Periodicity of Classical Ground States

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(Received 10 May 1983)

A model of classical particles in one space dimension with an elementary length and general finite-range interaction with hard core is considered. It is shown that such a model must have a periodic ground state.

PACS numbers: 05.70.Fh, 05.20.-y, 61.50.Em

One of the major unsolved problems in the study of matter is to understand why, at low temperature and pressure, there is a strong tendency for molecules to be highly ordered.[1,2] That is, it is unknown, *even heuristically*, why solids are crystalline. (The high-pressure problem is also unsolved, but is not considered here.) The first sucesses on the problem have appeared in the last few years[3-13] and consist of exact studies of specific models in one and two space dimensions. The techniques developed are rather restricted to the specific interactions considered. In this Letter we present the first such argument of a general nature. (General arguments are used in Duneau and Katz[14,15] but are not really relevant to this problem as they allow all critical points of the energy, not just ground states.) Our model is one-dimensional and allows general finite-range (including many-body) potentials with hard core—but with an elementary length in space. We show that all such systems have crystalline ground states.

Specifically, we consider "lattice gas" models, wherein particles can occupy sites in $\mathbf{Z}$. We allow limited multiple occupation; if we describe the state of a system by its sequence $\{z_j \mid j \in Z\}$ of occupation numbers, we assume $0 \leq z_j \leq \tilde{K} < \infty$ for all j. We assume an interaction of the following general type. For each ordered set of consecutive occupation numbers $\{z_j, z_{j+1}, \ldots, z_{j+k}\}$, $k \geq 0$, we have a (many-body) translation invariant energy, $f(z_j, \ldots, z_{j+k})$, between the $k+1$ sites, subject only to the finite-range condition $f(z_j, \ldots, z_{j+k}) = 0$ if $k \geq \tilde{R}$ for some fixed $\tilde{R} < \infty$. (This is equivalent to an arbitrary multiparticle interaction of range k.) To model systems at zero temperature (and arbitrary pressure, which is built into f and a chemical potential) we use "ground states" defined as follows. $\tilde{z} = \{\tilde{z}_j\}$ is a ground state if for every integer pair (k, l), $-\infty < k < \infty$, $-\infty < l < \infty$, $k \leq l$, the energy function

$$E_{k,l}(z) = \sum_{(k',l')}' f(z_{k'}, z_{k'+1}, \ldots, z_{l'})$$

[where the sum is over all pairs (k', l') where either $k \leq l' \leq l$ or $k \leq k' \leq l$ or both], considered as a function only of the variables z_j, $k \leq j \leq l$ (while $z_j = \tilde{z}_j$ for $j < k$ and $j > l$), attains an absolute minimum for $z_j = \tilde{z}_j$, $k \leq j \leq l$. This is a form of stability commonly used for infinite-particle models.[16-18]

With the definitions just given of system, class of interactions, and ground state we can establish the following result.

Theorem.—There exists a periodic ground state, with period at most $\tilde{R}^{\tilde{K}}$.

Proof.—By considering abutting sets of $\tilde{R}$ consecutive sites we can replace the model with an equivalent one described through new occupation variables z_j now bounded by $\tilde{R}^{\tilde{K}}$, and an interaction $g(z_j, \ldots, z_{j+k})$ which vanishes whenever $k \geq 2$. Thus we consider the new model with $R = 2$ and $K = \tilde{R}^{\tilde{K}}$. (The new variables describe blocks of old variables but because the new state space is larger, no information about particle configuration has been lost. Similarly the energy as a function of state is unchanged.) Let $z = \{z_j\}$ be a ground state. (Its existence is guaranteed by a standard compactness argument.) Define an infinite sequence of $(K+1)$ vectors, $w_k = \{w_k{}^j \mid 1 \leq j \leq K+1\}$, by $w_k{}^j = z_{k(K+1)+j}$, $k = 0, 1, \ldots$. From the pigeonhole principle there exists t in T and integers l, m, $1 \leq l < m \leq K+1$, such that for some subsequence $\{k_i\}$ of the integers we have, for all i, (a) $w_{k_i}{}^l = w_{k_i}{}^m = t$, and (b) $w_{k_i}{}^n$ is independent of i for $l \leq n \leq m$. That is, there is an infinite number of identical strings or blocks spaced along the line. We now give a method for moving these repeating blocks of coordinates about so as to produce other ground states. Define the state $z(1)$ by

$$z_j(1)=\begin{cases} z_j, & j\le k_0(K+1)+l,\\ z_j, & j\ge k_1(K+1)+m,\\ z_{j+(k_1-k_0)(K+1)+l-m}, & k_0(K+1)+m<j\le k_0(K+1)+m+(m-l),\\ z_{j+l-m}, & k_0(K+1)+m+(m-l)<j<k_1(K+1)+m.\end{cases}$$

This moves the repeating block in the k_1th segment to the left of the coordinates that previously lay between it and the repeating block in segment k_0. The repeating blocks are now in contact. Next we define states $z(n)$, $n\ge 2$, recursively by

$$z_j(n+1)=\begin{cases} z_j(n), & j\le k_0(K+1)+m+n(m-l),\\ z_j(n), & j\ge k_{n+1}(K+1)+m,\\ z^{(n)}_{j+(k_{n+1}-k_0)(K+1)+l-m-n(m-l)}, & k_0(K+1)+m+n(m-l)<j\le k_0(K+1)+m+(n+1)(m-l),\\ z^{(n)}_{j+l-m}, & k_0(K+1)+m+(n+1)(m-l)<j<k_{n+1}(K+1)+m.\end{cases}$$

Finally we define the periodic state $\tilde{z}$ by $\tilde{z}_j = z_{k_0(K+1)+l+j-n(m-l)}$, where $n=[j/(m-l)]$ and $-\infty<j<\infty$. It is easy to check that all $z(n)$ are ground states by using the fact that if $E_{k,l}(z)$ is minimized with $z_j=z_j^*$, $k\le j\le l$, then if $k\le k'\le l'\le l$, $E_{k',l'}(z)$ is also minimized when $z_j=z_j^*$, $k'\le j\le l'$. [Specifically, for $k=0$ and large enough l, the set of summands in $E_{k,l}(z(n))$ is identical to that in $E_{k,l}(z)$, while z and $z(n)$ have the same coordinates outside the interval.] So each transformation $z(n)\to z(n+1)$, $n=0,1,\ldots,$ leaves constant the total energy in the region surrounding the changed variables. Suppose then for our proposed ground state $\tilde{z}$ there was a local transformation A of variables that lowered the energy. Then there is some sufficiently large n such that A could be applied with the same effect to $z(n)$. But then the original state z, by hypothesis a ground state, could have its energy lowered by the transformation defined by the succession $z\to z(1)\to\ldots\to z(n)\to A(z(n))$, a contradiction. Thus our argument shows that $\tilde{z}$ is a (periodic) ground state, with period at most $K=\tilde{R}^{\tilde{k}}$. This completes the proof.

A ground state $\tilde{z}$ is said to be "isolated" if $E_{k,l}(z)$ attains a *unique* minimum, at $z=\tilde{z}$, for each k, l. Our proof shows the following:

Corollary.—Only periodic ground states can be isolated.

We gratefully acknowledge useful discussion with Ray Heitmann and partial support by National Science Foundation Grants No. MCS 81-01596 and No. Phy 81-07381.

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