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Correlations in Classical Ground States

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We prove that ground states have, generically, a certain degree of spatial symmetry.

KEY WORDS: Crystalline symmetry; ground states.

1. INTRODUCTION

It is a major unsolved problem to understand the cause of spatial symmetry (specifically crystalline symmetry) in low-temperature bulk matter.[1-5] The essence of the problem—why energy ground states tend to be periodic—has been essentially solved for one-dimensional models,[6,7] but there are what could be interpreted as "counterexamples" in two and three dimensions,[8-10] i.e., simple models which have quasiperiodic, *but no periodic*, ground states.

Periodic configurations are special in many ways. They exhibit *long range order* in that the configuration in one region determines the configuration even in very distant regions. Also, they are *homogeneous* in the sense that the configuration is essentially identical in any two congruent regions much larger than the period.

We will show that energy ground states tend to have this homogeneity property, at least in an average sense. This seems to be the first general, qualitative result on the spatial symmetry of ground states for dimensions higher than one.

2. NOTATION AND PRELIMINARY RESULTS

We consider classical lattice gas models on the n-dimensional cubic lattice $\mathbb{Z}^n$, $n \geq 1$, with $N \geq 1$ particle species and no multiple occupation of

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lattice sites. Microscopic states of the infinite system (henceforth called configurations) are described as follows. At each lattice site x the system can exist in one of $N+1$ states, one of which indicates "unoccupied" and the remainder of which refer to the N possible species that may occupy the site. A configuration of the infinite system is a function $f: x \in \mathbb{Z}^n \to f(x) \in \mathbb{R}^{N+1}$, where the $N+1$ coordinates $f_j(x)$ of $f(x)$ satisfy $f_j(x) = \delta_{j,k}$ if the system is in the kth state at site x. We use the sup norm on $\mathbb{Z}^n \subset \mathbb{R}^n$, so that if $x = (x_1,..., x_n)$, $\|x\|_\infty = \sup\{|x_j| \mid j = 1,..., n\}$. F denotes the family of nonempty finite ordered subsets of $\mathbb{Z}^n$. If $S \in F$ and f is a configuration, $f(S)$ represents the ordered product $\prod^0_{x \in S} f(x)$ so that the kth component $f_k(S)$ of $f(S)$ equals $f(x^k)$, where x^k is the kth site in S. For any finite set D, $c(D)$ denotes its cardinality. A function $g : S \in F \to g(S) \in W$ from F to a metric space W (with metric m) will be said to have limit $\bar{g} \in W$ as $S \to \infty$ if, given $\varepsilon > 0$, there exists $R > 0$ such that $m[g(S), \bar{g}] < \varepsilon$ for any cube $S = C_{x,b} \equiv \{y \in \mathbb{Z}^n \mid \|y - x\|_\infty \leqslant b\}$ such that $b > R$. In particular, a subset Y of $\mathbb{Z}^n$ is said to have relative density r if the function $S \in F \to c(Y \cap S)/c(S)$ has limit r as $S \to \infty$. A configuration is called quasiperiodic if, given $\varepsilon > 0$, there exists a periodic configuration (that is, periodic in n directions) which coincides with it off a set of relative density less than ε.

Next we need a more general version of fraction space.[8,10] First we put an equivalence relation on F; $S, S' \in F$ are equivalent if S and $S' + x$ are equal (as unordered sets) for some translation $x \in \mathbb{Z}^n$. Order the (countably many) equivalence classes, $\{E_j \mid j \in \mathbb{N}\}$, and from each E_j choose a representative S_j. Let K be the countable set $\{(j, k) \mid j \in \mathbb{N},\ k \in M(S_j)\}$ where $M(S_j) = \{g(S_j) \mid g \text{ a configuration}\}$. So, as k varies, (j, k) runs through the possible states of occupation of S_j. We will need the real separable Banach space $\bar{l}_1(K)$ of functions $T = \{T_q \mid q \in K\}$ with finite norm $\|T\|_1 \equiv \sum_{(j,k) \in K} |T_{(j,k)}|\, c(S_j)$ and its dual $l_\infty(K)$. On $l_\infty(K)$ we use two topologies, the dual norm $\|g\|_\infty \equiv \sup\{|g_q| \mid q \in K\}$ and the weak-* topology, the weak topology generated by the linear functionals in $\bar{l}_1(K)$. Between $T \in \bar{l}_1(K)$ and $g \in l_\infty(K)$ the duality is denoted $T(g) \equiv \sum_{(j,k) \in K} T_{(j,k)}\, g_{(j,k)}\, c(S_j)$. The unit ball $l^1_\infty(K) = \{g \in l_\infty(K) \mid \|g\|_\infty \leqslant 1\}$ is metrizable and compact in the weak-* topology.[11] For a metric on this ball we use

$$m(g, g') \equiv \sum_{(j,k) \in K} |T^{(j,k)}(g - g')|\, (N+1)^{-2c(S_j) - j}$$

where $T^{(j,k)}$ is the characteristic function of the singleton $\{(j, k)\}$. Given a configuration f, a representative S_j and $V \in F$, we define

