state with G boundary conditions is a small perturbation of a periodic configuration of period $2 \cdot 6^n$. This means that the Gibbs state must either have period at least $2 \cdot 6^n$ or be totally nonperiodic.

I will follow closely the proof of the analogous theorem for an exponentially decaying interaction.[4]

I begin with introducing the contours. If S is the family of all tiles, and $|S| = 4529$, then $\mathscr{X} = S^{Z^2}$ is the infinite-volume configuration space of the system,

$$\mathscr{X}_\Lambda^G = \{X \in \mathscr{X}: \quad X(a) = G(a) \text{ if } a \in Z^2 - \Lambda\}$$

Let $X \in \mathscr{X}_\Lambda^G$,

$$\gamma(X) = \{(a, b): \quad U(X(a), (X(b)) > 0\}$$

$$V_m(a) = \{b \in Z^2: \quad \mathrm{dist}(a, b) \leqslant m\}$$

$$\Gamma_n(X) = \bigcup_{(a,b) \in \gamma(X)} V_{2 \cdot 6^n}(a)$$

$$|\Gamma_n(X)| = \mathrm{card}\{(a, b): \quad (a, b) \in \gamma(X)\}$$

$\Gamma_n(X)$ can be decomposed into a finite number of connected components called the contours of the configuration X. Each such contour α divides the lattice into one infinite connected component $\mathrm{Ext}\,\alpha$, called the exterior of the contour, and a finite number of disjoint connected components $\mathrm{Int}_i \alpha$, called the interiors of the contour, and the contour itself. A contour which is not contained in any interior of any other contour is called an exterior contour. Denote by $\Gamma_n^e(X)$ the set of all exterior contours of the configuration X.

Proposition 1. If $X \in \mathscr{X}_A^G$ and $X(a) \neq G(a)$, where $a \in L_n$, then a belongs either to one of the exterior contours of the configuration X or to an interior of one of the exterior contours.

One has the following bound for $\langle \mathrm{Pr}_a^G \rangle_A^G$:

$$\langle \mathrm{Pr}_a^G \rangle_A^G = \frac{\sum_{X \in \mathrm{Pr}_a^G \mathscr{X}_A^G} e^{-\beta H(X|G)}}{\sum_{X \in \mathscr{X}_A^G} e^{-\beta H(X|G)}} \leqslant \sum_{\alpha} \frac{\sum_{X \in \mathscr{X}_A^G,\, \alpha \in \Gamma_n^e(X)} e^{-\beta H(X|G)}}{\sum_{X \in \mathscr{X}_A^G} e^{-\beta H(X|G)}}$$

$$\equiv \sum_{\alpha} P(\alpha) = \sum_{l=1}^{\infty} \sum_{\alpha;\, |\alpha| = l} P(\alpha) \tag{1}$$

where the summation is over all connected sets α of Z^2 such that a belongs either to α or to its interior. $P(\alpha)$ is the probability of α being the exterior contour for some configuration in $\mathscr{X}_A^G$.

Observe that a projection on L_m, $m \leqslant n$, of every interior of every contour is a piece of a translated ground-state configuration G. Now let us construct a Peierls transformation. It translates a configuration on every interior of an exterior contour $\Gamma_n^e(X)$ and puts a ground-state configuration G on a contour itself in such a way that the contour is "erased": all pieces fit on L_m, $m \leqslant n$. Formally:

$$T\colon\ \mathscr{X}_A^{G\alpha} \to \mathscr{X}_A^G; \qquad \mathscr{X}_A^{G\alpha} = \{ Y \in \mathscr{X}_A^G\colon\ \alpha \in \Gamma_n^e(X) \}$$

$T(X) = X^*$, where X^* is defined as follows:

$$X^*_{|\mathrm{Ext}\,\alpha} = X_{|\mathrm{Ext}\,\alpha}, \qquad X^*_{|\alpha} = G_{|\alpha}, \qquad X^*_{|\mathrm{Int}_i\alpha} = \tau_i X_{|\mathrm{Int}_i\alpha} \tag{2}$$

where i runs over all interiors of α, and τ_i are lattice translations such that the orientations of crosses of X^* are the same as those of G on the part of every lattice L_m, $m = 1, 2,..., n$, contained in $\mathrm{Int}_i \alpha$.

