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HULL-GENERATING WALKS

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A hull-generating walk (HGW) is a type of kinetic random walk that generates the hull or perimeter of a percolation cluster, and thus has a fractal dimension of 1.75. Some examples of HGWs for site and bond percolation on a square lattice are described.

1. Introduction

A percolation cluster is a collection of occupied sites connected to each other by paths along nearest-neighbor pairs of sites, and surrounded inside and outside by vacant sites. (For bond percolation, this definition holds by reformulating the problem as site percolation on the covering lattice.) A closed circuit along the boundary of adjacent occupied and vacant sites is called a perimeter or the hull of the cluster. The term "hull" was first used by Mandelbrot [1] to describe the island of points enclosed by the external boundary of a cluster, but it has been generalized to refer to the boundary as well, and that meaning will be used here. One can have both external hulls, in which the occupied sites are on the inside and the vacant sites on the outside, and internal hulls, in which the occupied sites are on the outside and the vacant sites are on the inside.

Mandelbrot's influence on the study of percolation hulls goes far beyond the coining of the name, of course. The invention of fractals and the resulting interest in the study of growth processes and geometric properties has stimulated a great deal of work on percolation clusters and their hulls, which are among the simplest and most elegant of random fractals, and which result from many growth and epidemic models (see for example refs. [2–4]). While perimeters of percolation clusters have been studied for many years in the context of cluster statistics [5,6] or boundary properties [7], the introduction of fractals has led to substantial advances in the understanding of their properties.

Indeed, the fractal nature turned out to be the key to the discovery of expressions for all the critical exponents of percolation hulls. In their investigation of the scaling of percolation-gradient frontiers (hulls), Sapoval, Rosso and Gouyet [8] were led to the conjecture that the fractal dimension of the hull is exactly

$$D = 1 + 1/\nu = 1.75\,, \tag{1}$$

where $\nu = 4/3$ is the correlation-length exponent. This conjecture is supported by numerical studies [8–11]. Then, by scaling arguments, (1) was shown [10–12] to give simple values for the other critical exponents, such as $\gamma' = 2$ (for the mean hull-size exponent) and $\beta' = 1/3$. Finally, Saleur and Duplantier [13] derived exact expressions for these exponents from first principles, thus verifying (1) by scaling. Theoretical arguments for (1) have also been given by Bunde and Gouyet [14]. This work has shown that percolation hulls have simpler critical exponents than the clusters themselves.

Many types of kinetic random walks in two dimensions have been found to generate percolation-cluster hulls – often quite unexpectedly. What makes a given path a percolation-cluster hull is that it is generated with the same probability (weight) as it would be found on a lattice that has been randomly populated with occupied and vacant sites. In this paper I am concerned with these walks, which I call hull-generating walks (HGWs).

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In general, HGWs have the following properties:

(1) They are generated on a lattice that starts out completely blank (untested), except perhaps for one or two sites to start the walk.

(2) They leave a path of both occupied and vacant sites, or some equivalent representation of a cluster boundary.

(3) Their growth process is local (depending only upon a local set of sites) and kinetic (they grow step by step).

(4) They eventually close to form a completed loop (on an infinite lattice).

(5) Once they close, they are no longer kinetic in nature, meaning that their probability of growing (weight) is no longer dependent upon the starting point.

(6) When closed, their weight is that of the corresponding perimeter of a percolation cluster. If the occupied sites are on the outside, then the path represents an external perimeter, while if the occupied sites are in the inside then the path represents an internal perimeter.

(7) Their fractal dimension is 1.75.

