Tiling, periodicity, and crystals

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(Received 17 August 1984; accepted for publication 8 February 1985)

A result on nonperiodic tilings is generalized and related to the problem of the origin of crystalline symmetry.

I. INTRODUCTION

It is a very general physical phenomenon that the molecular configurations of matter tend to be crystalline, i.e., periodic, at low temperature (and any pressure, specifically low pressure). There is a major gap in the understanding of this phenomenon[1–4] and it is of a mathematical character of independent interest, as described below.

Using statistical mechanics one can model matter as follows. The possible state of each molecule is viewed as a random variable with the joint distribution of (many molecule) configurations given by a standard Gibbs ensemble, a known probability measure. At low temperature and pressure the measure is concentrated (uniformly) on those configurations with minimal total energy, where the total energy of a configuration is the sum over energy distributions from pairs (and to a minor extent by triplets, etc.) of neighboring molecules. Thus in this low-temperature, low-pressure limit the variables in a sense lose their randomness and one sees that configurations minimizing such a sum are expected to have a strong tendency to be periodic. The feature we wish to emphasize is that solutions of some general class of minimization problems should necessarily exhibit nontrivial symmetries.

It is a major open question in physics to understand the generality in which this scheme (the "crystal problem") is true and the basic mechanisms behind it.[1–4] Aside from its relevance to physics this problem is also of mathematical significance in its relation to the many optimization problems, such as the isoperimetric problem, for which solutions exhibit symmetries which are not easily understood. For the isoperimetric and some related problems a method due to Steiner has elucidated the symmetry of the solutions.[5] Such an approach would be welcome for the crystal problem; perhaps its shadow has appeared.[6]

The first real progress in the crystal problem has emerged in the last decade and consists mostly of rather specific (classical mechanical) models in one and two space dimensions, usually modeling molecular-bonded solids.[6–19] The mathematical framework is the following. One considers a countable family of variables, $\{z_j \mid j \in N\}$, each having values in some space W of the form $W = X \times S$, where X is "physical space," usually either $\mathbb{R}^d$ or a discrete analog such as $\mathbb{Z}^d$, and S is an "internal space," often finite. In this paper we will only consider classical discrete models, with $X = \mathbb{Z}^d$ and $S = \{1, 2, \ldots, N\}$. Since physically two variables may not simultaneously have common X coordinates it is convenient to use $\mathbb{Z}^d$ itself to index the variables. We will only consider two-body, translation-invariant, finite-range potential energy functions, that is, real symmetric ("potential") functions V on $W' \times W'$, $W' \equiv X \times S$, such that for all u, z, w in $\mathbb{Z}^d$ and s, t in S

$$V[(z, s), (w, t)] = V[(z + u, s), (w + u, t)], \tag{1}$$

$$V[(z, s), (w, t)] = 0 \quad \text{unless } 1 \leqslant |z - w|_\infty \leqslant D, \quad D \text{ a fixed constant.} \tag{2}$$

($|V|_p$ denotes the p norm of $V \in \mathbb{Z}^d$; we will be using only $p = 1, \infty$.) Since we are analyzing infinite-molecule configurations the total energy is not directly accessible; we define "ground states" in the DLR sense[20,21] as follows. A "configuration" $f' \in S^{\mathbb{Z}^d} \equiv T$ is a "ground state with respect to (a given potential) V", ($f' \in T_V$), if for every finite subset C of $\mathbb{Z}^d$ and every other configuration f'' such that f'' and f' agree on all sites not in C, it follows that $E_{C,V}(f') \leqslant E_{C,V}(f'')$. Here $E_{C,V}$ is defined for an arbitrary f in T by

$$E_{C,V}(f) = \sum_{\{z,w\}} \sum_{\cap C \neq \varnothing} [V(z, f(z)), (w, f(w))].$$

Note that T_V is nonempty by a simple compactness argument. A configuration f will be called "r-periodic" ($f \in T'$), if there exist (at least) r linearly independent vectors v in $\mathbb{Z}^d$ such that $f(z + v) = f(z)$ for all z in $\mathbb{Z}^d$. Finally, $\tilde{T}_V$ denotes the set, perhaps empty (a situation usually called "frustration"), of $f \in T$ such that for all z, $w \in \mathbb{Z}^d$,

$$V[(z, f(z)), (w, f(w))] = \inf_{f' \in T} V[(z, f'(z)), (w, f'(w))].$$

Note that $\tilde{T}_v \subseteq T_v$ and that the inclusion is often proper even when $\tilde{T}_V$ is nonempty.

