THERMODYNAMICS OF RANDOM TILING QUASICRYSTALS

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ABSTRACT

Random tiling models in two and three dimensions, equipped with a matching rule interaction, are studied by Monte Carlo (MC) simulations. An accelerated MC algorithm due to G. Barkema is used, which allows to make a MC move at every time step. By entropic sampling techniques, the entropy as a function of energy is determined for different system sizes, and the specific heat is computed from the entropy. By direct MC simulations, the phasonic diffusion constant and certain order parameters are measured. All our results consistently support the existence of a phason unlocking transition at $\beta \approx 1.3$ in the 3D case. In particular, the specific heat diverges at the same temperature at which the phasonic diffusion constant suddenly changes its slope. In 2D there is no sign of a phase transition.

1. Introduction

In this paper, the thermodynamic properties of 2D octagonal and 3D icosahedral random tilings[1] are studied by Monte Carlo (MC) simulations. For both tiling models an interaction energy is used which has a perfectly ordered, quasiperiodic ground state. This interaction is based on the alternation condition[2] (AC), which requires that tiles of the same shape but pointing to different sides must alternate along any lane of tiles[2]. An interaction energy of 0.5 units is attributed to every violation of the AC, i.e., to any two consecutive tiles of the same shape pointing to the same side of the lane. In the case of the octagonal tiling, the usual periodic approximants with square unit cells are used, which are compatible with the AC[3], so that the ground state energy for these approximants is zero. Moreover, it can be shown[3] that any tiling not violating the AC and having the same periodicity is one of those approximants. In the icosahedral case, on the other hand, there are no periodic approximants without violations of the AC. In this paper, the usual approximants with cubic unit cells are used. An approximant of order p/q has an energy of $12p$, which is the ground state energy. More precisely, in any of the twelve lane directions not parallel to an edge of the unit cell there exists exactly one such lane, containing $2p$ AC violations. Lanes parallel to the unit cell edges do not show any AC violations. The $24p$ AC violations are forced by the boundary conditions and cannot be decreased. This is also confirmed by our simulation results. Note that the density of AC violations decreases with increasing order of the approximant, and finally vanishes for the perfectly icosahedral tiling. It is conjectured[2] that a tiling without any AC violations is perfectly quasiperiodic and icosahedrally symmetric.

It is expected[4] that in 2D the quasiperiodic ground state is unstable at positive temperatures, the equilibrium phase being a random tiling phase. In 3D, however, the ordered ground state should be stable for a whole range of temperatures, and a phason unlocking transition from an ordered, quasiperiodic phase to a random tiling phase is expected to occur at some finite temperature. This has also been confirmed by MC simulations[5,6]. It is this phase transition which is the primary objective of this paper. We are particularly

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interested in the behaviour of the phasonic diffusion constant[7] across this phase transition. Phason assisted diffusion is a diffusion channel specific to quasicrystals[7]. It is expected to be very sensitive to the degree of order in the structure. So far, in 3D the phasonic diffusion constant has been determined only at infinite temperature[8], whereas in 2D also finite temperature results are available[9,10] – but in 2D there is no phase transition. In the following, we shall first discuss our simulation techniques, and then present our results.

2. Simulation Techniques

Our MC dynamics is basically the one used by Tang[11]. An elementary MC step consists of local rearrangements of tiles, called flips. The tiles to be rearranged are, in the 2D case, a square and two rhombi forming a hexagon, and in the 3D case two fat and two skinny rhombohedra forming a rhombic dodecahedron. For an elementary MC step, a tiling site is chosen at random. If it is inside a hexagon or dodecahedron, the energy cost ΔE of the flip is computed, and the site is flipped with a probability $\min(1, e^{-\beta\Delta E})$, where β is the inverse temperature. MC steps in which a non-flippable site is chosen are counted too, but the tiling is left unchanged. After each attempted flip, the physical time is advanced by $1/N$, where N is the number of vertices in the system, so that a complete MC sweep takes one unit of time. It is easy to see that this procedure satisfies detailed balance.