HGWs were first introduced by Ziff, Cummings, and Stell [15,16] for the specific purpose of generating percolation cluster perimeters. They were independently found to result from quite different considerations. Kremer and Lyklema [17] devised an indefinitely growing self-avoiding walk (IGSAW) on a square lattice which satisfies properties (1)–(3) above, but not the rest because the walks never close. However, Weinrib and Trugman [12] studied a similar walk on a honeycomb lattice, which they call the smart kinetic walk (SKW), and found that it is precisely a HGW for site percolation on the dual (triangular) lattice. Gunn and Ortuño [18] considered a random system of sites on a lattice that have the property of rotating the direction of a walk passing through them by given amounts, and found under certain circumstances that the paths are equivalent to a HGW for bond percolation on the square lattice. A similar walk was used by Grassberger [11]. Recently, Roux et al. [19] have introduced a step-by-step tiling process that is equivalent to the Gunn and Ortuño model and also to the representation by Saleur and Duplantier [13], and thus is equivalent to the bond-percolation HGW. These models will be described in more detail below.

HGWs are useful for finding the percolation threshold [10,20]: in fact using the gradient-probability method [20] they appear to be the most efficient Monte Carlo way to find p_c. HGWs allow one to generate the hull of the backbone of a percolation cluster [21], and also the "accessible perimeter" of Grossman and Aharony [22], as discussed below. Coniglio et al. [23] and later Duplantier and Saleur [24] and Bradley [25] have argued that the HGW is appropriate to represent a two-dimensional polymer chain at the θ or θ' point, and so these walks are more than just a mathematical curiosity but have physical significance as well.

In general, a HGW can be constructed for a given system by the following procedure [15]: First devise an algorithm to trace out the perimeter of an existing cluster. Then repeat the same algorithm on a blank (untested) lattice, with the modification that when the state of any site that is still untested is needed, that site is made "occupied" with probability p and "vacant" otherwise, and the algorithm is continued according to that decision. Moreover, the state of the site must be remembered so that if it is ever visited again it will be treated the same way. The perimeter produced by this walk has the same weight as the corresponding perimeter on a populated lattice, because, in random percolation, the state of a site (or bond) is assigned with statistical independence, and it is irrelevant whether the choise of the state is made beforehand or during the walk.

An interesting aspect of the HGW is the behavior when p is increased beyond p_c. For $p<p_c$, external hulls are more likely, while for $p>p_c$ the internal hulls are more likely [15]. However, the existence of the infinite cluster is not evident – there is no hull associated with it. The internal hulls that are produced when $p>p_c$ may be holes within the infinite cluster, or holes within a larger finite cluster. There is a natural symmetry for the behavior of the walks about p_c, which for site percolation on the triangular lattice and bond percolation on the square lattice is perfect because of the identity of matching lattices.

By considering different lattices and definitions of the perimeter, a great variety of HGWs can be constructed, all of which satisfy properties (1)–(7) above. Furthermore, even for the same system one can devise different walks that generate the perimeter. This will be illustrated by some examples of HGWs for site and bond percolation on a square lattice.

2. Site percolation on a square lattice

In fig. 1 a simple cluster of five occupied sites (shaded circles) and nine vacant sites (open circles) for site percolation on a square lattice is shown. First consider the walk that follows the occupied sites at the boundary, which is illustrated in fig. 1a. To follow that boundary, the walker moves from occupied site to occupied site, always keeping vacant sites to its right. The walker "looks" first to the right, then straight, then left, then back, where "straight" is the direction of the previous step. The HGW that results from this process follows the following rule on a initially untested lattice: If the site being looked at is

(1) occupied: the walker moves to it;

(2) vacant: the walker looks to the next site in counter-clockwise order;

