Configurational Entropy of Codimension-One Tilings and Directed Membranes

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Received July 15, 1996; final December 18, 1996

The calculation of random tiling configurational entropy amounts to an enumeration of partitions. A geometrical description of the configuration space is given in terms of integral points in a high-dimensional space, and the entropy is deduced from the integral volume of a convex polytope. In some cases the latter volume can be expressed in a compact multiplicative formula, and in all cases in terms of binomial series, the origin of which is given a geometrical meaning. Our results mainly concern codimension-one tilings, but can also be extended to higher codimension tilings. We also discuss the link between free-boundary- and fixed-boundary-condition problems.

KEY WORDS: Quasicrystals; configurational entropy; partitions; random tilings.

1. INTRODUCTION

Quasicrystalline materials revealing exotic symmetries were discovered more than 10 years ago. A great deal of work has been devoted to understanding their structure at the atomic level. Even though one can estimate that in the best cases only 70–80% of the atomic locations are known, this can already be seen as a success, considering the initial complexity of the problem. Among the many questions which are still open, the origin of the stability in these noncrystallographic metallic alloys is not clearly understood. However, several models have been proposed to explain this stability. One of the most popular consists in considering quasicrystals as particular instances of Hume-Rothery alloys. Indeed, these phases appear to be stabilized when their stoichiometry amounts to almost definite values.

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for the ratio of electrons per atom. In the language of quasicrystals, this is associated with Fermi surfaces close to boundaries of pseudo-Brillouin zones, the latter being defined with respect to the most intense diffraction peaks.

A second often-considered explanation is that of an entropically stabilized material, the random tiling model. The underlying problem can be easily settled (as was initially done) under the simplifying assumption that the complexity of the structure is coded in the arrangement of tiles (for instance, simple rhombi in 2D or rhombohedra in 3D). Once the best arrangement of tiles is found (e.g., which minimizes the free energy), the last step toward atomic models is made by an atomic decoration of the tiles. Note that this way of modeling the structure (with each cell of a given type receiving the same atomic decoration) does not exhaust all the possible atomic structures, but is believed to give plausible averaged structures. In the “maximally” random tiling model, the free energy only depends on its configurational entropy contribution, which amounts to a combinatorial problem. Note that, in the simplest case of rhombus tilings on a triangular grid (which is not strictly speaking related to quasicrystal problems, but retains part of their complexity), Blôte and Hilhorst showed that the entropy amounts to that of the ground state of an Ising antiferromagnet on a triangular lattice.

More realistic models should take into account an energy term that is a function of the tile configuration. There could even be a phase transition between a low-temperature phase, whose stability would be mostly driven by interaction energies (favoring a perfect quasicrystal order), and a higher temperature phase, entropically stabilized, whose disorder would nevertheless not destroy the Bragg-like diffraction peaks (in 3D) which are the signature of the quasiperiodic order.

Even though, on physical grounds, we do not particularly favor the entropic stabilization mechanism as opposed to the electronic quantum effect, we shall focus in this paper on the combinatorial problem which underlies this entropic model. Indeed, this problem of “statistical mechanics of tilings” appears to be extremely interesting. The paradigmatic models of quasicrystals are the Fibonacci chain in 1D, the Penrose tiling in 2D, and their generalized icosahedral versions in 3D. The standard method for generating these $d$-dimensional structures consists in a selection of sites and tiles in a $D$-dimensional ($D > d$) lattice according to certain rules, followed by a projection onto a suitable $d$-dimensional Euclidean subspace (we say that we have a $D \to d$ problem). A main difference between the quasiperiodic and the simplest crystalline arrangements (e.g., the periodic chain and square and cubic tilings in 1D, 2D, and 3D, respectively) is the possibility in the former of limited local rearrangements (“reshuffling”) of