Comment on "Cluster Approach to Quasicrystals"

In a recent Letter [1], Jeong and Steinhardt propose a cluster based approach to explain the stability of quasicrystals. The basic idea is to energetically favor only a few important clusters occurring in the structure, instead of all allowed clusters up to a given size, as one would do in a matching rule approach. Minimization of the energy then favors overlaps of such clusters, which leads to correlations. In Ref. [1] it was demonstrated that with a proper choice of clusters and their associated energies it is possible to obtain different kinds of ground states, such as perfectly quasiperiodic structures, weak matching rule structures, and random tiling structures.

The most interesting perhaps are interactions leading to a perfectly ordered ground state, and I shall consider only such interactions in this Comment. I shall demonstrate that by using the cluster approach instead of the more traditional matching rule approach it is not possible, in general, to reduce the range of the interactions needed to stabilize a perfectly quasiperiodic structure. The cluster approach may allow to reduce considerably the *number* of different clusters that have to be given low energy – which can be quite an achievement –, but it cannot be used to reduce *minimal size* of these clusters.

The arguments leading to this conclusion are very general, but I shall explain them with an example, the 3D Penrose tiling, which is obtained as a cut of physical space through a 6D lattice decorated with atomic surfaces. When physical space is moved so that it leaves one atomic surface, it enters at the same time another atomic surface, so that the corresponding vertex just jumps to a nearby place, thereby rearranging four tiles forming a rhombic dodecahedron. We say that the contents of the dodecahedron is flipped. At the very same time, a whole infinity of dodecahedra, all lying on a single plane, are flipped as well, in a correlated way. Apart from the interior of these dodecahedra, the structures just before and just after the flip are identical and mirror symmetric about a plane through the centers of the dodecahedra.

It is now clear that any interaction which is to stabilize the 3D Penrose tiling, whether it involves all clusters up to a given size, or only a few of them, must have a range sufficiently big so that all flipping dodecahedra are coupled to each other by interaction clusters, because otherwise some subset of the dodecahedra could be flipped independently of the rest of the dodecahedra, without affecting the density of any interaction cluster. Such a partial flip would therefore disorder the tiling without costing any energy. Moreover, not only the dodecahedra on a perfect mirror plane have a mirror symmetric environment. In fact, any dodecahedron with an interior vertex sufficiently close to the boundary of its atomic surface has a mirror symmetric environment, and can therefore be flipped without energy cost. Such dodecahedra have a finite density in the quasicrystal.

The above arguments do not directly show that interactions with too short a range necessarily lead to random tiling structures. They just show that there is an ensemble of disordered states which are energetically degenerate with the structure we wanted to stabilize. This ensemble might consist of weak matching rule structures. It appears very likely though that the disorder can proliferate and produce a random tiling structure.

Unfortunately, the minimal matching rule radius for the 3D Penrose tiling, below which no matching rules exist, is not rigorously known, although there are strong indications that the alternation condition [2] represents a set of genuine, perfect matching rules. The alternation condition can be enforced by specifying allowed clusters up to a diameter of about five tile edge lengths, which is roughly the same as the lower bound derived above.

The arguments presented here are very general and can be applied to any quasicrystal [3]. In particular, a lower bound on the minimal range of interactions can always be derived. Experience from various examples [3] shows that at least for relatively simple tilings the minimal matching rule radius is often close to this lower bound. As the lower bound holds for any kind of interaction, the cluster approach cannot reduce the minimal interaction range.

The Penrose tiling treated in Ref. [1] was a fortunate case because it allows for extremely short range matching rules, which is rather exceptional. It was therefore possible to stabilize the structure by energetically preferring a few simple and *small* clusters. Other structures needing longer range matching rules will need longer range interactions also in the cluster approach, although the number of clusters needed might be greatly reduced in that way.

I would like to thank P. Steinhardt and H.-C. Jeong for providing me with their results prior to publication, and for interesting discussions on the cluster approach to quasicrystals. This work was supported by the Swiss Nationalfonds, and by DOE grant DE-FG02-89ER-45405.

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PACS NOs: 61.44.+p, 61.50.Ks, 05.50.+q

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