Since the average probability of accepting a proposed flip becomes rather small at low temperatures, we use an accelerated version of the algorithm described above, which is due to G. Barkema[12]. It is completely equivalent to the standard algorithm. The basic idea is to make a flip at every time step, i.e., to avoid any rejection of a proposed flip. In order to maintain detailed balance, two conditions must be satisfied: flippable sites must be chosen with the correct relative probability, which is proportional to $\min(1, e^{-\beta\Delta E})$, and are then flipped with certainty, and after each flip the physical time must be incremented by the average survival time of the state before the flip, in order to compensate for not rejecting any flips. This average survival time is equal to $1/Np_0$, where p_0 is the probability of leaving the state unchanged in the next attempted MC move in the standard algorithm. In order to implement this accelerated algorithm, it is necessary to know the energy cost of all possible flips at any time, and one must be able to chose those flips with the correct relative probabilities. This creates some bookkeeping overhead, but at low temperatures this overhead is by far compensated by not having to reject any flips after a costly computation of the energy cost of an attempted flip.

The accelerated algorithm is used to measure directly the thermodynamic properties of the random tiling system, such as the specific heat, as well as to measure some order parameters of the system. Particular attention is payed to phason assisted diffusion, for which the diffusion constant has been measured. In addition to such direct measurements, the accelerated algorithm can also be used in combination with entropic sampling techniques[13]. With entropic sampling, the Boltzmann probability distribution $e^{-\beta E}$ is replaced by the (initially unknown) distribution $e^{-S(E)}$, where $S(E)$ is the entropy of the system. This probability distribution has the property that all possible energies of the system occur with equal probabilities. This can be used in the simulation: in an iterative procedure, the entropy function $S(E)$ is adapted until a uniform energy distribution is reached[13]. In this way, the entropy $S(E)$ can be obtained directly, and various thermodynamic properties can be computed from it. The accelerated algorithm can easily be combined with entropic sampling. The most efficient way is to integrate the time spent at the different (discrete) energy values, and to adapt $S(E)$ so that these times become uniformly distributed. The acceleration proves particularly useful for those energy ranges where the entropy varies rapidly, i.e., near the boundaries of the spectrum.

3. Results

In Fig. 1, the diffusion constant D, as obtained in direct MC simulations, is shown for different sample sizes as a function of inverse temperature (Arrhenius plot). In the octagonal case, there is an unphysical diffusion mechanism which dominates at low temperatures. It makes use of the periodic boundary conditions, but is suppressed for large enough sample sizes at any fixed temperature. We have eliminated the effect of this unphysical mechanism by finite size scaling. The limiting curve shows a very smooth behaviour. In the icosahedral case, however, the diffusion constant shows a sudden change in slope at $\beta \approx 1.3$, which becomes more pronounced with increasing system size. This change in slope can be interpreted in terms of a phase transition (see below). In the icosahedral case, finite size effects are important even at relatively large temperatures. For both systems, the behaviour of the diffusion constant can be understood in terms of a correlated random walk model[14].

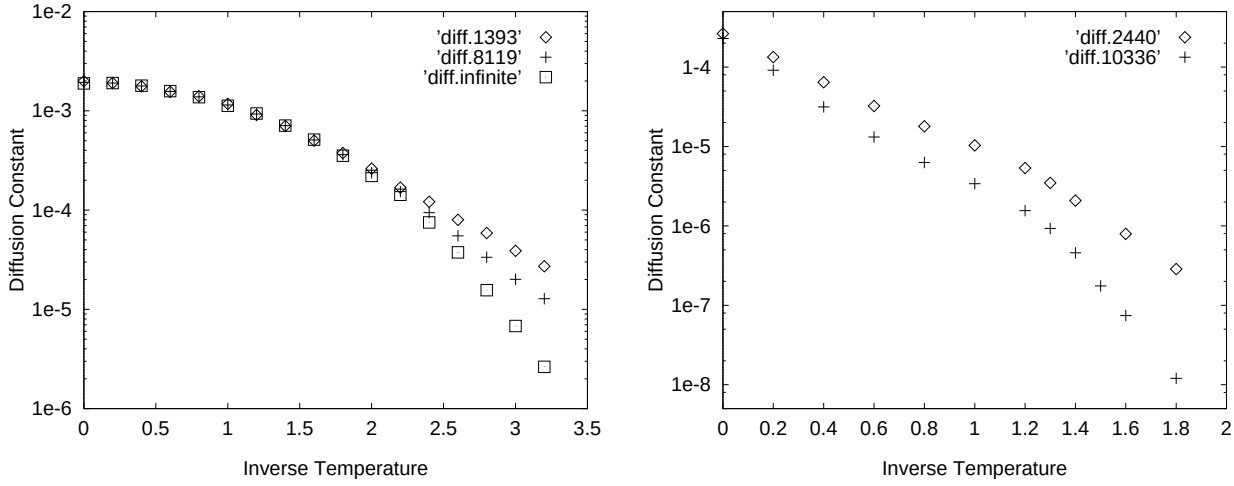

Fig. 1. Diffusion constant as a function of inverse temperature in logarithmic scale (Arrhenius plot), for different sizes of the octagonal (left) and the icosahedral tiling (right).