(3) untested: the site is made "occupied" with

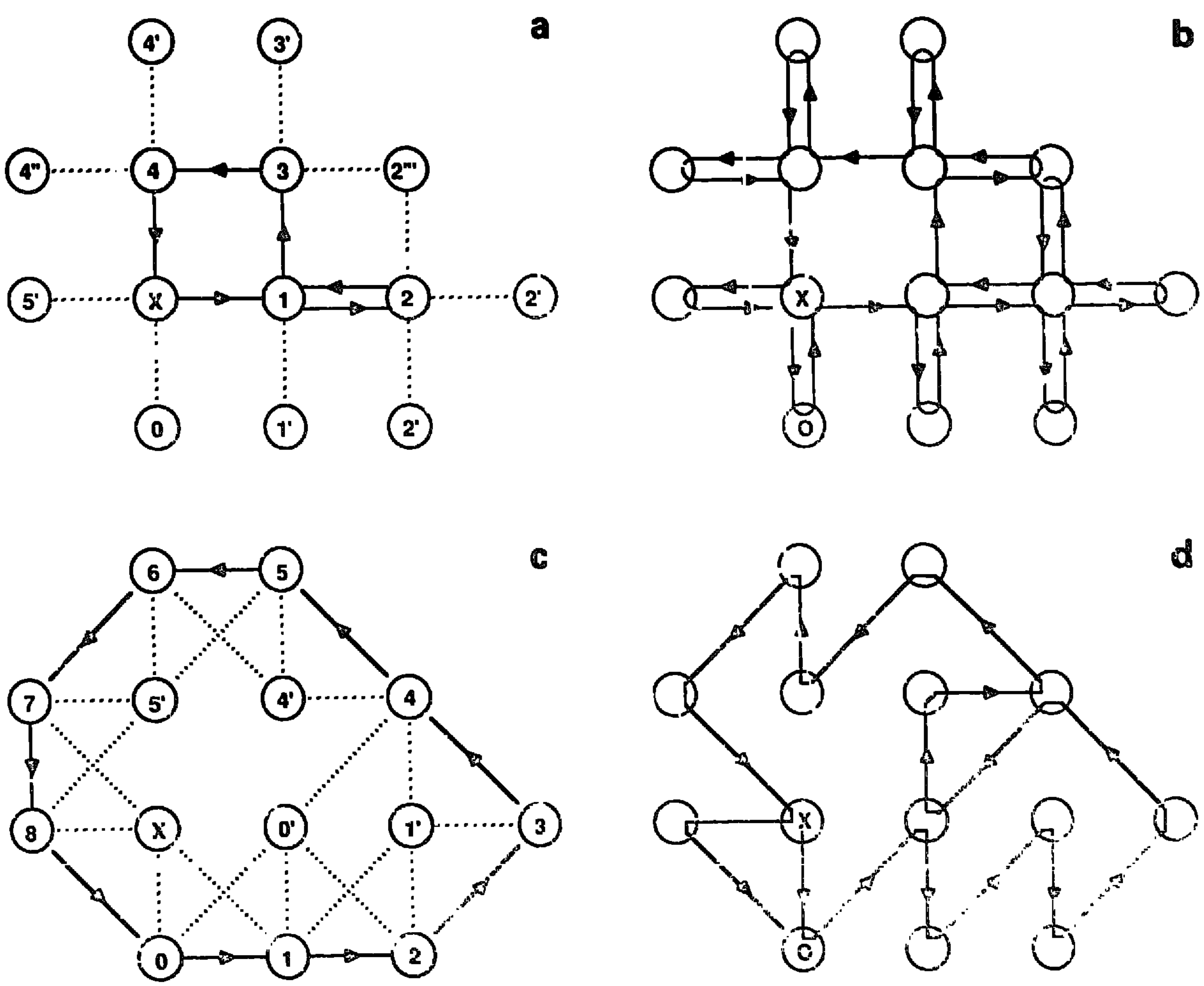

Fig. 1. Site percolation on a square lattice: (a) the walk that connects occupied sites (shaded circles) of the perimeter, (b) the equivalent "blind ant" walk, (c) the generic walk that moves along the vacant sites (open circles) of the perimeter, and (d) a new more efficient walk that goes along diagonals from vacant sites and vertical and horizontal lines from occupied sites.

probability p and (1) is followed, otherwise the site is made "vacant" and (2) is followed.

The walk is started by placing down the occupied–vacant site pair (marked X and O in fig. 1a), and finishes when the walker returns to X and attempts to go in the direction of the first step. Also in fig. 1a, the occupied sites are numbered according to the order in which they are created, and the vacant sites are labelled with a prime, double prime, etc., and a number corresponding to the occupied site where the walker was when the vacant site was created. Thus after the walker reaches occupied site 1, the vacant site 1′ is first created, before the occupied site 2 is created. Because of the three vacant sites created around 2, the walker must backtrack to site 1, which is allowed here. When the walker reaches occupied site 3, it first looks to the right and sees 2″, which was already made vacant before, and so goes on to site 3′ – and so on. This walk was simulated very extensively in refs. [10,15,20], where the scaling relations and (1) were verified, and the value of p_c (square) was found, all to high accuracy.

