

Self-avoiding walks on a Penrose lattice

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1986 J. Phys. A: Math. Gen. 19 L405

(<http://iopscience.iop.org/0305-4470/19/7/008>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 31/05/2010 at 19:30

Please note that [terms and conditions apply](#).

LETTER TO THE EDITOR

Self-avoiding walks on a Penrose lattice

L Schimmele and M Föhnle

Institut für Physik, Max-Planck-Institut für Metallforschung, 7000 Stuttgart 80, West Germany

Received 6 February 1986

Abstract. Direct real space renormalisation group procedures are constructed to calculate the self-avoiding walk exponent ν on a two-dimensional Penrose lattice. This lattice is neither translationally invariant nor hierarchical, but still self-similar, and therefore calls for a renormalisation group treatment. Within the accuracy of a small cell calculation the obtained values of ν are consistent with the universal value of ν in two dimensions which is believed to be close to $\nu = 0.75$.

Recently the existence of metallic phases has been reported (Shechtman *et al* 1984, Urban *et al* 1985) which exhibit electron diffraction spots of remarkable sharpness although they do not have translational invariance. The experimental findings can be interpreted if one assumes that the atoms are situated at the lattice points of a quasicrystal. The quasicrystals are more ordered than the amorphous structures. Although they have no translational order, they still have perfect long-range bond orientational order along each lattice vector direction (Penrose 1974, Gardner 1977, Mackay 1982, Kramer 1982, Zia and Dallas 1985, Levine and Steinhardt 1984). On the other hand they are considerably less ordered than crystals. For example, if we introduce 'bonds' between neighbouring atoms the number of bonds meeting at a lattice point varies from lattice point to lattice point with no obvious regularity.

There has already been considerable interest for many years in the investigation of phase transitions and critical phenomena (e.g. magnetic phase transitions) for systems with structural disorder (Stinchcombe 1983, Föhnle 1985). The question of how the critical exponents and the non-universal properties at the critical temperature are influenced by the kind and degree of disorder is still not settled. It would therefore be useful to study critical phenomena when the underlying structure is of the quasicrystalline type which is intermediate between a crystalline and an amorphous phase. In addition the quasicrystalline lattices seem to be especially suited to serve as model systems for theoretical investigations since they are, like crystalline lattices, self-similar in the sense that one can eliminate a subset of the lattice points and obtain another quasicrystalline lattice with nearest-neighbour distances increased by a constant factor (Gardner 1977, Levin and Steinhardt 1984). This property offers the possibility of using real space renormalisation group (RSRG) methods to describe critical properties on such lattices. To learn about the problems inherent in the construction of a real space renormalisation procedure on a lattice which is neither translationally invariant nor hierarchical we study as an example direct renormalisation group procedures for self-avoiding random walks (SAW) on a quasicrystalline lattice.)

For our investigations we have chosen a special two-dimensional quasicrystalline lattice, which is formed by the vertices of a so-called Penrose tiling (Penrose 1974, Gardner 1977). The tiling is made up of two shapes, called 'kites' and 'darts' (see figure 1) with q as many kites as darts in an infinite tiling, where $q = (1 + \sqrt{5})/2$ is the golden ratio. If we consider the edges of the kites and darts as being bonds, two bond lengths appear which again are in the proportion q . To perform a direct RSRG procedure for SAW we first construct a decimated lattice by partitioning the original lattice into cells. These cells which again have the form of kites and darts both cover the lattice and lead again to a Penrose lattice when the original lattice points which are not corners of the cells are eliminated. The decimated lattice differs from the original one merely by a rescaling of all lengths by a scale factor b .

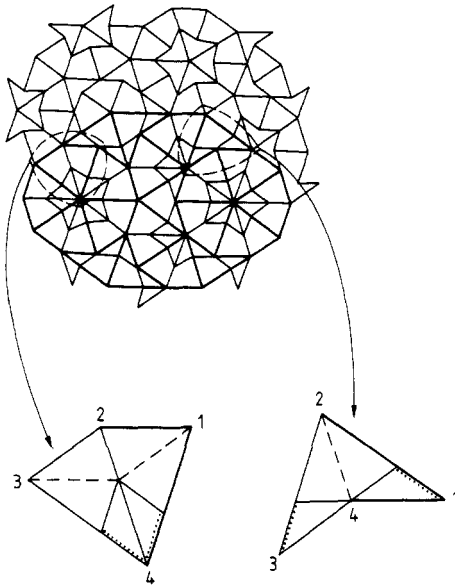


Figure 1. Penrose tiling and cell reconstruction of the lattice.

