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LETTER TO THE EDITOR

How low temperature causes long-range order

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Abstract. We show that for almost all interactions, that is, generically, ground states of classical lattice gas models must have either long-range order or be completely uniform.

It is a traditionally accepted experimental fact that at low temperature and sufficient pressure all known materials form crystals, i.e. structures with some spatial symmetries. It is a long-standing open problem to understand the mechanism responsible for the microscopic periodicity [1–5]. A detailed description of this crystal problem and a review of old and recent results can be found in [6].

The equilibrium behaviour of systems of many interacting particles results from a competition between energy and entropy, i.e. the minimisation of free energy. At very low temperatures the probability distribution on the set of all particle configurations—the standard grand canonical ensemble—is concentrated on those configurations with minimal energy since the entropy contribution to the free energy is negligible. At this point the basic question is: why should particle configurations with minimal energy necessarily be periodic or exhibit some sort of long-range order? We will give a simple answer to this question.

In classical lattice gas models one considers 'configurations' of interacting particles on, say, the three-dimensional simple cubic lattice, with at most one particle per lattice site. By a 'ground state' we mean a limit, as temperature goes to zero, of the translation-invariant grand canonical probability distribution on the set of all configurations, and by a 'ground-state configuration' we mean any configuration in the support of the ground state. Only recently have simple examples (i.e. interactions), due to Radin [7–12], been given which have no periodic ground-state configurations. Even these models, however, exhibit long-range positional order in the manner of quasicrystals. It is therefore natural to look for long-range order as a substitute for crystallinity [6]. By long-range order we mean that the correlation function $\rho(a, b; \boldsymbol{x})$, which represents the relative probability of having local states a and b separated by the spatial vector $\boldsymbol{x}$, satisfies

$$|\rho(a, b; \boldsymbol{x}) - \rho(a)\rho(b)| \nrightarrow 0 \qquad (1)$$

as $|\boldsymbol{x}| \to \infty$ for some a and b, which means that the local states in distant regions are not independent. We prove that for almost every interaction the translation-invariant ground-state distribution (known to be unique [13]) either has long-range order or is completely uniform, i.e. the density of state a $\rho(a) = 1$ for some local state a. The argument is as follows. Most interactions are close to interactions of the form $W + \theta(n)$, where W is some finite-range interaction and $\theta(n)$ is the interaction between two particles at a distance n along the axes of the lattice and with the coupling constant equal to $-1/\sqrt{n}$. The presence of the latter interaction allows the creation of cell walls at a distance n, separating identical particle configurations (the energy cost per lattice site of such walls is proportional to $1/n$) and therefore enforcing long-range order.

Let us now describe these models and the proof in more detail. Let $V(\boldsymbol{x})$ be the translation-invariant interaction energy between particles separated by the spatial vector $\boldsymbol{x}$, where $V(\boldsymbol{o})$ is the chemical potential. We allow those interactions V for which

$$\|V\| \equiv \sum_{x \in Z^3} |V(\boldsymbol{x})| < \infty \tag{2}$$

with $\|V\|$ being the measure of the size of V—the norm on the Banach space of interactions. It corresponds to the restriction that the sum of the energies of interaction of any fixed particle with all other particles be finite. Let W be an interaction with finite range r, i.e. $W(\boldsymbol{x}) = 0$ if $|\boldsymbol{x}| > r$. Notice that the set of all finite-range interactions is dense in the set of all interactions. We will show that if V is 'close enough' to an interaction of a special form, then there is a high degree of periodicity in the ground state of V. Let $\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3$ be the usual basis in Z^3, and for each positive integer n let $\theta(n)$ be the two-body interaction: $\theta(n)(\boldsymbol{x}) = -1/\sqrt{n}$ if $\boldsymbol{x} = n\boldsymbol{x}_i$ for some i, and otherwise 0. $\theta(n)$ tries to force the lattice sites at a distance n along the axes to be occupied, i.e. to enforce period n. Obviously, $\|\theta(n)\| = 3/\sqrt{n}$. Let $X(n)$ be a periodic configuration with period n along the axes of the lattice, with density of particles as close as possible to ρ, the density in the ground state $\mu(V)$ of V, and with minimal (among all such periodic configurations) energy per site with respect to V. Let $Y(V)$ be any configuration in the support of the ground-state distribution $\mu(V)$. Let $\rho_V(o, o; \boldsymbol{x})$ be the relative probability of having two occupied sites separated by the vector $\boldsymbol{x}$. For any configuration X and interaction V let $e_V(X)$ be the energy per site in X with respect to V (assuming it exists). Note that $e_{V+U}(X) = e_V(X) + e_U(X)$ and $|e_V(X)| \leq \|V\|$. With this notation we have, for any interaction V,

