Commun. Math. Phys. 107, 577–586 (1986)

Communications in Mathematical Physics

Many Phases in Systems without Periodic Ground States

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Abstract. The low temperature behavior of systems without periodic ground states is investigated. It is shown by using Peierls' argument that in some models the translational symmetry is broken. In particular, an infinite range model with infinitely many Gibbs states is constructed.

1. Introduction

One of the unsolved problems of statistical mechanics is to understand the causes of crystalline symmetry in low temperature matter [1]. Here we discuss specific classical lattice gas models in two dimensions. Namely, each site of the square lattice can be occupied by one of several different particles. The particles interact through two-body potentials and low temperature behavior of such systems results from the competition between energy and entropy, i.e., the minimization of the free energy.

Before discussing the finite temperature region it is important to investigate the ground states of the system, i.e., the configurations of particles with minimal potential energy per lattice site. A major question here is: does every classical lattice system always possess at least one periodic ground state? This problem was studied by Radin [2–4] and the answer is no. There are examples of models which do not have periodic ground states. They are based on Berger's [5] and Robinson's [6] results on nonperiodic tilings of the plane with a finite family of certain tiles. Such models do possess, however, so-called q-periodic ground states. A configuration of particles is q-periodic if when a certain fraction of them is ignored the rest of the configuration is periodic; the smaller the fraction, the larger the period.

The next step is to prove or disprove that in such systems the q-periodic structure can survive at low temperatures giving rise to a q-periodic Gibbs state. We have to keep in mind, however, that in contradistinction to the ground states there is always at least one translational invariant Gibbs state at any nonzero temperature. We have not resolved this problem. Instead we answer here the following more modest question: do systems without periodic ground states exhibit phase transitions? In other words: are there at least two Gibbs states at low temperatures? The answer to the question as stated above is trivially positive. Imagine a two-dimensional model without periodic ground states placed above a two-dimensional ferromagnetic Ising model without being coupled to it. Obviously such a model does not have periodic ground states. On the other hand, because of the presence of the ferromagnetic Ising model, there are at least two Gibbs states at low temperatures.

In Sect. 2 of this paper we investigate a model which cannot be decoupled in the above sense (it has too few coupling constants). We use Robinson's tiles and introduce an interaction which forces some periodic structure (with period larger than one lattice spacing) to appear in every ground state. Then we add a weaker interaction such that this periodic structure is filled out with a nonperiodic pattern. Using Peierls' argument we can show that the periodic structure survives at low temperatures. The translational symmetry is broken; there is a Gibbs state which is non-translational invariant.

In Sect. 3 we construct a specific model with two-body infinite range interaction (decreasing at infinity sufficiently fast) without periodic ground states and with infinitely many Gibbs states on the phase diagram. We prove that there is an infinite sequence of temperatures T_n such that if $T < T_n$, then a corresponding Gibbs state has a minimal period at least 2^{n+1} in both directions. Two possibilities arise. Either all T_n's are different so there are infinitely many phase transitions or there is a temperature at which there exists a nonperiodic Gibbs state – a q-periodic Gibbs state. We are unable to determine which possibility actually happens. It would be interesting to construct a model with finite range interaction without periodic ground states and with a q-periodic Gibbs state at low temperatures. A possible candidate would be a model with just q-periodic ground states as in the second example. The Robinson tile model has some ground states which are not q-periodic.

2. Finite Range Interaction Model

We investigate here the low temperature behavior of a certain classical lattice gas model on a square lattice. Section 2.1 contains the description of the different particles and interaction between them. In Sect. 2.2 the main theorem is formulated: the breakdown of the translational symmetry at low temperatures. Section 2.3 contains the proof of the theorem. More specifically, we construct the Peierls transformation to obtain the standard exponential bound for the probabilities of certain excitations from the ground state. Our transformation is not injective but we can bound appropriately its kernel from above. The standard bound for the number of connected excitations finishes the proof.