A self-similar reconstruction of the lattice, where the lengths are rescaled by a factor q , is indicated by the bold lines in figure 1 (see also Gardner 1977)†. An enlargement of the resulting cells is shown in the lower part of figure 1. The full internal lines as well as those parts of the border lines of the cell which are not accompanied by a dotted line are the bonds of the original lattice (for the meaning of the broken lines see below). In addition to the small cell reconstruction with a rescaling parameter $b = q$, we also use a subdivision into larger cells. This can be achieved by simply repeating the rescaling process with the lattice obtained after the first steps. This leads to a rescaling parameter $b = q^2$ with respect to the original lattice.

We then proceed further by using the methods developed for translationally invariant lattices, which have been described previously by several authors (Shapiro

† The rescaled lattice is indeed one of the uncountable number of infinite Penrose tilings, but usually it is not the same pattern as the original one. Since, however, every finite region in any Penrose pattern is contained somewhere inside every other pattern (Gardner 1977) all Penrose patterns can be regarded as equivalent for our purposes.

1978, de Queiroz and Chaves 1980, Redner and Reynolds 1981, Family 1980, Stanley *et al* 1982, Napiorkowski *et al* 1979, Malakis 1980). Similar methods have also been applied for SAW on hierarchical fractal lattices (Rammal *et al* 1984, Ben-Avraham and Havlin 1984). The quantity of interest is the root mean square end-to-end distance of SAW of N steps (canonical ensemble), which diverges for $N \rightarrow \infty$ as N^ν , $\langle R^2 \rangle_N^{1/2} \sim N^\nu$. In order to study the SAW problem as a critical phenomenon, a grand canonical ensemble is introduced, where averages over all possible walks of arbitrary many steps are considered (Shapiro 1978). To define the grand canonical averages, a weight (fugacity) K is attributed to each step of the SAW respectively, i.e. the SAW is described by a set $[K]$ of weights. The steps are along the short and long bonds of the Penrose lattice. Because we consider random SAW, we assume that the weights for those steps on the original lattice are equivalent. Possibly additional steps may be considered corresponding to additional bonds created by the decimation transformation. For example, the 'diagonal' bond 2-4 in the enlarged kite of figure 1 is created by a walk along the bonds of the original Penrose lattice, but there is no such diagonal bond in the kites of the original lattice. We can proceed by either discarding these additional bonds in the enlarged lattice, or by having introduced them already in the original lattice (broken lines in figure 1); see below. Because we do not allow a step along these additional bonds on the original lattice, we attribute to them a zero weight in the original lattice.

By comparing walks and their corresponding weights on the original and the decimated lattice recursion relations (renormalisation transformation) $\{K\} \rightarrow \{K'\}$ for the weights are constructed. The exponent ν is given by (see the articles quoted above)

$$\nu = \ln b / \ln \lambda_1 \quad (1)$$

where λ_1 is the relevant eigenvalue $\lambda_1 > 1$ of the renormalisation transformation linearised at the fixed point $\{K^*\}$ of the transformation.

Formulated in this way, the SAW problem becomes 'critical': when the value K for the weight of the allowed steps in the original lattice approaches a critical value $K_c = 1/\bar{z}$ from below (\bar{z} is an effective coordination number; see e.g. McKenzie (1976) or Sykes *et al* (1972)), then the root mean square end-to-end distance ξ of the SAW in the grand canonical ensemble diverges as $(K_c - K)^{-\nu}$, where the quantity ν is identical to that appearing in $\langle R^2 \rangle_N^{1/2} \sim N^\nu$.

We use a two-parameter and in addition a four-parameter RSRG procedure. In the two-parameter case we renormalise the fugacities K_s for a short bond and L_l for a long bond ($K_s = K_l$ on the original lattice). In the four-parameter case in addition a fugacity D_k for a diagonal bond in the kite (broken lines in the lower part of figure 1) and a fugacity D_d for a diagonal bond in the dart (dotted lines in figure 1) are introduced ($D_k = D_d = 0$ in the original lattice). The new bonds in the decimated lattice are attributed to the cells as indicated in figure 1 by the heavy border lines, i.e. the bonds 1-2 and 1-4 are attributed to the cells shown in the lower part of figure 1, whereas the bonds 2-3 and 3-4 are attributed to neighbouring cells. In this way each bond in the Penrose lattice is attributed to one and only one cell.

To construct recursion relations for the fugacities we proceed in close analogy to de Queiroz and Chaves (1980), Redner and Reynolds (1981) and Family (1980) (see also Stanley *et al* 1982) who used a 'corner rule' weight function. Thereby a specific corner of the cell is chosen to be the starting point of a SAW, and all walks leaving the cell via a certain edge of the cell rescale to a specific bond on the decimated lattice. Two complications occur compared to translationally invariant lattices. First, there

are now two cells and we obtain different recursion relations for the fugacities depending on whether we have constructed them for the kite or the dart. We therefore average the recursion relations obtained for the two shapes according to their relative occurrence. This procedure seems to be reasonable because the attribution of a bond in the lattice to a cell is not unique and because there should be an averaging anyway when the decimation transformation is repeatedly applied. It is, however, by no means rigorous. The second complication is that the two endpoints of a bond are inequivalent because they have different surroundings. We therefore construct two recursion relations for the fugacities associated with a certain bond in a certain cell by taking either one or the other endpoint of the rescaled bond as the fixed starting point for SAW in the sense of the corner rule. Again the two contributions must be averaged.