In the context of tiling theory Robinson has proven by explicit example[22] that for any $N \geqslant 56$ and $d \geqslant 2$ there exist "nearest neighbor" [see (3) below] potentials V such that $\tilde{T}_V$ is not empty but that no configuration in $\tilde{T}_V$ is $(d-1)$ periodic. The structure of V is as follows. Two subsets K_i of $S \times S$ are determined, and V has the properties (1), (2), and (with $\{e_i\}$ the usual basis of $\mathbb{Z}^d$)

$$V[(z, s), (w, t)] = 0, \quad \text{if } |z - w|_1 > 1, \tag{3}$$

$$V[(z, s), (w, t)] = -1, \quad \text{if } z - w = e_i \text{ and } (s, t) \in K_i, \quad i = 1, 2, \tag{4}$$

$$V[(z, s), (w, t)] > -1, \quad \text{if } z - w = e_i \text{ and } (s, t) \notin K_i \text{ or } i \geqslant 3. \tag{5}$$

[It is almost immediate to translate examples from tiling notation to the above notation. But note that this requires special features in the tiling example to be able to associate it with some simple lattice, such as $\mathbb{Z}^d$, and finite S; this seems to exclude examples such as those of Penrose (see Ref. 23).]

 0022-2488/85/061342-03$02.50

II. EXTENSION

One purpose of this paper is to generalize the tiling result from $\tilde{T}_V \cap T^{d-1} = \emptyset$ (and $\tilde{T}_V \neq \emptyset$) to $T_V \cap T^{d-1} = \emptyset$.

Proposition: For any $N \geqslant 56$ and $d \geqslant 2$ there are potentials satisfying (1)–(5) for which there are no r-periodic ground states for $r \geqslant d-1$.

Proof: Suppose $\tilde{f} \in T_V \cap T^{d-1}$ for a potential V satisfying (1)–(5). For simplicity we will assume $d=2$ and that $\tilde{f}$ is periodic along an elementary lattice direction, say horizontally; the general case follows easily. This means $\tilde{f}$ consists of a vertical strip, repeated horizontally. Since the strip has finite width the situation is essentially one-dimensional and it then follows immediately from Ref. 6 that there exists $f' \in T_V \cap T^2$. From the above tiling result it then follows that for some z, w, $|z-w|_1 = 1$, $V[(z, f'(z)), (w, f'(w))] > -1$ and, f' being two-periodic, there must be a nonzero *density* of such pairs. But then for any large enough "square" subset C of $\mathbb{Z}^d$, $E_{C,V}(f') > E_{C,V}(f'')$, where f'' coincides with any $f \in \tilde{T}_V$ inside C and with f' outside C. This contradiction with $f' \in T_V$ proves our claim.

Note: Ammann has produced an example, verified in detail by Robinson[24] reducing the (tiling) bound on N from 56 to 16. This immediately carries through for our generalization. The first tiling result of this type (requiring a large N) is due to Berger.[25]

The above examples are somewhat surprising "counterexamples" to the vague thesis of the opening paragraphs. Perhaps they can be attributed to some "unphysical" manner in which the potential V exploits the *shape* of the molecules, shape here being understood either in the literal sense of the tiles or in the general sense of an internal degree of freedom. With this in mind we pose the following reformulation, which emphasizes the invariance group of V.

