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LETTER TO THE EDITOR

Walks on the Penrose lattice

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Abstract. We performed extensive Monte Carlo simulations for different types of walks (random walks, ideal chains and self-avoiding walks) on the Penrose quasilattice. The critical exponent ν—for each process—is found to be the same as for periodic two-dimensional lattices, thus universality seems to hold also for the Penrose tiling.

The discovery of quasicrystals [1] has started intensive theoretical activity to understand their structure and to generalize concepts developed for periodic lattices (for a recent review see [2]). Quasilattices have local symmetries [3] (five-fold rotations, icosahedral point group etc.) which are forbidden in regular, periodic lattices. Furthermore they exhibit strong long-range correlations, which are absent in other types of irregular systems (liquids, glasses). In spite of some similarities quasilattices are also essentially different from other types of lattices with long-range correlations (fractals, directed lattices) or from problems with randomness or dilution.

One interesting question concerning quasicrystals is how the irregular structure of the lattice influences the form of critical correlations, whether they keep their universal form observed on different, periodic lattices with the same spatial dimension. Until now studies of this problem have been mainly restricted to lattices with one-dimensional aperiodicity. Exact results are available for the quantum mechanical phase transition of the one-dimensional transverse Ising model on the Fibonacci lattice and on some other aperiodic lattices. For a class of lattices (Fibonacci and related sequences) a phase transition with universal, Ising type critical exponents is observed [4–7], while for some hierarhical sequences the transition is washed out by the presence of too high barriers [8]. The observations for the one-dimensional XY model are essentially the same [8], and one expects also the same type of properties of the thermodynamical phase transition of two-dimensional layered Ising systems where the aperiodicity is restricted only to one direction [9].

For two-dimensional pentagonal quasiperiodic lattices (such as the Penrose lattice [10]) the known results are scarce. Godrèche *et al* [11] have studied the Ising model on the Penrose lattice (PL) by means of the Migdal–Kadanoff scheme, and

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found a phase transition similar to the usual one encountered on periodic lattices. Monte Carlo simulations on the Ising model [12, 13] and on the percolation problem [14] have given numerical evidence for universality on the PL. On the other hand Korepin [15] has constructed exactly solvable vertex models with appropriate rules on the PL.

In the present letter we consider another cooperative process on the PL: we investigate the asymptotic behaviour of different types of walks, such as random walks (RW), ideal chains (IC) and self-avoiding walks (SAW). We note that different types of walks on irregular lattices (fractals [16], random systems [17], percolation clusters [18] etc) have become subject of intensive investigations recently. A RW describes the diffusion process through the lattice, while IC and SAW are considered to be idealised and 'realistic' models, respectively, of a single polymer chain in a good solvent [19]. Furthermore, the SAW being the $n = 0$ limit of the $O(n)$ model [19], this process makes a connection with magnetic phase transitions on the PL. Since SAW usually can be studied with higher accuracy comparing to other magnetic systems, we hope to get clearer evidence for the existence/non-existence of universality on the PL.

In this letter we investigate the asymptotic behaviour of the square of the end-to-end distance

$$\langle R_N^2 \rangle = AN^{2\nu} \tag{1}$$

for walks with N steps. We use a Monte Carlo (MC) simulation method (for a review see [20]), in which the underlying lattice for each walk is generated separately, by randomly choosing the angle of the projection in the projection method of de Bruijn [21]. Thus each walk has a different starting point and local environment, such that the averaging with respect to the starting points of the walks has automatically been performed. We note that quasilattices with higher local symmetries were excluded, such as the so-called singular and exceptionally singular lattices [21].

The Penrose tiling we consider is built up of two rhombuses with the same edge a, and has an inhomogeneous coordination number with possible values $q_i = 3, 4, 5, 6$ and 7; its value on average is four. Thus the length of a step is always the same; however the possible orientations of the step are determined by the local environment of the given point. In the following, first results on the two relatively simpler processes (RW and IC) are presented, while properties of the SAW are discussed afterwards.