To be specific, in the two-parameter case there are two contributions from the *kite* that rescale to a *long bond*:

(α) all SAW within the cell that start at corner 1 and leave the cell by way of the edge 3-4 \dagger ,

(β) all SAW that start at corner 4 and leave the cell by way of edge 1-2;
secondly there are two contributions from the *dart*, i.e.

(α) SAW that start at corner 1 and leave the cell by way of edge 2-3,

(β) SAW that start at corner 2 and leave the cell by way of edge 1-4.

Thereby each step along a short or a long bond in the original lattice introduces a factor K_s or K_l , respectively. Similarly for the *short bond* we have two contributions from the *kite*

(α) SAW starting at 1 and leaving the cell by way of edge 2-3,

(β) SAW starting at 2 and leaving the cell by way of edge 1-4

and two contributions from the *dart*, i.e.

(α) SAW going from 1 to edge 3-4,

(β) SAW going from 4 to edge 1-2.

The rules given above are still not completely sufficient to determine the recursion relations. This is because some of the cell walks could be attributed according to these rules to a long bond as well as to a short bond. To avoid double counting we therefore have introduced a parameter α . If $\alpha = 0$ all these doubtful walks are attributed to a long bond, whereas for $\alpha = 1$ they are chosen to rescale to a short bond.

The same rules apply also to the four-parameter case except that the walks starting at corner 4 and ending at 2 or vice versa are chosen now to rescale to a diagonal bond in the kite (D_k) or in the dart (D_d), respectively. In this case the diagonal bonds must of course be taken into account from the outset and therefore additional cell walks compared to the two-parameter case are possible. As before a parameter α has to be introduced to avoid double counting, although this problem is less severe in this case. The rules given above are of course applicable to arbitrary cell sizes.

We have treated the two-parameter RSRG method for two cell sizes $b = q$ and $b = q^2$; the four-parameter RSRG method, however, has only been treated for the small cell $b = q$. We give here the resulting recursion relations only for the two-parameter case and for $b = q$. We obtain

$$K_l' = p_k \{ p_l^{k-1} [2(K_l K_s^2 + K_l^2 K_s)] + p_l^{k-4} [2K_l^2 K_s + (1 - \alpha)(K_l K_s + K_l^3 K_s)] \} \\ + p_d \{ p_l^{d-1} (K_l^2 K_s + K_l K_s) + p_l^{d-2} [K_l^2 K_s + (1 - \alpha) K_l K_s] \} \quad (2a)$$

\dagger Steps in the original lattice along the edges 1-2 and 1-4 are counted to be within the cell whereas steps along the edges 2-3 or 3-4 are not allowed because they are attributed to neighbouring cells.

$$K'_s = p_k \{ p_s^{k,1} (K_1 + K_1 K_s^2) + p_s^{k,2} [K_1 + K_1 K_s^2 + K_s^2 + \alpha (K_1 K_s + K_1^3 K_s)] \} + p_d [p_s^{d,1} K_1 + p_s^{d,4} (K_1 + K_s + \alpha K_1 K_s)]. \tag{2b}$$

In (2) the contributions from kite and dart to the recursion relations are weighted by p_k and p_d , where $p_k/p_d = q$ and $p_k = p_d = 1$. The weights $p_{l(s)}^{k(d),i}$ used to calculate the averages over the two starting points i ($i = 1, 4$ or $1, 2$) for a long (l) or short (s) bond in the kite (k) or dart (d) have been chosen according to an *effective* number of directions in the rescaled lattice from which corner i can be approached (the bond for which the recursion relation is constructed has to be excluded in calculating this number)†. Explicitly these quantities which have a weak dependence on the weights are given by

$$p_{l(s)}^{k(s),i} = \frac{x_{l(s)}^{k(d),i}}{x_{l(s)}^{k(d),i} + x_{l(s)}^{k(d),j}} \tag{3a}$$

(i, j are the two endpoints of a bond), with

$$x_1^{k(d),i} = \sum_{\alpha} p_{y_{\alpha}, z_{\alpha}}^{k(d),i} [y_{\alpha} K_s + (z_{\alpha} - 1) K_l] \tag{3b}$$

$$x_s^{k(d),i} = \sum_{\alpha} p_{y_{\alpha}, z_{\alpha}}^{k(d),i} [(y_{\alpha} - 1) K_s + z_{\alpha} K_l]$$

for the two-parameter case, where $p_{y_{\alpha}, z_{\alpha}}^{k(d),i}$ is the probability that y_{α} short and z_{α} long bonds meet at the corner i of the kite (or dart). The probabilities $p_{y_{\alpha}, z_{\alpha}}^{k(d),i}$ for the different coordination configurations α have been determined by simply counting their relative occurrence on a finite Penrose tiling of several hundred lattice points. The weights in the case of the four-parameter RSRG are determined in the same way. The only difference is the inclusion of the diagonal bonds in the calculation of the $x_{l(s)}^{k(d),i}$.