In this algorithm it is assumed that the walker is able to "look" at a neighboring site before deciding to move to it. In this case the walker is called a "myopic" ant [4]. If the walker does not have this ability (it is a "blind" ant), then it must move to every site in the perimeter, and the walk of fig. 1b results. Here a vacant site rotates the walk by π, while an occupied site rotates it by $-\pi/4$, and evidently this is a walk of the Gunn–Ortuño type.

The basic idea behind the walk of fig. 1b can be used to define a "generic" walk for any site-percolation problem: the vacant sites send the walker back ($\Delta\theta=\pi$) while an occupied site rotates the walk to the next direction of the lattice. (I arbitrarily use negative θ to define the next direction here.) A similar walk along the vacant sites can be made by going to the dual lattice and reversing the roles of the sites.

In fig. 1c the generic walk that joins the vacant sites of this same cluster is shown. The vacant sites satisfy the connectivity of the dual lattice, which in this case is the square lattice with nearest-neighbor and next-nearest-neighbor communication.

Inspection of figs. 1b and 1c shows that many of the steps are redundant in that a walker sometimes goes to a site that is guarranteed to be of a certain state by virtue of the walker's previous position. In fig. 1d a simpler, more efficient walk that visits both the occupied and vacant sites of a perimeter is shown. In this walk, the occupied sites rotate the walk to the first vertical or horizontal direction to the right, and the vacant sites rotate it to the first diagonal direction to the left. The angles of rotation are thus not fixed but either $\pm\pi/2$ or $\pm 3\pi/4$ depending upon the direction from which the site is approached. The asymmetry between the occupied and vacant sites reflects the different nature of these two sites on this lattice.

3. Bond percolation on a square lattice

A great variety of HGWs for bond percolation on a square lattice have been found, and I will briefly describe them here.

In fig. 2a a bond-percolation cluster with five occupied bonds (solid lines) and ten vacant bonds (shaded lines) is shown. The arrows follow a step-by-step path from bond center to bond center that traces out the boundary of this cluster.

In fig. 2b the same process is shown on the equivalent covering site-percolation lattice, where the sites are placed at the centers of the bonds and each site is connected to six other sites. The path of the connected arrows is precisely the walk of Gunn and Ortuño [18] in a system containing sites that rotate the walk by either $-\pi/2$ or $\pi/2$, corresponding to the occupied bonds and the vacant bonds, respectively. In contrast, the generic walk for this system is shown in fig. 2c, which is evidently more complicated. A generic walk can also be constructed that steps from vacant site to vacant site, analogous to fig. 1c. Notice that in fig. 2b the walker checks only the diagonals of the lattice.

Manna and Guttmann [26] have pointed out that the paths of connected arrows in fig. 2a or 2b are kinetic growth trails (KGTs) [27], also called growing self-avoiding trails (GSATs) [28], on the directed