III. FRACTION SPACE

Let G be a group of l_∞ isometries acting on $\mathbb{Z}^d$, and assume G contains all translations of $\mathbb{Z}^d$. We emphasize two examples: (1) $G_1 = \mathbb{Z}^d$; and (2) G_2 is generated by $\mathbb{Z}^d$ and the reflections through the d planes $z_j = 0$ and the $d(d-1)$ planes $z_j = \pm z_k, j \neq k$. Extend the action of G to $\mathbb{Z}^d \times \mathbb{Z}^d$ by $g(w, z) = (g(w), g(z))$ and let m be the number of orbits of G in $A \equiv \{(w, z) \mid 1 \leqslant |w-z|_\infty \leqslant D\}$. For each f in T^d define $p(f)$ in ("fraction space") $L \equiv \mathbb{R}^{mN^2}$ with coordinate $p(f)_{N^2 j+k}$ being the relative fraction of those points (z, w), in the jth orbit of G in A, such that $(f(z), f(w))$ is the k th point in $S \times S$; here $j = 0, \ldots, m-1$ and $k = 1, \ldots, N^2$. Given a potential V satisfying (2) and invariant under G, i.e.,

$$V[(z, s), (w, t)] = V[(g(z), s), (g(w), t)], \quad \text{for all } g \text{ in } G, \tag{1'}$$

we define $q(V)$ in $L^* = \mathbb{R}^{mN^2}$ with coordinates $q(V)_{N^2 j+k} = V[(z, s), (w, t)]$, where (z, w) lies in the jth orbit of G in A and (s, t) is the k th element in $S \times S$. Let $P = \{p(f) \mid f \in T^d\}$, and let $t(j)$ be the relative fraction in A of points in the jth orbit of G. With this notation the energy per particle is

$$e_V(f) = \sum_{j=0}^{m-1} \sum_{k=1}^{N^2} t(j)\, p(f)_{N^2 j+k}\, q(V)_{N^2 j+k},$$

which we denote by the inner product $\langle p(f), q(V) \rangle$. Now it is a theorem of Sinai[19,21] that f in T^d is a ground state for V if and only if

$$e_V(f) = \inf_{f' \in T^d} e_V(f'),$$

i.e., if and only if $p(f)$ lies in a hyperplane of support for P, of the family (labeled by c) of parallel hyperplanes $\langle p, q(V) \rangle = c$, with the least c. Consider the following problem: For a given invariance group G, and every V satisfying (1'), (2), $D \geqslant 1$, and d, $N \geqslant 2$, does there exist a ground state f for V in T^d? Note that the role of a given potential is precisely to select a given direction in L, so the problem of the existence of such an f in T^d becomes the following.

Problem: For given G (and all $D \geqslant 1$, d, $N \geqslant 2$) does P contain all the exposed points of its closure?

We have seen in the above proposition that this does not hold for $G = G_1$ (at least since we allow $N \geqslant 16$). It is an open problem whether or not this holds for $G = G_2$.

We conclude with the following argument which solves the problem for G_2 under the severe restriction that $D = 1$.

Let $\hat{T}^d$ be the set of all $\hat{f}$ in T^d invariant under reflections through all the hyperplanes of the form $z_j = n$, n in $\mathbb{Z}$. There are exactly N^{2^d} such $\hat{f}$, corresponding to the possible restrictions of an f to the unit cube $K = \{z \in \mathbb{Z}^d \mid z_j = 0 \text{ or } 1\}$. Given f in T^d as h runs through the translation group $\mathbb{Z}^d$ the restriction of the f to the translate $h(K)$ agrees with each of the restrictions of $\hat{f}$ to K with a well-defined frequency, which we denote $H_f(\hat{f})$. It is then easy to check that

$$p(f) = \sum_{\hat{f} \in \hat{T}^d} p(\hat{f}) H_f(\hat{f}),$$

proving our assertion.

IV. CONCLUSION

This last formulation deemphasizes the role of the interaction apart from its spatial invariance group, and this together with construction of "fraction space" unifies important aspects of the crystal problem and tiling theory in a common, simple, algebraic framework. However, this will eventually need generalization. Since molecules with complicated shapes do exist (though presumably not of the type of the tiles referred to above!) it is clear that eventually one must investigate invariance groups acting on $\mathbb{Z}^d \times S$ not just $\mathbb{Z}^d$.

ACKNOWLEDGMENTS

We wish to thank Gary Hamrick, Ray Heitmann, Robert Maier, and David Saltman for useful conversations and Raphael Robinson for showing us some of his unpublished results on tilings.

This research was supported in part by National Science Foundation Grant No. MCS 81-01596.

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