$$(S_j, V) \equiv \{x \in \mathbb{Z}^n \mid (S_j + x) \cap V \neq \varnothing\} \subset \mathbb{Z}^n$$

and $S_V(f) \in l^1_\infty(K)$ by

$$S_V(f)_{(j,k)} \equiv \frac{1}{c(S_j)\,c(V)} \sum_{t \in (S_j,V)} \prod_{m=1}^{c(S_j)} [f_m(S_j+t), k_m]$$

where $[g, g']$ denotes the usual inner product of g, g' in $\mathbb{R}^{N+1}$. We think of $S_V(f)_{(j,k)}$ as the average number (out of all translations of S_j which intersect the "box" V) of times the occupation status k of S_j occurs in the configuration f. A configuration f is said to be averageable if the function $V \in F \to S_V(f) \in l^1_\infty(K)$ has a limit [denoted $\bar{S}(f)$] as $V \to \infty$ in the sense defined above, where $l^1_\infty(K)$ is equipped with its weak-* topology. Note that periodic and quasiperiodic configurations are averageable. Let $B_0 \equiv \{\bar{S}(f) \mid f$ a periodic configuration$\}$, and define (the generalized fraction space) B to be the weak-* closure of B_0 in $l_\infty(K)$. B will always be assumed to have the metric weak-* topology from $l^1_\infty(K)$ and it is thus compact. We will need the fact that it is also convex.

Lemma 1. B is convex.

Proof. Given p and p' in B, and $\varepsilon > 0$, choose periodic configurations f and f' such that $m[\bar{S}(f), p] < \varepsilon/4$ and $m[\bar{S}(f'), p'] < \varepsilon/4$. For each positive integer k we partition $\mathbb{Z}^n$ into "even" and "odd" cubes (checkerboard fashion) of the form $\{C_{x,k} \mid x_j = (2k+1)\,n_j$ for some integer $n_j\}$ where such a $C_{x,k}$ is called odd (respectively, even) if $\sum_j n_j$ is odd (respectively, even). Let f^k be the periodic configuration which on every odd cube is (the translation of) the restriction of f to $C_{0,k}$, and which on every even cube is (the translation of) the restriction of f' to $C_{0,k}$. It follows easily that $m\{\bar{S}(f^k), [\bar{S}(f) + \bar{S}(f')]/2\}$ has limit zero as $k \to \infty$. Therefore, for large enough k, $m[\bar{S}(f^k), (p+p')/2] < \varepsilon$, which proves the lemma.

Lemma 2. Given any configurations f, f' which agree on the cube $V = C_{x,b}$, and vector $T^{(j,k)}$ of $\bar{l}_1(K)$

$$|T^{(j,k)}[S_V(f) - S_V(f')]| \leqslant \min\{t(n,j)/b,\, c(S_j)\}$$

for some number $t(n, j)$ which depends only on the dimension n and the diameter of S_j.

Proof. The result follows easily by counting the fraction of translations of S_j which intersect both V and $\mathbb{Z}^n \backslash V$ (the only ones on which f and f' can differ) out of all translations which intersect V. The fraction is one of surface to volume.

Lemma 3. If f is an averageable configuration $\bar{S}(f) \in B$.

Proof. This follows immediately from Lemma 2.

Elements of $\tilde{I}_1(K)$ will be called interactions since by duality with $l_\infty(K)$ they consist of translation invariant assignments of (many-body) energies to each finite subset of $\mathbb{Z}^n$. Given an interaction T, a configuration f is said to be a ground state[12] for T if for every $V \in F$ and every f' which agrees with f on $\mathbb{Z}^n \backslash V$, $T[S_V(f)] \leqslant T[S_V(f')]$. Further, we define $e(T) = \inf\{T(p) \mid p \in B\}$. A point p in B is said to be exposed by T if $T(p) < T(p')$ for all $p' \in B$, $p' \neq p$. Note that an exposed point of B is necessarily a convex extreme point of B.

3. MAIN RESULTS

Theorem 1. If f is a ground state for T, then $\lim_{V \to \infty} T[S_V(f)] = e(T)$.

Proof. Assume the conclusion false. Then for some $\varepsilon > 0$ and every positive integer k, there exists a cube $V(k) = C_{x(k), b(k)}$ with $b(k) > k$ such that $|T[S_{V(k)}(f)] - e(T)| > \varepsilon$. If for infinitely many of these $V(k)$ it was true that $T[S_{V(k)}(f)] < e(T) - \varepsilon$, Lemma 2 would imply, for some periodic $\tilde{f}$, that $T[\bar{S}(\tilde{f})] < e(T) - \varepsilon/2$, which would contradict the definition of $e(T)$. It follows that for infinitely many k, $T[S_{V(k)}(f)] > e(T) + \varepsilon$. But then choose a periodic configuration f' such that $|T[\bar{S}(f')] - e(T)]| < \varepsilon/4$. For k large enough, $T[S_{V(k)}(f')] < e(T) + \varepsilon/2$. Let f^k be defined to coincide with f' in $V(k)$ and with f in $\mathbb{Z}^n \backslash V(k)$. Then for k large enough, Lemma 2 implies that $|T[S_{V(k)}(f^k) - S_{V(k)}(f')]| < \varepsilon/4$, so that

$$T[S_{V(k)}(f^k)] < e(T) + 3\varepsilon/4 < T[S_{V(k)}(f)]$$

which contradicts f being a ground state for T, and proves the result.