The possible configurations for RW and IC are the same and—for regular lattices—they are even equivalent, since they have equal statistical weights in this case, while for lattices with inhomogeneous coordination number the two processes have different statistical weights. For an IC the statistical weight of all chains with the same length is the same; however for the RW it is proportional to the inverse product of the coordination numbers of the visited sites: $\prod_i q_i^{-1}$. We note that in the case of fractals there is a controversy over whether the IC and RW belong to the same universality class or not [16].

To address this problem in the case of the PL we studied the average square end-to-end distance for walks up to a length of $N = 1000$. For each length the average was taken over $M = 40\,000$ generated walks. Results for IC and RW are drawn in figure 1 on a log–log scale. One can see that the resulting points are lying on a straight line with equal slope in both cases, such that the slopes—within the error of the estimation—correspond to the value on regular lattices: $2\nu_{\rm RW} = 2\nu_{\rm IC} = 1.0 \pm 0.005$.

Different types of correlations between successive steps of the two processes, however, result in different amplitudes in equation (1). This quantity can generally

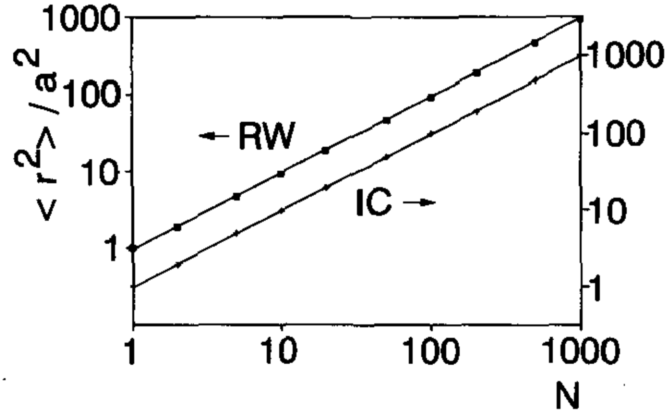

Figure 1. Average square end-to-end distance as a function of the length of the walk for IC and RW on a log–log scale. The straight lines through the data have slope 1. (Note the scales on the vertical axes are shifted for the two processes.)

be written as $A = a^2(1 - f)$, where a is the lattice spacing and f is a correlation factor. On periodic lattices, where the successive steps are uncorrelated, $f = 0$. On the PL we found weak correlations for IC—$f_{\mathrm{IC}} = 0.015 \pm 0.005$—while for RW the observed correlations are stronger: $f_{\mathrm{RW}} = 0.060 \pm 0.005$. This behaviour is possibly connected to the fact, that on the PL there is relatively higher probability for a random walker to go backwards than to go ahead compared with the probabilities on a regular lattice.

Now we turn to discuss results of SAW. In this case we generated $M = 100\,000$ walks up to a length of $N = 200$ by the extended biased sampling method [20]. A plot of the average square end-to-end distance versus the number of steps on a log–log scale on figure 2 reveals that the points in average are lying on a straight line, the slope of which is close to the regular lattice value $2\nu_{\mathrm{SAW}} = 1.5$ [22]. However, the relative noise of the obtained results is increasing with the order, therefore one needs sophisticated methods for an accurate determination of the critical exponent ν.

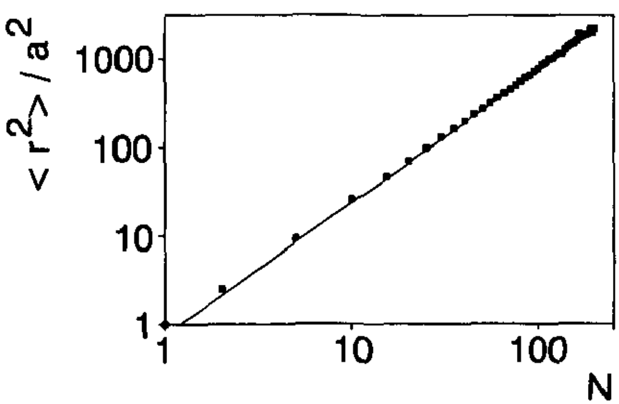

Figure 2. Average square end-to-end distance as a function of the length of the walk for SAW on a log–log scale. The straight line through the data has a slope 1.5.