2.1. Description of the Model

Each site, say a, of the square lattice can be occupied by one of the 56 different particles – Robinson's tiles denoted $X(a)$ [6]. We describe now the Robinson tiles;

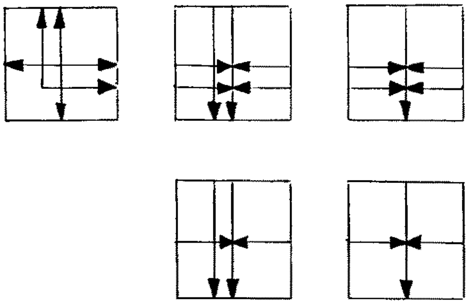

Fig. 1

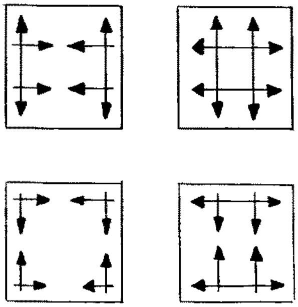

Fig. 2

we follow [6] closely. There are five 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 are combined with the parity marking at the lower left in Fig. 2. Vertical arms (the direction of the central arrow) 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 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 must alternate both horizontally and vertically in the manner shown in Fig. 2. This is exactly the periodic structure which will survive at low temperatures.

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

$$U_{ab}(X) \equiv U(X(a), X(b)) = \begin{cases} 0 & \text{if } X(a) \text{ and } X(b) \text{ match,} \\ 1 & \text{if } X(a) \text{ and } X(b) \text{ do not match,} \\ & \text{but the parity markings match,} \\ N>1 & \text{if the parity markings of } X(a) \\ & \text{and } X(b) \text{ do not match.} \end{cases}$$

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:

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

where X and Y are two infinite volume configurations which differ only on a finite subset of the lattice. It can be proven [4] that there are no periodic ground states in such a model; you cannot tile the plane periodically with these particular tiles. There are, however, q-periodic ground states such that every bond is "satisfied" – every two nearest neighbor tiles match. For a complete description of the ground states see [6].

2.2. *The Main Theorem*

Denote by $\mathscr{G}$ the family of ground states. Let $G \in \mathscr{G}$, Λ be a finite subset of the square lattice, and $\langle \ \rangle_\Lambda^G$ be a finite volume Gibbs state with G boundary conditions. Let $\langle \ \rangle^G$ be a cluster point of $\langle \ \rangle_\Lambda^G$ when $\Lambda \to \mathbb{Z}^2$ and Pr_a^G the projection on all configurations with the parity marking at a different from the parity marking of $G(a)$.

Theorem.

$$\langle Pr_a^G \rangle^G < \varepsilon(\beta) \to 0 \quad \textit{when} \quad \beta \to \infty,$$

where β is the inverse temperature.

Corollary. *There are at least four extremal Gibbs states at low temperatures.*

2.3. *The Proof*

We begin by introducing the contours. If S is the family of all tiles, and $|S| = 56$, then $\mathscr{X} = S^{\mathbb{Z}^2}$ is the infinite volume configuration space of the system.

$$\mathscr{X}_\Lambda^G = \{X \in \mathscr{X} : X(a) = G(a) \text{ if } a \in \Lambda^c \equiv \mathbb{Z}^2 \backslash \Lambda\}.$$

Let $X \in \mathscr{X}^G$;

$$\gamma(X) = \{(a,b) : U(X(a), X(b)) = N\},$$

$$(a,b)^* = (a^*, b^*);\ a^*, b^* \in \mathbb{Z}^{2*} \quad \text{(the dual lattice)},$$

$$\gamma^*(X) = \{(a,b)^* : (a,b) \in \gamma(X)\}.$$

Consider a graph $\Gamma_X = (V_X, E_X)$, where

$$V_X = \{a^* \in \mathbb{Z}^{2*} \text{ such that } b^* \in \mathbb{Z}^{2*} \text{ and } (a^*, b^*) \in \gamma^*(X)\},$$

$$E_X \equiv \gamma^*(X).$$

Let Γ_X^c be the set of connected components of Γ_X, called the contours of the configuration X. It is easy to see that every vertex belongs to at least two edges (cf., the proof of Proposition 2.1). Because of that, every contour α divides $\mathbb{Z}^2$ into one infinite connected component Ext_α, called the exterior of α, and a finite number of finite disjoint connected components $\mathrm{Int}_i\alpha$, called interiors of α. Two sites of the lattice are connected if they are nearest neighbors.