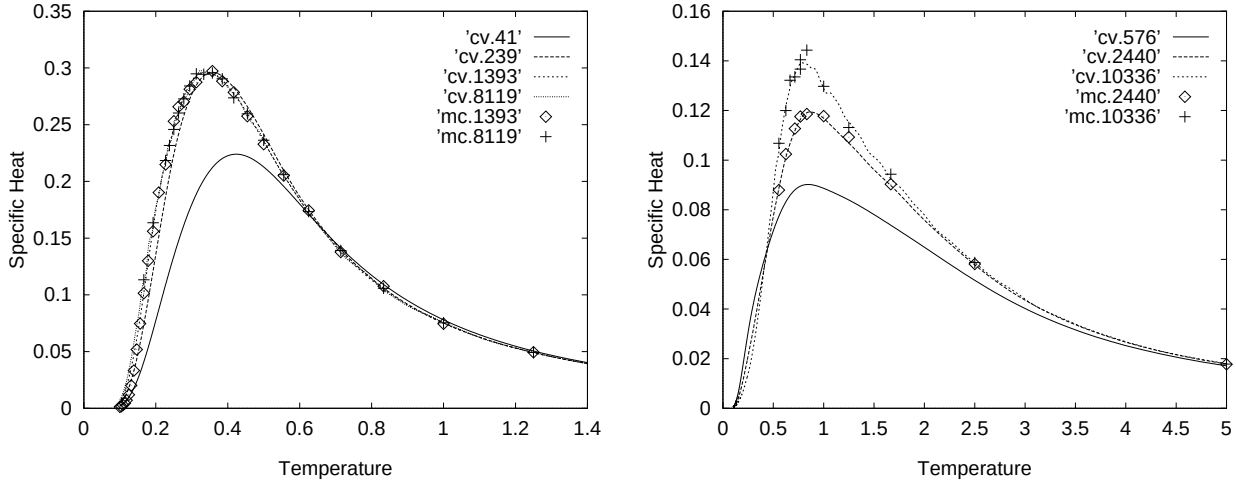

Fig. 2. Specific heat as a function of temperature, for different sizes of the octagonal (left) and the icosahedral tiling (right). Curves are from entropic sampling simulations, whereas points are from direct MC simulations.

In Fig. 2, the specific heat for different system sizes is shown. The curves are computed from $S(E)$, which was determined by entropic sampling. With only moderate computational effort, remarkably smooth specific heat curves could be obtained. Only for the

largest samples and near the maximum the curves are somewhat noisy. For many temperatures the specific heat has been determined also in direct MC simulations. These specific heat values are perfectly compatible with the entropic sampling results. It is most remarkable that in the octagonal case the specific heat per vertex converges very rapidly. Even the result for the 239-approximant is already very close to the limit. On the other hand, in the icosahedral case the specific heat seams to diverge slowly, at the same temperature where the diffusion constant shows a sudden change in slope. Moreover, we have confirmed the result of Dotera and Steinhardt[6] that the susceptibility associated with the sheet magnetization[6] rapidly diverges with system size, again at the very same temperature. These three features are clear indications of a phase transition at this temperature.

From the entropic sampling results the entropy per vertex at infinite temperature, σ_0, can easily be determined: it is simply the maximum of $S(E)/N$. With finite size scaling we obtain in the infinite system limit a value of $\sigma_0 = 0.432(1)$ for the octagonal case, and a value of $\sigma_0 = 0.2470(5)$ for the icosahedral case. These values are compatible with previous results[15,10,16], although in the octagonal case a small discrepancy remains[15]

4. Conclusions

Direct MC simulations and entropic sampling simulations for octagonal and icosahedral random tiling systems have been presented. In the icosahedral case, all our results consistently suggest the existence of a phason unlocking transition at a unique, finite temperature. In particular, the specific heat and the susceptibility of the sheet magnetization both diverge at the same temperature where the phasonic diffusion constant shows a sudden change of slope. In the octagonal case, on the other hand, there is no sign of a phase transition. More detailed results will be presented elsewhere.

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