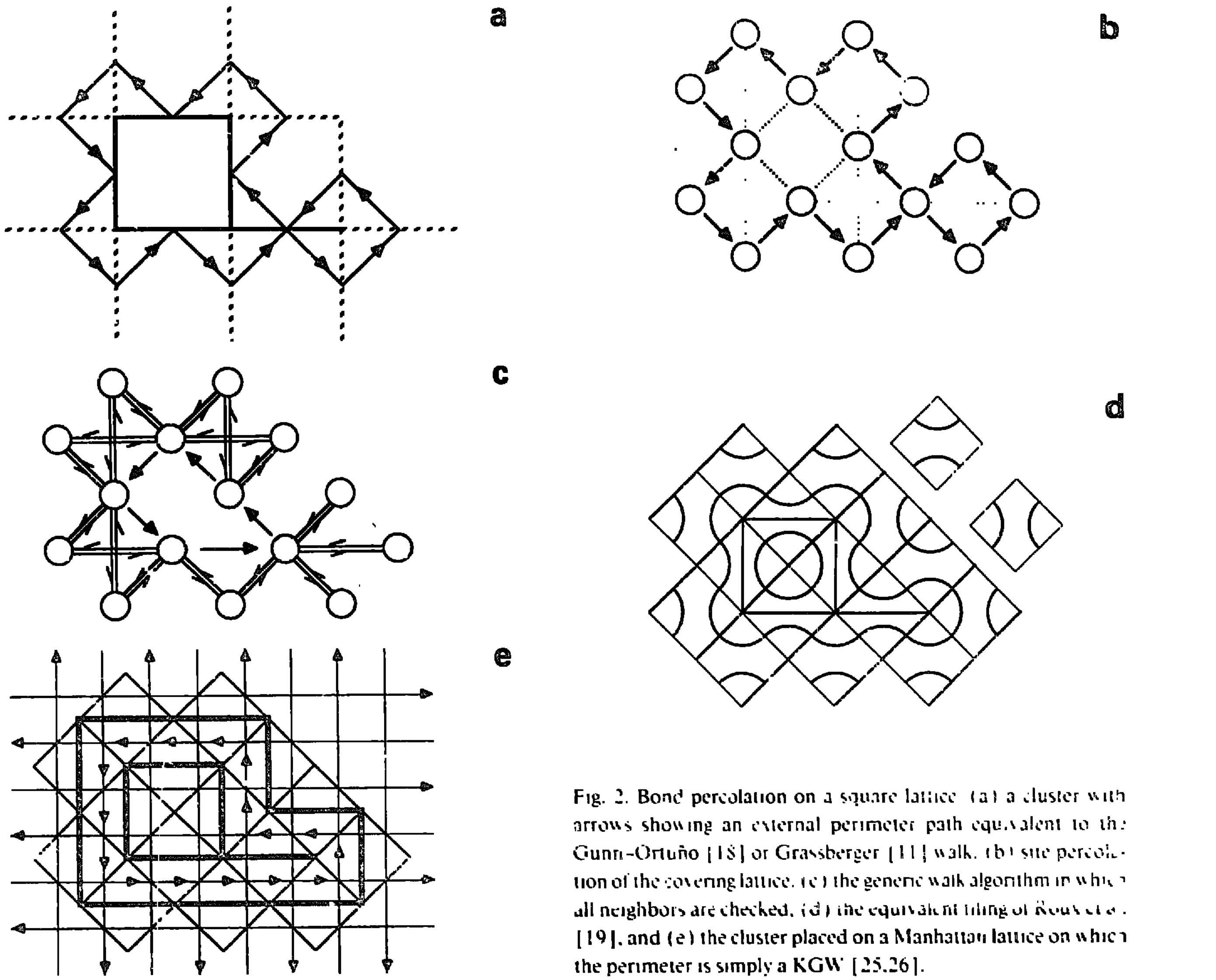

Fig. 2. Bond percolation on a square lattice: (a) a cluster with arrows showing an external perimeter path equivalent to the Gunn–Ortuño [18] or Grassberger [11] walk, (b) site percolation of the covering lattice, (c) the generic walk algorithm in which all neighbors are checked, (d) the equivalent tiling of Roux et al. [19], and (e) the cluster placed on a Manhattan lattice on which the perimeter is simply a KGW [25,26].

L-lattice, in which at each site there is a pair of arrows pointing in and a pair pointing out. A KGT is a kinetic walk on a lattice that can visit each site without restriction but each bond only once. On the L-lattice, the KGT is automatically a SKW because it never gets trapped except to close.