Proposition 2.1. *Let $X \in \mathscr{X}_\Lambda^G$ and assume the parity marking of $X(a)$ is different from the parity marking of $G(a)$. Then there exists a contour of X such that a belongs to one of its interiors.*

Proof. Pick any $b\in\mathbb{Z}^2\backslash\Lambda$. If the proposition is not true then one can construct a path on the lattice starting at b and ending at a such that it never crosses an element of $\gamma^*(X)$. This is obviously impossible. □

We have the following bound for $\langle Pr_a^G\rangle_\Lambda^G$:

$$\langle Pr_a^G\rangle_\Lambda^G=\frac{\sum\limits_{X\in Pr_a^G\mathscr{X}_\Lambda^G} e^{-\beta H(X|G)}}{\sum\limits_{X\in\mathscr{X}_\Lambda^G} e^{-\beta H(X|G)}}\leqq\sum_\alpha\frac{\sum\limits_{X\in\mathscr{X}_\Lambda^G,\,\alpha\in\Gamma_X^c} e^{-\beta H(X|G)}}{\sum\limits_{X\in\mathscr{X}_\Lambda^G} e^{-\beta H(X|G)}}$$

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

where the summation is over all finite connected graphs on $\mathbb{Z}^{2*}$ such that a belongs to one of its interiors and $|\alpha|$ is the number of edges in α.

To bound $P(\alpha)$ from above we construct the following Peierls transformation.

$$T:\mathscr{X}_\Lambda^{G\alpha}\to\mathscr{X}_\Lambda^G\,;\qquad \mathscr{X}_\Lambda^{G\alpha}=\{X\in\mathscr{X}_\Lambda^G:\alpha\in\Gamma_X\}\,.$$

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

$$X^*_{|\mathrm{Ext}\alpha}=X_{|\mathrm{Ext}\alpha}\,,\qquad X^*_{|\mathrm{Int}_i\alpha\backslash\partial\mathrm{Int}_i\alpha}=\tau_{a_i}X_{|\mathrm{Int}_i\alpha\backslash\partial\mathrm{Int}_i\alpha}\,, \tag{2}$$

$X^*_{|\partial\mathrm{Int}_i\alpha}$ is such that the parity markings match all the neighboring parity markings and otherwise is arbitrarily fixed. τ_{a_i} are lattice translations which make the above choice possible and i runs over all the interiors of α,

$$\partial\,\mathrm{Int}_i\alpha=\{a\in\mathrm{Int}_i\alpha:\mathrm{dist}(a,\mathbb{Z}^2\backslash\mathrm{Int}_i\alpha)\leqq 1\}\,.$$

Certainly if $N\geqq 5$ then

$$H(X^*|G)\leqq H(X|G)-|\alpha|\,. \tag{3}$$

Proposition 2.2.

$$\mathrm{card}(\mathrm{Ker}\,T)\leqq 2^{|\alpha|}\cdot 56^{2|\alpha|}\,.$$

Proof. The number of finite disjoint connected components $\mathrm{Int}_i\alpha$ is obviously bounded by $|\alpha|/2$. Then we have 4 different (including the identity) possible translations τ_{a_i}. Finally we have to take into account the boundary of $\mathrm{Int}_i\alpha$. This introduces the factor $56^{2|\alpha|}$. □

Combining (1) and Proposition 2.2 we get the following Peierls estimate.

Proposition 2.3.

$$P(\alpha)\leqq 2^{|\alpha|}56^{2|\alpha|}e^{-\beta|\alpha|}\,.$$

Proof.

$$P(\alpha)\leqq\frac{\mathrm{card}(\mathrm{Ker}\,T)\cdot\sum\limits_{X^*\in T(Pr_a^G\mathscr{X}_\Lambda^G)} e^{-\beta H(X^*|G)-\beta|\alpha|}}{\sum\limits_{X^*\in T(Pr_a^G\mathscr{X}_\Lambda^G)} e^{-\beta H(X^*|G)}}\leqq 2^{|\alpha|}56^{2|\alpha|}e^{-\beta|\alpha|}\,. \quad □$$

The following estimate was proven by Holsztynski and Slawny [7].

