CLUSTER MAXIMIZATION, NON-LOCALITY, AND RANDOM TILINGS

C.L. HENLEY
Dept. of Physics, Cornell University, Ithaca, NY 14853-2501, USA

Jeong and Steinhardt (JS) implement local rules by selecting the sub-ensemble of tilings which have the maximum occurrences of a chosen pattern (“cluster”) C. It is unknown how to prove that a given C implies a given sub-ensemble; counterexamples given here demonstrate this problem is nonlocal, and show the JS results depend on periodic boundary conditions. Sub-ensembles which are random tilings of supertiles are at least as interesting, mathematically and physically, as the ideal cases emphasized by JS; the case C = star-decagon is explored here. Finally, I suggest minimizing the frequency of chosen intersite distances as a more physical alternative to the cluster approach.

1 Introduction

Although the “random-tiling” and “local-rules” scenarios give rather different pictures of the stabilization of quasicrystal order, they are hard to distinguish since they both predict Bragg peaks and quasiperiodicity in projections of 3D slabs. Before this question can be settled, we must understand how the microscopic structural energy favors the quasicrystal structure. One common assumption is a decorated tiling, implicitly assuming the tilings are all degenerate (= random tiling) within a rather coarse energy resolution, as is consistent with existing pseudobinary pair potentials. On a finer energy scale, the tile-tile effective Hamiltonian might either favor a periodic crystal (so the quasicrystal is an entropically stabilized random tiling), or else a quasiperiodic tiling. Some interatomic potentials are known that (in simulations) produce decorated quasicrystal random tilings upon cooling.

Jeong and Steinhardt (JS) idealized the tile Hamiltonian so as to define restricted tilings: in their simplest cases, they choose a “cluster” C and take the subsensembles of tilings that maximize its frequency. I will call such a prescription a “maximizing rule” (in analogy to “matching rule”.) The tiling is specified much more economically this way than by enumerating the complete “R-atlas” of allowed local patterns. For several different cases, JS inferred the subsensembles from images of the ground states obtained in simulations. The fact that JS obtained random tilings while searching for quasiperiodic ones suggests that the former cases are more common than the latter.

The original JS paper – and work it inspired – has a major gap: we
Figure 1: (a). Tiles of SD packing (centers marked; one SD is outlined), (b). Unit cell of packing with maximum cluster density (hexagon tile), coexisting with domain of fat rhombi.

don’t know how to prove mathematically that the subsensemble is optimal for the given Hamiltonian. JS in fact accomplished such a proof, but only for a certain (fairly large) C, copies of which can cover the entire tiling (with overlaps allowed). This gap is shared with most atomic quasicrystal models; a general understanding of the relation of Hamiltonian to tiling would have immediate applications in predicting quasicrystal structures.

Among the examples found by JS, symmetric cluster rules such as $C_{B/T}$ or the star-decagon $C_{SD}$ gave random tilings; quasiperiodicity could be forced only for rather special C’s that break the 5-fold rotational symmetry. Conceivably this could be realized by vacancy alternations in the inner Al$_{12}$ shell of a Mackay Icosahedron, or in the “δ” (six-dimensional body center) sites.

2 Supertiling maximizing the SD-cluster

The random tiling cases are, perhaps, even harder than the quasiperiodic ones, since the optimum is not a quasi-unique pattern, but a degenerate ensemble. Such cases might model changes in symmetry due to supertile formation which give superlattice-like diffraction. As an explicit example, I now specialize to the “star-decagon” cluster $C_{SD}$ (called “$C_D$” by JS).

The random tiling which describes the JS results for $C_{SD}$ is formed by the supertiles A,B,C outlined in Fig. 1(a), which add to form a “boat” shape. Supertiles 2A+2B can be combined to make a “hexagon” as in Fig. 1(b). (Here we can draw the B triangle hypotenuses in two ways in the interior, but we must count them both as the same tiling.) One could also create a 5-pointed “star” with $C_{SD}$ on each vertex (the top part of Fig. 1(a) is a fragment of this star.) The A-B-C tilings have as a subset the random tilings of boat, hexagon, and
star (which I called “two-level tiling”\(\square\)), which in turn have include the Penrose single-arrow-edge tiling. Using this, the ideal SD frequency in a connected tiling is found to be \(\tau^{-3}/\sqrt{5}\) clusters per vertex.