In fig. 2d the random tiling model of Roux et al. [19] is shown. In this model, the two tiles shown in the upper right-hand corner of that figure are randomly placed with equal probability on a square lattice (rotated by $\pi/2$ here) and connected paths are formed. The tiles evidently have the effect of rotating the direction of the walk as in fig. 2b, and thus this process is equivalent to the bond HGW, as shown by Duplantier [29], and Manna and Guttmann [26]. Note that the two tiles do not correspond directly to occupied and vacant sites, however. If one thinks of the lattice as being a checkerboard, then the occupied sites will correspond to tiles of one type on the white squares but the tiles of the opposite type on black squares [29]. Roux et al. [19] always found criticality for any mixture of the two tiles randomly put on all squares, since they thus always created an equal number of vacant and occupied bonds (however, placed with a spatial bias towards different colors on the checkerboard).

In fig. 2e the cluster is placed on an underlying Manhattan lattice with half the lattice spacing of the percolation lattice. The arrows of the walk around the cluster are seen to obey the restrictions of this lattice, as shown by Bradley [25] and by Manna and Guttmann [26]. Each step on this lattice corresponds to either a cut of a vacant bond or a step parallel to an occupied bond. Because of the properties of the Manhattan lattice at each step there are two possible directions to continue. The walk is a simple kinetic growth walk (KGW). A KGW is a walk which steps with equal probability to any neighboring site that was not previously visited [30–32]. On the Manhattan lattice, the KGW is therefore a SKW [25,26].

In summary the following walks are HGWs for bond percolation on a square lattice:

(1) The generic walk on the covering site lattice, which can be constructed to step between either the occupied (fig. 2c) or vacant sites.

(2) The paths on the $\pm\pi/2$ model of Gunn and Ortuño [18].

(3) Hull percolation on the random tiling of Roux et al. [19].

(4) The KGT (or GSAT) on an L-lattice [26].

(5) The KGW on a Manhattan lattice [25,26].

4. Discussion

Thus, we have seen that many walk-forming processes, which have mostly arisen independently from a variety of problems, are in fact different forms of HGW. This paper has been mainly a pedagogical review, although the walk of fig. 1d is a new and efficient HGW for site percolation hulls. A tiling procedure to generate these paths can also be given, although it is not as elegant as the tiling for bond percolation. This walk can also be generalized for site–bond percolation.

The perimeters considered here are related, but not identical, to the accessible perimeter introduced by Grossman and Aharony [22]. The accessible perimeter is the external perimeter of a cluster that can be probed by a particle of a given size moving along a path of nearest-neighbor vacant sites from infinity. When this particle is sufficiently large (depending upon the lattice), the invaginations of the cluster are cut off and the remaining hull is found to have a fractal dimension of $\approx 4/3$ rather than the 7/4 of the complete perimeter, and thus of a different universality class. Note that for a perimeter generated by the HGW, we can define the accessible perimeter as all sites that can be reached from infinity without crossing any path of the HGW, which is thus a definition independent of the size of a probe particle and the type of lattice. To generate the accessible perimeter by a walk process, one must first generate the complete perimeter in the usual way with a HGW, and then carry out another scouting walk around the perimeter to identify the "hull" of the hull [21,22]. In fact, this new hull is more in the spirit of Mandelbrot's original definition of the word than the more common usage as any perimeter, and furthermore the fractal dimension (4/3) is exactly identical to the value conjectured by Mandelbrot [1] for the Brown hull (which is the accessible perimeter of the Brown trail), based upon the value for the self-avoiding random walk. There is no local walk that can generate the accessible perimeter from scratch, which is perhaps related to its being of a different universality class.

The connections between HGWs and KGWs, SKWs, IGSAWs, etc. are numerous but their exact nature is dependent upon the specific lattice and system being considered. In many cases, such walks are not precisely HGWs but of the same universality class. One example is the IGSAW of Kremer and Lyklema [17] on a square lattice. While the growing end of the IGSAW never gets trapped, the non-growing end easily does [17]. In contrast, for the IGSAW (or the SKW) on the honeycomb lattice introduced in ref. [12] neither end will get trapped and the walk will always eventually close, because it is a HGW.