Proposition 2:

$$H(X^* | G) \leqslant H(X | G) - |\alpha|/2$$

Proof. The present Peierls transformation certainly lowers the energy associated with L_m, $m \leqslant n$, by $|\alpha|$. However, it may introduce some misfits connected with higher sublattices. Because of the existence of plain edges propagating in every two out of three corridors between crosses, the broken bond may be introduced at most in every second cube $V_n(a)$. ▮

One has the following estimate for the kernel of the Peierls transformation.

Proposition 3. One has $\mathrm{card}(\mathrm{Ker}\ T) \leqslant (2 \cdot 6^n)^{|\alpha|}\, 4529^{32 \cdot 6^{2n} |\alpha|}$

Proof. The number of finite disjoint connected components $\mathrm{Int}_i \alpha$ is obviously bounded by $|\alpha|/2$. Then we have $(2 \cdot 6^n)^2$ possible translations τ_i. Finally, we have to take into account the boundary of $\mathrm{Int}_i \alpha$ and the contour itself. This introduces the factor $4529^{2(2 \cdot 2 \cdot 6^n)^2 |\alpha|}$. ▮

Combining (1) and Propositions 2 and 3 gives the following Peierls estimate.

Proposition 4:

$$P(\alpha) \leqslant (2 \cdot 6^n)^{|\alpha|}\, 4529^{32 \cdot 6^{2n} |\alpha|} e^{-\beta |\alpha|/2}$$

Proof:

$$P(\alpha) \leqslant \frac{\mathrm{card}(\mathrm{Ker}\ T) \cdot \sum_{X^* \in T(Pr_a^G \mathscr{X}_\Lambda^G)} e^{-\beta H(X^* \mid G) - \beta |\alpha|/2}}{\sum_{X^* \in T(Pr_a^G \mathscr{X}_\Lambda^G)} e^{-\beta H(X^* \mid G)}}$$
$$\leqslant (2 \cdot 6^n)^{|\alpha|}\, 4529^{32 \cdot 6^{2n} |\alpha|} e^{-\beta |\alpha|/2} \quad ▮$$

The following estimate was proven by Holsztynski and Slawny.[18]

Proposition 5. The number of connected subsets $|\alpha| = l$ of Z^2 such that the fixed site of the lattice belongs either to α or to its interior and in addition α is a contour of some configuration is bounded above by $[A(n)\, l + B(n)]^2\, C(n)^{2l-2}$, where $A(n)$, $B(n)$, and $C(n)$ depend only upon n.

This shows that

$$\langle \mathrm{Pr}_a^G \rangle_\Lambda^G \leqslant \sum_{l=1}^{\infty} [A(n)\, l + B(n)]^2\, C(n)^{2l-2}\, (2 \cdot 6^n)^{|\alpha|}\, 4529^{32 \cdot 6^{2n} |\alpha|} e^{-\beta l/2} \quad (3)$$

uniformly in Λ.

The series converges and goes to 0 when $\beta \to \infty$ and hence Theorem 2 is proven

5. CONCLUSIONS

The importance of the given example is that it gives strong evidence that finite-range interactions are capable of forcing nonperiodicity not only in ground states, but at low temperatures as well. It is an important open problem to construct a quasiperiodic equilibrium state of many interacting particles at positive temperature.

It was proven recently that classical lattice gas models with ordered but nonperiodic ground states are not that rare. In fact, they form a generic set in the space of summable interactions[19-21]; however, these results really only concern medium-range interactions, not finite range as described here.

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