Proposition 2.4. *The number of connected graphs on $\mathbb{Z}^2$ with ℓ edges and such that a fixed site a belongs to one of its interiors is bounded above by $(A\ell+B)^2\cdot C^{2\ell-2}$, where A, B, and C are constants.*

Finally:

$$\langle P_a^G\rangle_\Lambda^G \leqq \sum_{\ell=1}^{\infty}(A\ell+B)^2C^{2\ell-2}2^\ell 56^{2\ell}e^{-\beta\ell}\leqq\varepsilon(\beta)\to 0$$

when $\beta\to\infty$ independently of Λ.

This finishes the proof of the main theorem.

3. Infinite Range Interaction Model

We construct here a model on the square lattice with an infinite range two-body interaction decreasing at infinity sufficiently fast. We follow the scheme of the previous section. Namely, in Sect. 3.1 we describe our model. In Sect. 3.2 we formulate the main theorem which is proven in Sect. 3.3.

3.1. Description of the Model

The description of the set of particles which can occupy the sites of the lattice is based on Robinson's tiles. We use the four parity markings shown in Fig. 2. Again, the crosses are combined with the parity marking at the lower left. The parity marking at the upper right constitutes a tile by itself or is combined with a cross. Two remaining parity markings constitute tiles by themselves. Taking into account four cross orientations there are all together eleven different tiles. Now let us define the interaction. If the parity markings of two adjacent tiles do not match, they contribute positive energy E_0 to the system. Then we introduce an interaction between crosses. Two crosses at a distance 2^n, $n=1,2,\ldots$ contribute the positive energy E_{2n} if they are not in the same relative orientation as any of the two adjacent crosses in Fig. 3. Two crosses at a distance $2^n\sqrt{2}$, $n=0,1,2,\ldots$ contribute the positive energy E_{2n+1} if they are in the same relative orientation as two diagonally adjacent crosses in Fig. 4. Finally, if the lattice site is occupied by a cross, then a lattice site at a distance $2^n\sqrt{2}$, $n=0,1,2,\ldots$ and facing the cross in the way the dots face the nearest crosses in Fig. 3 should be occupied by another cross; otherwise the positive energy contribution is E_{2n+1}. All other interactions are zero. E_k's satisfy the following relation:

$$12\sum_{i>k}2^{2k+4}\cdot 2^i\cdot E_i<E_k/2\,,\qquad k=0,1,2,\ldots, \tag{4}$$

hence the interaction can decrease at infinity arbitrarily fast. It is easy to see (cf., the proof of Proposition 3.2) that the ground states (without line defects) of this interaction are exactly the q-periodic ground states of the previous model. Namely, let G be one of these ground states. G defines in a natural way an infinite sequence of square lattices $\mathbb{L}_n\subset\mathbb{L}=\mathbb{Z}^2$ with the lattice spacing 2^n, $n=1,2,\ldots$ such that if $a\in\mathbb{L}_n$ then $G(a)$ is a cross. Moreover, the pattern of orientations of crosses on each lattice is as in Fig. 3. If the pattern is chosen on the lattice $\mathbb{L}_n$ then $\mathbb{L}_{n+1}$ consists of