Theorem 1 is not too surprising since it shows that (in a strong sense) periodic boundary conditions do not affect energy density. That ground states tend to be averageable, which refers to correlations in the configurations, is less obvious since interactions with degenerate ground states can certainly have ground states which are not averageable—for example when chemical potentials (which appear as one-body interactions in our notation) allow coexistence of different pure phases. One might expect, however, that such degeneracy is a relatively rare phenomenon. To prove this we need to sharpen the usual notion of pure phase to correspond not just to extreme points[13,14,12] but to exposed points.

Our main result follows.

Theorem 2. Assume $p \in B$ is exposed by the interaction T. Then every ground state f of T is averageable, and $\bar{S}(f) = p$.

Proof. Assume the conclusion false. Then there exists $\varepsilon > 0$ such that for every positive integer k there exists a cube $V(k) = C_{x(k),b(k)}$ with $b(k) > k$ such that $m[S_{V(k)}(f), p] > \varepsilon$. By compactness, some subsequence $S_{V(k')}(f)$ has a limit q in B. But from Theorem 1, $T[S_{V(k')}(f)] \to e(T)$, and so $T(q) = e(T)$. Since p is exposed by T, $q = p$ which contradicts $m[S_{V(k)}(f), p] > \varepsilon$ and proves the result.

Theorem 3. The set of interactions for which all ground states are averageable is generic—it contains a dense G_δ in $\bar{\mathcal{I}}_1(K)$ (in the norm topology).

Proof. Assume the interaction T does not expose a point of B. Then there exists $p^1, p^2 \in B$, and $T' \in \bar{\mathcal{I}}_1(K)$ such that $T(p^1) = T(p^2) = e(T)$ and $T'(p^2) < T'(p^1)$. Then, with p^3 representing either p^1 or p^2, and sgn ε denoting the sign of ε

$$\begin{aligned}[e(T+\varepsilon T') - e(T)]/\varepsilon &= (\inf\{(T+\varepsilon T')(p) - T(p^3) \mid p \in B\})/\varepsilon \\ &= \operatorname{sgn} \varepsilon \inf\{[T(p-p^3)/|\varepsilon| + \operatorname{sgn} \varepsilon\, T'(p)] \mid p \in B\}\end{aligned}$$

If $\varepsilon > 0$ the right-hand side is at least as small as the value $T'(p^2)$ achieved when $p = p^3 = p^2$. If $\varepsilon < 0$, the right-hand side is at least as large as the value $T'(p^1)$ achieved when $p = p^3 = p^1$. So

$$\lim_{\varepsilon \downarrow 0} [e(T+\varepsilon T') - e(T)]/\varepsilon \leqslant T'(p^2) \qquad \text{and}$$

$$T'(p^2) < T'(p^1) \leqslant \lim_{\varepsilon \uparrow 0} [e(T+\varepsilon T') - e(T)]/\varepsilon$$

which implies that the function $e: T \in \bar{\mathcal{I}}_1(K) \to e(T)$ is not Gâteaux differentiable at T. Since e is finite-valued, continuous, and concave, Mazur's theorem[15,16] shows that the set on which e is Gâteaux-differentiable contains a dense G_δ, which completes the proof.

4. CONCLUSION

We have proven that, generically, ground state configurations are "averageable." To clarify this, consider an averageable configuration f. For simplicity assume the dimension $n = 1$ and that there is $N = 1$ species of particle; each site x of $\mathbb{Z}$ is assigned the value 0 (unoccupied) or 1 (occupied) by f. Averageability implies that given any finite subset S of $\mathbb{Z}$, say $S = \{x_1, x_2, x_3\}$ with $x_1 < x_2 < x_3$, and any occupation values, say $x_1 \sim 0$, $x_2 \sim 0$, $x_3 \sim 1$, there is a "frequency" p with the following property. Given $\varepsilon > 0$ there is a length L such that for *every* finite interval $I \subseteq \mathbb{Z}$ of length larger than L (I centered anywhere in $\mathbb{Z}$; this uniformity is crucial), if you translate $\{x_1, x_2, x_3\}$ about within I, the fraction of times a translation of $\{x_1, x_2, x_3\}$ inherits from f the values $\{0, 0, 1\}$ will be within ε of p. In other words, every pair of sufficiently large regions of an averageable configuration have nearly identical average correlations (that is, correlations averaged over the regions.)

We have shown that, generically, ground states have this sort of *statistical homogeneity*. As noted in the introduction, this should be contrasted with the notion of *long range order*, which means that (even) greatly separated regions are correlated. It is our hope that the above results on statistical homogeneity of ground states will help to prove results about long range order, and in particular periodicity, of ground states.

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