CRYSTALS AND QUASICRYSTALS: A LATTICE GAS MODEL ☆

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We give an example of a lattice gas model with a completely symmetric, short-range, two-body interaction which has quasiperiodic, but no periodic, ground states.

The discovery of quasicrystalline solids [1] has increased interest in the fundamental problem [2–6] of understanding the causes of spatial (crystalline) symmetry in low temperature matter. It is generally believed that (for simple substances) matter becomes crystalline, as temperature is lowered at fixed pressure, due to a transfer of influence in the Gibbs free energy from entropy to (potential) energy; by some (unknown) mechanism many body states of low potential energy are forced to be crystalline. Besides the experimental evidence of real matter this is also found to hold in computer simulation of realistic models as well as the various toy models used throughout statistical mechanics. We should note however that for models with degenerate ground states, or in low dimensional models, the presence of periodic ground states can be swamped by entropy effects at all nonzero temperatures; this does not however negate the need to understand why minimization of potential energy by itself (i.e. without entropy competition) leads to crystalline symmetry.

To date results [7–22] on this "crystal problem" have concentrated on classical rather than quantum models, in one and two space dimensions, and lately on discrete (i.e. lattice gas or spin) rather than continuum models. Roughly the status of the problem is as follows. The one dimensional problem is essentially solved [19, 20]. Among two dimensional models a class of models is known to have periodic ground states [15,21] and, using Berger's result [23] on nonperiodic tilings (better known through the simpler examples of Amman [24], Penrose [24] and Robinson [24,25]) isolated, specific toy models are known [21] which do not have periodic ground states. These latter are lattice gas models of several particle species on the square lattice in two (or higher) dimensions, with nearest neighbor, translation invariant two body interactions. The interactions are covariant but not invariant under the lattice symmetries (such as 90° rotations). The noninvariance of the interactions can be thought of as associated with nonsymmetric "shapes" of the particles, which influence spirals out from the particles at low energy thus forbidding any periodic ground states but allowing "quasiperiodic" ground states. (A periodic array is a "ground state" if it achieves the minimum energy density amongst all periodic arrays. An array is quasiperiodic if for any $0 < \epsilon < 1$ when a certain fraction ϵ of particles are ignored the rest of the array is periodic; the smaller the ϵ, the larger the period.)

In this letter we refine the above example significantly by showing that the result – a (lattice gas) model with quasiperiodic but no periodic ground states – can come from translational invariant, two body, finite range interactions with the full symmetry of the (two dimensional, square) lattice; between each pair of lattice gas species the interaction will only depend on the spatial separation (and in fact the range will be less than three lattice spacings).

Two of the published results referred to above are: (1) An example of a lattice gas model with 16 particle species, a nearest neighbor interaction, and with

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quasiperiodic but no periodic ground states [21];
(2) A proof that for a lattice gas model with N species, if the interaction is at most nearest and next nearest neighbor and is symmetric under reflection through the lines $x = 0, y = 0$ and $x = \pm y$ then it must have a periodic ground state [21].

A new symmetry result is the following.

Proposition. For an N species lattice gas model on the square lattice, if the (two body or even many body) interaction is finite range, translation invariant (this can be weakened slightly), vanishes except between particles parallel to an axis and is symmetric with respect to one or both of the lines $x = \pm y$, then it has a periodic ground state.

Proof. Considering interactions just among particles on the x-axis, we know [19] there is a periodic ground state $\{S(x)\}$, where $S(x)$ denotes the species at site x. It then follows immediately that a periodic ground state for the full system is either $S(x,y) = S(x+y)$ or $S(x,y) = S(x-y)$, depending whether $x = y$ or $x = -y$ is a symmetry line for the interaction; here $S(x,y)$ denotes the species at the site (x,y).

Thus an interaction which is sufficiently symmetric and short range must have a periodic ground state. We next give an example of a fully symmetric interaction of slightly longer range (still less than three lattice spacings) with quasiperiodic but no periodic ground states.