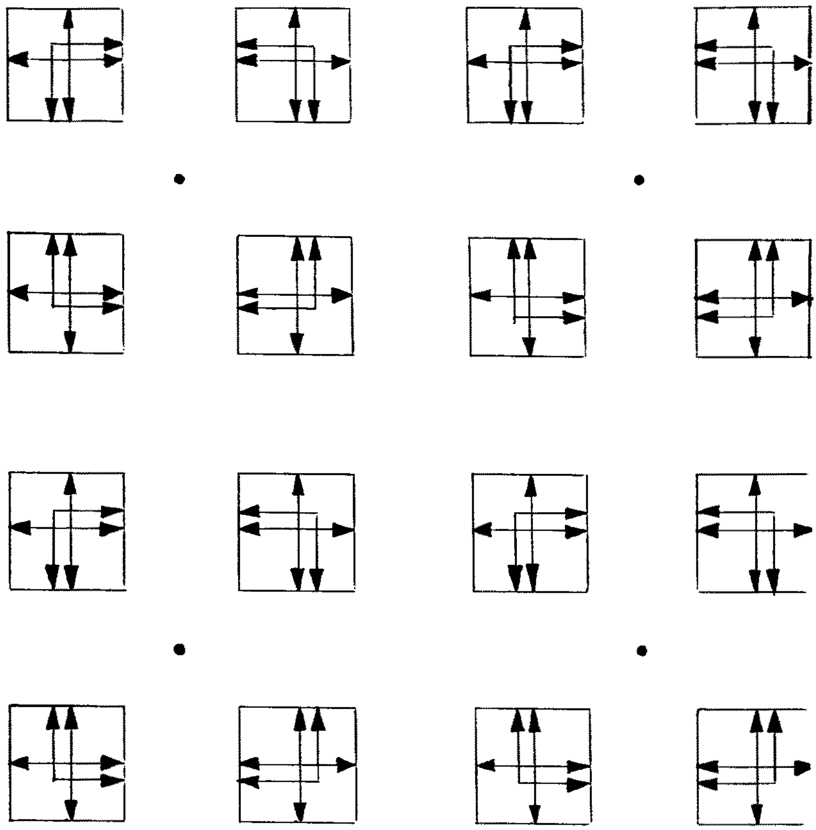

Fig. 3

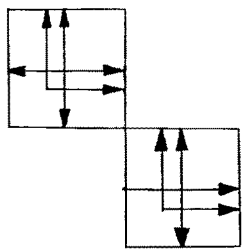

Fig. 4

the sites represented by dots in Fig. 3 (the centers of the squares whose vertices are occupied by crosses). Notice also that not all the bonds are "satisfied"; the energy of the ground state is positive, not zero as in the previous model.

3.2. The Main Theorem

Theorem. *There is an increasing sequence of inverse temperatures β_n, such that if $\beta > \beta_n$ then*

$$\langle Pr_a^G \rangle^G < \varepsilon(\beta) \to 0 \quad \textit{when} \quad \beta \to \infty ,$$

where $a \in \mathbb{L}_n$ *and* Pr_a^G *is the projection on all configurations which are different from* $G(a)$ *at* a.

Corollary. *If* $\beta > \beta_n$ *there are at least* $(2^{n+1})^2$ *extremal Gibbs states.*

3.3. The Proof

To prove the theorem we introduce first a slightly different notion of contours.

Let $X \in \mathscr{X}_A^G$,

$$\begin{aligned}\gamma_n(X) = \{a \in \mathbb{L}, &\text{ such that there is } b \in \mathbb{L} \\ &\text{and } U(X(a), X(b)) \geqq E_{2n} \\ &\text{and there are no crosses between} \\ &a \text{ and } b \text{ if } \operatorname{dist}(a,b) = 2^k,\ k = 0, 1, \ldots, n \\ &\text{and there are just crosses between} \\ &a \text{ and } b \text{ if } \operatorname{dist}(a,b) = 2^k\sqrt{2},\ k = 0, 1, \ldots, n-1 \\ &\text{and } X(a), X(b) \text{ are crosses}\}.\end{aligned}$$

[One may consider the alternate many-body interaction model in which the interaction has all the restrictions in the definition of $\gamma_n(X)$. Everything goes through exactly in the same way and is technically much easier.]

Now let us introduce some other notions:

$$|\gamma_n(X)| = \operatorname{card}\{(a,b) : a, b \in \gamma_n(X) \text{ and } U(X(a), X(b)) > 0\},$$

$$V_m(a) = \{b \in \mathbb{L} : \operatorname{dist}(a,b) \leqq m\},$$

$$\Gamma_n(X) = \bigcup_{\alpha \in \gamma_n(X)} V_{2^{n+1}}(a).$$

$\Gamma_n(X)$ can be decomposed into the finite number of connected components called the contours of the configuration X. Each such contour, α, divides the lattice into one infinite connected component Ext_α, called the exterior of the contour, and the 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 the interior of any other contour is called an exterior contour. Denote by $\Gamma_n^e(X)$ the set of the exterior contours of the configuration X.