$$\begin{aligned} e_V(X(n)) &= e_{\theta(n)}(X(n)) + e_W(X(n)) + e_{V-\theta(n)-W}(X(n)) \\ &\leq -3\rho/\sqrt{n} + 3c/n^{7/2} + e_W(X(n)) + \|V - \theta(n) - W\| \end{aligned} \tag{3}$$

where $|c| < 1$ and comes from the error in approximating ρ in $X(n)$, and

$$\begin{aligned} e_V(Y(V)) &= e_{\theta(n)}(Y(V)) + e_W(Y(V)) + e_{V-\theta(n)-W}(Y(V)) \\ &\geq -\sum_{i=1}^{3} \rho_V(o, o; n\boldsymbol{x}_i)/\sqrt{n} + [e_W(X(n)) - 3r\|W\|/n] - \|V - \theta(n) - W\| \end{aligned} \tag{4}$$

where the term in the bracket is an estimate of the energy cost of creating the walls of the unit cells of $X(n)$. Using $e_V(Y(V)) \leq e_V(X(n))$, and assuming $\|V - \theta(n) - W\| < 3r\|W\|/n$ we have

$$\sum_{i=1}^{3} \rho_V(o, o; n\boldsymbol{x}_i) \geq 3\rho - 9r\|W\|/\sqrt{n} - 3c/n^3. \tag{5}$$

Define $n(W)$ to be the smallest integer such that $(n(W))^{1/2}$ is greater than $9r\|W\|$, $C_k(W)$ to be the set of all interactions V such that $\|V - \theta(kn(W)) - W\| < 3r\|W\|/kn(W)$ and $B_m \equiv \bigcup_W \bigcup_{k \geq m} C_k(W)$. Note that each B_m is open and dense in the set of all interactions. We showed that strong correlations (in the form of (5)) at a distance m hold for every interaction in B_m. Long (infinite) correlations are obtained after intersecting these sets with respect to all distances. Therefore $B \equiv \bigcap_{m \geq 1} B_m$ is generic in the set of all interactions, i.e. it contains 'almost all' interactions [14]. For every V in B and every $m>1$ there is some $k \geqslant m$ and interaction W_m such that $\| V-\theta(kn(W_m))-W_m \| < 3r \| W_m \| / kn(W_m)$ and so from (5)

$$\sum_{i=1}^{3} \rho_V(o, o; kn(W_m)x_i) \geqslant 3\rho - 1/\sqrt{m} - 3c/m^3 \qquad (6)$$

so in order that V be 'clustering', i.e. that $\rho_V(o, o; x) \to \rho^2$ as $|x| \to \infty$ it must be that $\rho = 1$ or 0, i.e. either all sites are full or all are empty. This completes our argument.

Obvious alterations of the proof would produce analogous results for general lattices in any dimension, and also for models allowing any fixed finite number of states (particle species, spins, etc) per site, and also allowing many-body interactions.

It can be proven [15] that the ground state for most interactions is in fact not perfectly periodic. It is shown in this letter that it has at least long-range order.

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