However, these tilings are optimal only under the constraint that the tiling is \emph{connected}, \ie every tile edge is fitted against another tile edge with no gaps. Let us try instead a more physically relevant game. Given many fat and skinny rhombi, with the ideal number ratio \(\tau \equiv (1 + \sqrt{5})/2\), what packing has the most clusters? It is actually a \emph{phase-separated} configuration, consisting of a domain of hexagons, plus a domain of fat rhombi (Fig. 1(b)). For every tile, we have \(1/7\tau^2\) hexagons (each with two SD clusters), and \(\sqrt{5}/7\tau^6 = 0.018\) Fat tiles left over, giving a frequency of \(2/7\tau^2\) clusters per tile which is 3.3\% better than the connected tiling.

For a covering cluster, an essentially local proof of optimization is workable\(\square\) (extended by a clever use of inflation). Contrariwise, in the \(C_{SD}\) case any local proof, based on counting and dividing areas, can be ruled out: the “phase separated” state of Fig. 1(b) always beats the random tiling. The optimization is inherently nonlocal; a proof must make essential use of the connectedness of the tiling, or the requirement that the mean phason strain be zero.

As an aside, I have studied the tilings defined by a covering rule: \emph{every skinny rhombus must be covered by (at least one) SD}. The A-B-C random tilings have this property. It is easy to show that, if there is even one adjoining pair of \emph{parallel} Fat tiles, then there is at most one SD in the whole tiling. Excluding that, it is then easy (by enumerating the possible surroundings of a corner of the SD cluster) to show we obtain just the random tiling made of the tiles in Fig. 1(a) together with one added kind of tile, a large star.

3 Critique of “cluster” picture and conclusion

Do \emph{max}-rules really have a more natural connection to an interatomic Hamiltonian than Penrose matching rules do? The total energy of a structure defines an effective potential of the atomic coordinates which – we assume – is dominated by few-body (up to 4-body) interactions among near neighbors, and two-body interactions to further neighbors. To favor a \(C\)-cluster of \(M\) tiles (and \textit{not} favor smaller fragments of that cluster) requires a potential term among atoms on \(O(M)\) tiles, that is among \emph{at least} \(O(M)\) atoms\(\square\). That seems implausible, although it is just what is postulated in models with a hierarchical electronic structure\(\square\).

\textsuperscript{a}Such an instability appears less likely when the energy has a cusp as a function of phason strain as observed by JS\(\square\) in the quasiperiodic (non-random tiling) cases (nonzero value of their “\(\alpha_2\)”) – but even then it cannot be ruled out.
I suggest instead to explore a version of the JS game which I’ll call “constraint” rules. Rather than favor a chosen local pattern, let us disfavor certain chosen inter-vertex distances and take the sub-ensemble in which they are forbidden (or if that is too restrictive, in which their frequency is minimized.) A few such constraints can very effectively limit the allowed local patterns\textsuperscript{11}. So, just like the “cluster” rules, this offers a more economical specification than the $R$-atlas.\textsuperscript{5} Again one expects that random super-tilings are more generic than quasiperiodic ones. And constraint rules are much more plausible, a priori, since they are naturally derived from interatomic pair Hamiltonians.

Acknowledgments

This work was supported by DOE contract DE-FG02-89ER-45405. I thank H.-C. Jeong and P. J. Steinhardt for discussions and for sending unpublished images from their simulations.

1. C. L. Henley, in in Quasicrystals: The State of the Art, ed. P. J. Steinhardt and D. P. DiVincenzo (World Scientific, Singapore, 1991), p. 429, and references therein.
2. M. Mihalkovič, W.-J. Zhu, C. L. Henley, and R. Phillips, Phys. Rev. B 53, 9021 (1996).
3. M. Dzugutov, Europhys. Lett. 31, 95 (1995); J. Roth and C. L. Henley, Philos. Mag. A 75, 861 (1997); and references therein.
4. H.-C. Jeong and P. J. Steinhardt, Phys. Rev. Lett. 73, 1943 (1994).
5. L. S. Levitov, Commun. Math. Phys. 119, 627 (1988).
6. F. Gähler and H.-C. Jeong, J. Phys. A 28, 1807 (1995).
7. H.-C. Jeong and P. J. Steinhardt, Phys. Rev. B 55, 3520 (1997); see also Nature 387, 431 (1996).
8. P. Gummelt, in Proc. of the 5th International Conf. on Quasicrystals, ed. C. Janot and R. Mosseri (World Scientific, Singapore, 1995), p. 84; Geometriae Dedicata 62, 1 (1996).
9. F. Lançon, L. Billard, S. Burkov, and M. de Boissieu, J. Phys. I France 4, 283 (1994).
10. C. Janot, J. Phys. Condens. Matt. 9, 1493 (1997).
11. J. L. Robertson and S. C. Moss, Z. Phys. B 83, 391 (1991), and references therein.