The possible use of different methods of series analysis [23] for series with stochastic coefficients has recently been critically tested by Dekeyser *et al* [24]. It was observed that after a smoothing transformation—corresponding to a partial summation of the series—even the simple ratio method gives reasonable estimates, sometimes better than other standard methods of series analysis (Padé approximants, differential approximants).

Therefore our results were first analysed by the ratio method after $s = 1,2,3,4$ and 5 partial summations. Estimates for the critical exponent 2ν as a function of $1/N$ are drawn in figure 3(*a*), while the statistical error of the estimates (calculated by dividing the 100 000 walks into 100 equal groups) is presented in figure 3(*b*). As expected, the statistical error of the estimates decreases with s, while at the same time the strength of the confluent singularity—demonstrated by the curvature of the estimates in figure 3(*a*)—increases. One may minimize the two sources of errors around $s = 3 - 5$, such that one obtains:

$$2\nu_{\text{SAW}} = 1.48 \pm 0.04 \tag{2}$$

while the amplitude in equation (1) is estimated as $A/a^2 = 0.79(1)$. We analysed the series also by the dlog Padé method, in which case the smoothing is ineffective [24]. By this method we obtained $2\nu_{\text{SAW}} = 1.53 \pm 0.05$, which is in agreement with the earlier estimate in equation (2).

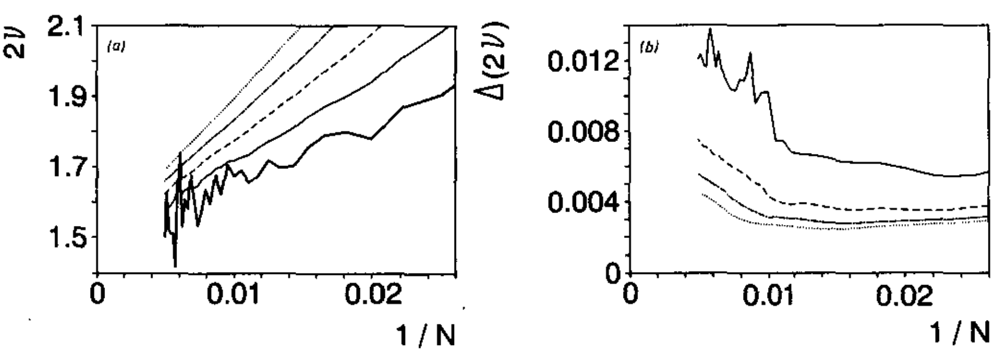

Figure 3. Average (*a*) and statistical error (*b*) for 2ν of SAW by the ratio method using various values of smoothing ($s = 1$ ——, $s = 2$ ——, $s = 3$ - - - -, $s = 4$ — · —, $s = 5$ · · · · · ·).

At this point we comment on the possible sources of errors in the estimation of ν_{SAW}. The statistical error of the MC-data is about 1–2% and slowly increasing with the length of the walk. By a partial summation—according to figure 3(*b*)—the stochasticity of the results can be considerably decreased, but at the same time the strength of the confluent singularity, the other important error of estimation is increasing. Finally, an extra source of error in the present case comparing with standard MC simulations is the inhomogeneity of the underlying Penrose lattice. The uncertainty coming from this effect is estimated to a few thousends on the basis of the accuracy of the statistical weigths of the different vertices of the Penrose lattice obtained in the simulation.

In conclusion with our MC simulation we have accurately demonstrated the universal behaviour of the SAW on the Penrose quasilattice. Our investigation—together with others made on similar magnetic models [12–14]—supports the general conjecture that magnetic phase transitions exhibit universal critical behaviour on the two-dimensional Penrose lattice.

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