NO INHERENT GLASSINESS IN A PENROSE TILING QUASICRYSTAL

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Abstract

Consideration of the structure of the Penrose pattern has led to speculation that a system with a Penrose tiling ground state might be subject to inherent glassy behavior. Monte Carlo simulations show, using a simple model of the energetics, that there is no inherent glassiness in the Penrose tiling. Thermodynamic quantities measured are completely reversible, displaying no observable hysteresis, and the system may be easily cooled from a highly disordered configuration into its lowest energy state.

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Although it is not yet clear what is the best theoretical description of the experimentally observed quasicrystals - materials with noncrystallographic orientational symmetry and relatively sharp diffraction peaks - it is clear that the quasiperiodic crystal model^{1, 2, 3, 4} suggests a very interesting potential new condensed matter phase. The Penrose tiling is the prototypical quasiperiodic crystal^{5, 6, 7, 8}.

In this paper we report studies of a thermodynamic model for which the Penrose tiling is the ground state. We first briefly describe properties of the Penrose tiling which lead to the suggestion that the Penrose pattern might display glassy behavior. We then describe Monte Carlo simulations which show that the thermodynamics of this model are completely reversible and that no inherent glassiness exists.

Why Glassy Behavior Might Be Expected

Figure 1 shows a portion of a Penrose tiling. The tiling is composed of fat and skinny rhombuses joined together by matching the double and single arrows along the rhombus edges as shown. Joining parallel rhombus edges creates five sets of "tracks" at 72 degree angles. A subset of these are shown. Each track may be decomposed into a series of "worms" consisting of strings of hexagonal arrangements of either two fat and one skinny or two skinny and one fat tiles. The figure shows one of these worms. These worms terminate at decagons, all of which have the structure of that highlighted in figure 1.

An elementary way to introduce disorder into the pattern is to "flip" a hexagon. Two such flips are illustrated in figure 2. Any tiling may be reached from any other by a suitable combination of flips (although energetically costly intermediate configurations may be required). Each flip introduces two matching rule violations as illustrated. Matching rule violations can travel easily within a worm without introducing further violations simply by successive flipping of hexagons. Thus, upon cooling from high temperatures, two violations within the same worm may easily annihilate.

The situation is quite different, however, for moving a matching rule violation through a decagon. The difficulty is illustrated in figure 3. In figure 3a a matching rule violation is present at edge A. We would like to move it through the decagon to edge B, perhaps so it can annihilate with a violation in the worm attached to edge B. Recall that at the completion of our rearrangements the decagon must still have the structure shown, although it may be rotated. (Otherwise we must introduce additional matching rule violations.) However, one quickly finds that it is impossible to rotate the decagon so as to move the violation at edge A to edge B without introducing violations in worms along other directions. (One such attempt is shown in figure 3b.)

Thus, the worms are tied together by decagons into a sort of traffic system. Because violations in two adjacent worms cannot annihilate without the creation of extra violations in other worms, one might speculate that the system would be difficult to cool from a disordered state back to a defect-free system (a kind of "gridlock") and might therefore be inherently glassy. That this is not the case is demonstrated in the simulations reported here.

Results of Monte Carlo Simulations

For our simulations we take a simple model of energetics in which a matching rule violation (whether single-single or double-double) is assigned unit energy. We heat and cool the system using a Monte Carlo simulation technique and check for lack of reversibility. The simulation procedure is to randomly choose a hexagon and then attempt to flip it. Flips are accepted or rejected according to a standard Metropolis algorithm. These hexagon flips may be shown to satisfy detailed balance.

Simulations were performed for systems of sizes 94 and 246 tiles with periodic boundary conditions. The sizes were chosen so as to obtain best periodic approximants⁹ to the Penrose tiling. Because of the periodic boundary conditions four matching rule violations are present in the lowest energy state of each periodic tiling.