Our results are summarised in table 1. The critical fugacity K_c is determined as the intersection of the critical surface connected to the fixed point K_1^*, K_s^* ($K_1^*, K_s^*, D_k^*, D_d^*$) with the axis $K_1 = K_s$ ($K_1 = K_s, D_k = D_d = 0$).

The spread in the numerical values for ν and K_c obtained for the two cell sizes and methods are comparable to that which one obtains from small cell renormalisation group methods for SAW, e.g. on a square lattice (Redner and Reynolds 1981, Stanley

Table 1. The results for the fixed point of the renormalisation group transformation, for ν and the critical fugacity K_c for the two-parameter and the four-parameter case and two cell sizes $b = q$ and $b = q^2$.

	α	K_1^*	K_s^*	D_k^*	D_d^*	ν	K_c
Small cell, 2 parameters	0	0.317	0.620			0.691	0.432
	1	0.237	0.880			0.636	0.476
Large cell, 2 parameters	0	0.368	0.659			0.726	0.475
	1	0.301	0.851			0.704	0.495
Small cell, 4 parameters	0	0.179	0.437	0.141	0.227	0.716	0.385
	1	0.171	0.459	0.146	0.231	0.712	0.388

† We also used equal weights for the contributions from the two bond endpoints. The resulting values of ν and the critical fugacity are not substantially changed thereby.

et al 1982, Malakis 1980). In addition the values for ν are as close to the conjectured universal value of $\nu = 0.75$ for two dimensions as can be expected for such small cell renormalisation group methods. Likewise the values for the critical fugacities are in reasonable agreement with the result expected for a lattice with an average coordination number of 4. In conclusion, it appears that position space renormalisation group procedures for SAW on quasicrystalline lattices can be constructed which give numerical estimates for ν and K_c which are of the same accuracy as can be achieved by these methods for SAW on translationally invariant lattices.

It can be hoped therefore that this desirable property can be carried over to position space renormalisation group treatments of other critical systems (e.g. the spin system) on quasicrystalline lattices.

References

- Ben-Avraham D and Havlin S 1984 *Phys. Rev. A* **29** 2309
 de Queiroz S L A and Chaves C M 1980 *Z. Phys. B* **40** 99
 Fähnle M 1985 *J. Phys. C: Solid State Phys.* **18** 181
 Family F 1980 *J. Phys. A: Math. Gen.* **13** L325
 Gardner M 1977 *Sci. Am.* **236** 110
 Kramer P 1982 *Acta Crystallogr. A* **38** 257
 Levine D and Steinhardt P J 1984 *Phys. Rev. Lett.* **53** 2477
 Malakis A 1980 *Physica* **104A** 427
 MacKay A L 1982 *Physica* **114A** 609
 McKenzie D S 1976 *Phys. Rep.* **27C** 35
 Napiorkowski M, Hauge E M and Hemmer P C 1979 *Phys. Lett.* **72A** 193
 Penrose R 1974 *Bull. Inst. Math. Appl.* **10** 266
 Rammal R, Toulouse G and Vannimenus J 1984 *J. Physique* **45** 389
 Redner S and Reynolds P J 1981 *J. Phys. A: Math. Gen.* **14** 2679
 Shapiro B 1978 *J. Phys. C: Solid State Phys.* **11** 2829
 Shechtman D, Blech I, Gratias D and Cahn J W 1984 *Phys. Rev. Lett.* **53** 1951
 Sykes M F, Guttman A J, Watts M G and Roberts P D 1972 *J. Phys. A: Gen. Phys.* **5** 653
 Stanley H E, Reynolds P J, Redner S and Family F 1982 in *Topics in Current Physics* vol 30, ed T W Burkhardt and J M L van Leeuwen (Berlin: Springer)
 Stinchcombe R B 1983 in *Phase Transitions and Critical Phenomena* vol 7, ed C Domb and J L Lebowitz (New York: Academic)
 Urban K, Moser N and Kronmüller H 1985 *Phys. Status Solidi a* **91** 411
 Zia R K P and Dallas W J 1985 *J. Phys. A: Math. Gen.* **18** L341