It is useful to make this distinction between "being of the same universality class as a HGW" and "being a type of a HGW", which is a stronger statement. As we have seen, there are many random walks that are a type of HGW, which means that any results of their simulation apply equally to percolation hulls. This can lead to ambiguity when refering to such walks – do they represent SKWs, or percolation hulls [23]? The answer depends upon the lattice – for site percolation on the triangular lattice the HGWs are both, while for the square lattice the HGW (fig. 1) is somewhat different than the SKW or IGSAW. I would also like to point out that in ref. [23], the very extensive simulations of ref. [10], which gave $1/D = 4/7 \pm 0.0005$, were misquoted to a much lower precision.

The various considerations given here for the square lattice can be applied to the many other two-dimensional lattices, including directed ones, to yield a great variety of interesting HGWs.

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References

[1] B.B. Mandelbrot, The Fractal Geometry of Nature (Freeman, San Francisco 1983) pp. 126–130, 132, 242.

[2] H.J. Herrmann, Phys. Rep. 136 (1986) 153.

[3] T. Vicsek, Fractal Growth Phenomena (World Scientific, Singapore, 1989).

[4] H.E. Stanley, in: On Growth and Form, H.E. Stanley and N. Ostrowsky, eds (Nijhoff, The Hague, 1986).

[5] P.G. de Gennes, P. Lafore and J.P. Millot, J. Phys. Chem. Solids 11 (1959) 105.

[6] M.E. Fisher and J. Essam, J. Math. Phys. 2 (1961) 609.

[7] G.R. Reich and P.L. Leath, J. Phys. C 11 (1978) 1155, 4017.

[8] B. Sapoval, M. Rosso and J.-F. Gouyet, J. Phys. (Paris) 46 (1985) L149.

[9] R. Voss, J. Phys. A 17 (1984) L373.

[10] R.M. Ziff, Phys. Rev. Lett. 56 (1986) 545.

[11] P. Grassberger, J. Phys. A 19 (1986) 2675.

[12] A. Weinrib and S.A. Trugman, Phys. Rev. B 31 (1985) 2993.

[13] H. Saleur and B. Duplantier, Phys. Rev. Lett. 58 (1987) 2325.

[14] A. Bunde and J.-F. Gouyet, J. Phys. A 18 (1985) L285.

[15] R.M. Ziff, P.T. Cummings and G. Stell, J. Phys. A 17 (1984) 3009.

[16] R.M. Ziff, presented at Statistical Mechanics Meeting at Rutgers, May, 1982, J. Stat. Phys. 28 (1982) 838.

[17] K. Kremer and J.W. Lyklema, Phys. Rev. Lett. 54 (1985) 267; J. Phys. A 18 (1985) 1515.

[18] J.M.F. Gunn and M. Ortuño, J. Phys. A 18 (1985) L1095.

[19] S. Roux, E. Guyon and D. Sornette, J. Phys. A 21 (1988) L475.

[20] R.M. Ziff and B. Sapoval, J. Phys. A 18 (1986) L1169.

[21] S.S. Manna, J. Phys. A 22 (1988) 433.

[22] T. Grossman and A. Aharony, J. Phys. A 19 (1986) L745; 20 (1987) L1193.

[23] A. Coniglio, N. Jan, I. Majid and H.E. Stanley, Phys. Rev. B 35 (1987) 3617.

[24] B. Duplantier and H. Saleur, Phys. Rev. Lett. 59 (1987) 539; 60 (1988) 1204; 61 (1988) 1521.

[25] R.M. Bradley, Phys. Rev. A 39 (1989) 3738.

[26] S.S. Manna and A.J. Guttmann, preprint (1988).

[27] A. Malakis, J. Phys. A 8 (1975) 1885.

[28] J.W. Lyklema, J. Phys. A 18 (1985) L617.

[29] B. Duplantier, J. Phys. A 21 (1989) 3969.

[30] J.W. Lyklema and K. Kremer, J. Phys. A 17 (1984) L691; 19 (1986) 279.

[31] I. Majid, N. Jan, A. Coniglio and H.E. Stanley, Phys. Rev. Lett. 52 (1984) 1257.

[32] S. Hemmer and P.C. Hemmer, J. Chem. Phys. 81 (1984) 584.