Results from heating from the lowest energy state and cooling from a highly disordered configuration are shown in figures 4-6. Figure 4 displays number of violations (or total energy)

as a function of temperature. Figures 5 and 6 depict the perpendicular space quantities $\langle h^2 \rangle$ and $\langle h_z^2 \rangle$ as a function of temperature. These quantities are defined with respect to the five-dimensional representation of the tiling. Qualitatively, they measure fluctuations associated with single and double arrow violations respectively.

Precisely, we may define the five dimensional coordinates $\{n_\alpha(\mathbf{r})\}$ of a tile vertex by counting, from an arbitrary origin, the number of positive steps minus the number of negative steps taken in each of the five pentagonal directions in order to arrive at the vertex at position $\mathbf{r}$. The vertex indicated in figure 7, for example, has five-dimensional coordinates (2 2 -1 -2 0). Given these indices we then define

$$\mathbf{h}(\mathbf{r}) = \sum_{\alpha=0}^4 n_\alpha(\mathbf{r}) \mathbf{e}_\alpha^\perp \quad (1)$$

$$h_z(\mathbf{r}) = \sum_{\alpha=0}^4 n_\alpha(\mathbf{r}) \quad (2)$$

where

$$\mathbf{e}_\alpha^\perp = \left(\cos \frac{4\pi\alpha}{5}, \sin \frac{4\pi\alpha}{5} \right) \quad (3)$$

These quantities are called the phason variables or perpendicular coordinates. The fluctuation quantities $\langle h^2 \rangle$ and $\langle h_z^2 \rangle$ are then defined by

$$\langle h^2 \rangle = \frac{1}{N} \sum_{\mathbf{r}} \langle (\mathbf{h}(\mathbf{r}) - \bar{\mathbf{h}})^2 \rangle \quad (4)$$

$$\langle h_z^2 \rangle = \frac{1}{N} \sum_{\mathbf{r}} \langle (h_z(\mathbf{r}) - \bar{h}_z)^2 \rangle \quad (5)$$

where $\bar{h}$ and $\bar{h}_z$ are the average values for a given configuration of $h(\mathbf{r})$ and $h_z(\mathbf{r})$ respectively and the sum is over all tiling vertices designated by their positions $\{\mathbf{r}\}$. (In our system these quantities must be modified slightly to account for the phason strain introduced by the periodic boundary conditions.)

As can be seen by inspecting Figures 4-6, all of the measured quantities are reversible, with hysteresis unobservable. Indeed, we have performed several of these heating and cooling runs for each size and have always been able to cool easily down to our lowest energy configuration with only 4 matching rule violations.

Thus we conclude that the Penrose pattern is not inherently glassy. These results do not preclude, of course, the observation of long equilibration times in real materials with quasiperiodic ground states. The basic hexagon flips performed here would, in a real system, correspond to particle rearrangements which may occur very slowly in real systems.

Further results on the phase diagram of this thermodynamic Penrose tiling model will be reported in a forthcoming longer publication ¹¹.

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Figure Captions

Figure 1: A fragment of a Penrose tiling of arrowed rhombuses. A set of tracks are shown. The light shading highlights a string of hexagons or "worm". All worms terminate on decagons of the type highlighted by the dark shading.

Figure 2: An illustration of a hexagon flip within a worm. The hexagons highlighted in the worm on the left have been flipped in the worm on the right.

Figure 3: a) An illustration of a terminating decagon with a matching rule violation at point A b) The violation at point A cannot be moved to point B without introducing additional matching rule violations. One attempt to move the violation to point B is shown.

Figure 4: Number of matching rule violations (or total energy) as a function of temperature for heating and cooling runs.

Figure 5: Perpendicular space fluctuations $\langle h^2 \rangle$ as a function of temperature for heating and cooling runs.

Figure 6: Perpendicular space fluctuations $\langle h_z^2 \rangle$ as a function of temperature for heating and cooling runs.

Figure 7: Illustration of the method for determining the five-dimensional coordinates $\{n_\alpha\}$ of the point A with reference to the origin O.

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Figure 1

Figure 2

Figure 3a

Figure 3b

Figure 4

Figure 5

Figure 6

Figure 7

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