We take as our starting point the example of Robinson [25] of a set of ten (families of) square tiles which, with rotations and reflections allowed and with given matching rules (which describe which tiles may abut, edge to edge) permit tilings of the plane but only quasiperiodically, not periodically. These tiles can be thought of as squares of side length 4; of ten families (the tiles in a given family being rotations and/or reflections of one "prototype" of the family) labeled 1 to 10. Choosing a fixed prototype of each family and using the lower left hand corner of each prototype as an origin of coordinates, we decompose each prototype into 16 unit squares, labeled by the coordinates of their lower left hand corners. So we have 160 distinguishable types of unit squares, for which, e.g., the symbol [4;(3,3)] refers to the square in the upper right hand corner of the fourth prototype. Denoting the tiles " molecules" and the unit squares "atoms", we will define interactions between the atoms such that the lowest energy state of a large collection of atoms will necessitate the atoms combining into molecules of the above families, and with the molecules obeying Robinson's matching rules which imply nonperiodicity. This is done as follows.

Interactions between atoms will be nonzero only if they (i.e. their centers) have separation at most $\sqrt{5}$. (Atoms may not overlap, must each be centered on the sites of a fixed square lattice, and must have edges parallel to the axes; the only effective separations are thus $1, \sqrt{2}, 2$ and $\sqrt{5}$.) The values of the interactions at the given separations will be one of two numbers, L (for low energy) or H (for high energy), where $L < 0$ and $L < H$. For each given atom type we need to know its interaction with each of the 160 atom types, at each of the four distances. This is obtained for a given atom A by first embedding A in "its molecule" – i.e. [2;(0,1)] in prototype 2 – and then surrounding this molecule with any eight molecules (not just prototypes) which observe Robinson's matching rules with this center molecule. Then atom A has interaction L with an atom of type B at a given distance $d = 1, \sqrt{2}, 2$ or $\sqrt{5}$ if and only if in at least one of these constructions an atom of type B appears at distance d from A. We now need to show that these interactions have the desired properties.

First we divide the atoms into three "classes"; "interior" atoms, which have coordinates within their molecules (1,1), (1,2), (2,1) or (2,2); "corner" atoms, which have coordinates (0,0), (0,3), (3,0) or (3,3); and "edge" atoms, which are the remainder. We note three obvious general facts about the interactions (the last of which reflects a simple but special feature of Robinson's example).

(A) The interaction between two atoms of a given class at separation $d = 2$ is H.

(B) The interaction between two corner atoms at separation $d = \sqrt{5}$ is H.

(C) The interaction between two identical edge atoms at separation $d = \sqrt{2}$ is H.

We know by construction that it is possible to fill the plane with atoms such that every interaction has value L (energy density $10L$); we will call any such arrangement a "ground state". We need to show there are no periodic ground states.

Lemma 1. If an interior atom is surrounded by eight atoms, with all interactions having value L, then the arrangement is identical to part of a molecule in the family associated with the atom.

Proof. This follows very easily using (A) and consideration of the definition of the interactions.

Lemma 2. If an interior atom appears in a ground state it appears embedded in a molecule of its family.

Proof. The proof consists of four applications of lemma 1.

Lemma 3. If a corner or edge atom appears in a ground state it appears embedded in a molecule of its family.

Proof. Consider the eight atoms surrounding the atom in question. If any of the eight is an interior atom, the result follows from lemma 2. That one of the eight must be an interior atom follows by contradiction using (B).

We now know that every ground state is composed of molecules. The fact that these molecules are not overlapping, or fail to abut in the desired way (i.e. corner to corner) follows easily from (A). Finally one sees that abutting molecules must obey Robinson's matching rules by considering two edge atoms at separation $d = 1$, one from each abutting molecule, and using (C). Thus any periodic array has a finite density of high energy interactions (i.e. an energy density higher than $10L$) and so cannot be a ground state.

To summarize: we have given an example of a translation invariant, two body interaction in a 160-species lattice gas model on the square lattice. The interaction is of short range (less than three lattice spacings), completely symmetric – only a function of the separation between particles – and yet it has quasiperiodic ground states but no periodic ground states. This result seems counterintuitive; in fact it squarely contradicts one of the key arguments in Anderson's recent and influential book, ref. [6].

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