Proposition 3.1. *If* $X \in \mathscr{X}_A^G$ *and* $X(a) \neq G(a)$, *where* $a \in \mathbb{L}_n$, *then* a *belongs either to one of the exterior contours of the configuration* X *or to the interior of one of the exterior contours.*

Proof. Use induction with respect to n. Walk on the lattice $\mathbb{L}_n$ and compare the proof of Proposition 2.1. □

Once again

$$\langle Pr_a^G \rangle_A^G \leqq \sum_{\ell=1}^{\infty} \sum_{\alpha;\, |\alpha| = \ell} P(a),$$

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

Now we construct a Peierls transformation.

$$T: \mathscr{X}_\Lambda^{G\alpha} \to \mathscr{X}_\Lambda^G; \qquad \mathscr{X}_\Lambda^{G\alpha} = \{x \in \mathscr{X}_\Lambda^G : \alpha \in \Gamma_n^e(X)\}.$$

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

$$X^*_{|\mathrm{Ext}_\alpha} = X_{|\mathrm{Ext}_\alpha}, \qquad X^*_{|\alpha} = G_{|\alpha}, \qquad X^*_{|\mathrm{Int}_i\alpha} = \tau_{a_i} X_{|\mathrm{Int}_i\alpha}, \tag{5}$$

where i runs over all the interiors of α and τ_{a_i} are lattice translations such that the orientations of crosses of X^* are the same as of G on the part of every lattice $\mathbb{L}_k$ $k = 1, 2, \ldots, n$ contained in $\mathrm{Int}_i\alpha$, and the parity markings match.

Proposition 3.2.

$$H(X^*|G) \leqq H(X|G) - \frac{|\alpha| E_n}{2}.$$

Proof. The cardinality of α is bounded above by $(2 \cdot 2^{n+1})^2 |\alpha|$. The presence of 2^i in (4) is caused by the $\mathrm{Int}_i\alpha$-interiors of α and the corresponding translations τ_{α_i}. 12 in (4) stands for the four directions on $\mathbb{Z}^2$ and three different kinds of interaction. X^* is constructed stepwise. Using the procedure described in (5) we remove the contours of X contained in α and involving the nearest neighbor interaction. Then we remove the contours intersecting α and involving the interaction of strength $E_1, E_2, \ldots$ up to E_{2n}, one energy level at a time. The proposition follows from (4). □

At the same time the proposition proves that the q-periodic configurations described above are really the only ground states (without line defects) of the system.

The kernel of the Peierls transformation is bounded above by

$$(2^{n+1})^{|\alpha|} \cdot 11^{(2^{n+1} \cdot 2)^2 \cdot 2|\alpha|}$$

for exactly the same reasons as in Proposition 2.2.

The number of connected subsets α of $\mathbb{Z}^2$ such that the fixed site of the lattice belongs either to this subset or to its interior, and in addition α is a contour of some configuration, and $|\alpha| = \ell$, can be bounded above by

$$[A(n)\ell + B(n)]^2 C(n)^{2\ell - 2},$$

where $A(n)$, $B(n)$, and $C(n)$ depend only upon n. Again we use here the result of Holsztynski and Slawny [7].

This shows that

$$\langle Pr_a^G \rangle_\Lambda^G \leq \sum_{\ell=1}^{\infty} [A(n)\ell + B(n)]^2 C(n)^{2\ell-2} \cdot (2^{n+1})^\ell \cdot 11^{(2^{n+1} \cdot 2)^2 \cdot 2\ell} \cdot e^{(-\beta \ell E_n)/2},$$

and hence the main theorem of this section is proven.

Acknowledgements. I would like to thank Charles Radin for introducing to me the systems without periodic ground states and for many fruitful discussions and critical comments.

References

1. Simon, B.: Fifteen problems in mathematical physics. Perspectives in mathematics: Anniversary of Oberwolfach 1984. Basel: Birkhäuser 1984
2. Radin, C.: Tiling, periodicity, and crystals. J. Math. Phys. **26**, 1342–1344 (1985)
3. Radin, C.: Crystals and quasicrystals: A lattice gas model. Phys. Letts. **114**A, 381–383 (1986)
4. Radin, C.: Correlations in classical ground states. J. Stat. Phys. (to appear)
5. Berger, R.: The undecidability of the domino problem. Mem. Am. Math. Soc. **66** (1966)
6. Robinson, R.M.: Undecidability and nonperiodicity for tilings of the plane. Invent. Math. **12**, 177–209 (1971)
7. Holsztynski, W., Slawny, J.: Phase transitions in ferromagnetic spin systems. Commun. Math. Phys. **66**, 147–166 (1979)

Communicated by J. Fröhlich

Received February 25, 1986; in revised form July 3, 1986