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Some general relations between dressed self-avoiding walks and percolation perimeters on lattices

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Abstract. We show for some simple examples the relations between some recently proposed dressed self-avoiding walks and site percolation. Connection between matching pairs and dressed walk generators is specified and some features of the corresponding bond percolation problem are given. The case of surface generators for dressed self-avoiding surfaces is briefly examined.

1. Introduction

The self-avoiding random walks (SAW) are known (de Gennes 1979) to be a convenient model for linear polymers with excluded volume interaction. Many extensions of the SAW have recently appeared, in particular in relation to kinetic growing models. Majid *et al* (1984) discussed the kinetic growing walk (KGW) where a random walker can only step to the sites not visited before. Ziff *et al* (1984) introduced a two-sided walk which generates the perimeters of site percolation clusters and Weinrib and Trugman (1985) showed that these perimeter walks present the same asymptotic behaviour as two other practically equivalent KGW, their smart kinetic walk (SKW) and the indefinitely growing self-avoiding walk (IGSAW) (Kremer and Lyklema 1985). The perimeter walks of Ziff *et al* (1984) appeared to be a particular case of a more general class of self-avoiding walks described in Gouyet *et al* (1987) which we called dressed self-avoiding walks (DSAW). All these walks have the same fractal dimension $d_{\rm H} = \frac{7}{4}$ (Sapoval *et al* 1985, Bunde and Gouyet 1985, Gouyet *et al* 1986, 1987) if they are not submitted to 'too strong constraints', i.e. if there is no long-range correlation between steps.

The purpose of this paper is to show for some simple examples the relations that exist between such DSAW and an underlying percolation problem. In particular any perimeter walk can be considered as a DSAW. In this case the generators of the walk are directly related to the matching-pair structure of the considered percolation problem. But the reciprocal is not true—all dressed self-avoiding walks cannot be associated with a percolation problem. This will become clear in §2 for some examples.

Dressed self-avoiding surfaces and a three-dimensional generalisation of the DSAW are briefly introduced in § 3. In addition we briefly examine in appendix 1 the case of perimeter generation in the bond percolation problem; in this case the perimeter is not associated with a DSAW and is more similar to a 'squig' fractal (Mandelbrot 1984). Appendix 2 is devoted to some remarks on approximate calculations of percolation thresholds from DSAW generators.

2. General considerations on DSAW generators on a lattice

A general definition of a DSAW can be found in Gouyet *et al* (1987). Given a 2D graph L, the walk takes place on the dual graph L^D and at each step the adjacent sites on L are occupied (dressed), for instance, by a white particle on the left and a black particle on the right (see figure 1). The walk is then continued in such a way that white (black) particles always remain on the left (right) of the walk. The walker cannot walk again on its own path. If no other possibilities occur then the walk closes. After a sufficient number of steps, when no particular constraint is added, all the walks become rings.

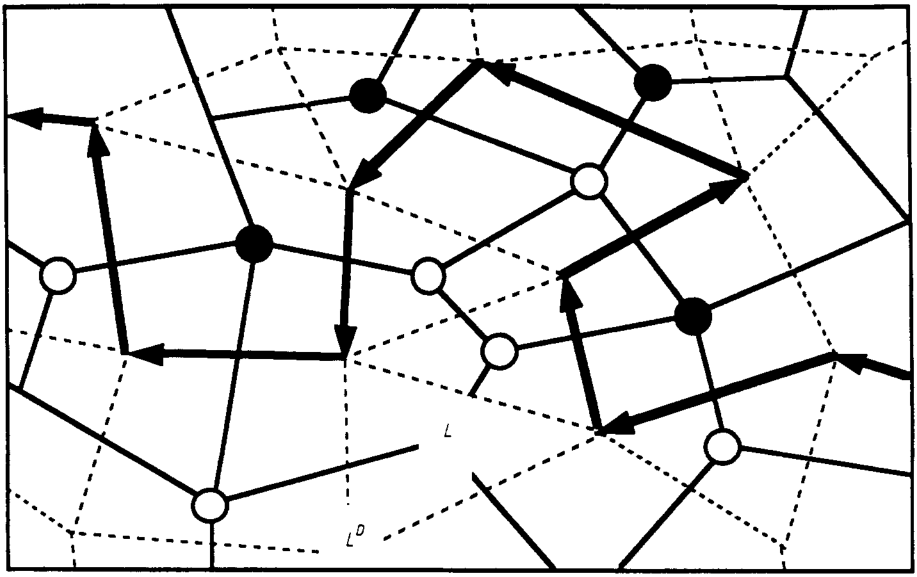
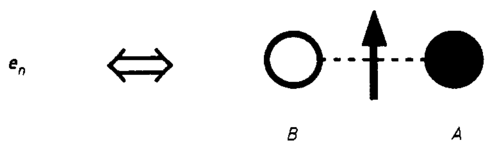


Figure 1. This figure represents a dressed self-avoiding walk on an arbitrary random lattice L (full lines). The successive steps of the walk are arrows placed on the dual lattice L^D (broken lines). The arrows are dressed with black and white particles (see text).

A dressed step e_n will simply be a step of the walk dressed with one white particle on its left and one black particle on its right, n indicating the position of the step in the walk:



A generator $G = \{e_{n-1}, e_n\}$ of a DSAW will then be formed by at least two successive dressed steps, respectively the entrance door and exit door of a polygon on the lattice L. Except for the case of triangular polygons, occupation of the corners and connections between these corners must be specified. Depending on the lattice L, different possibilities can occur. Some of them have been described in Gouyet *et al* (1987) in the case of the square lattice. Here we will examine these possibilities in more detail.

(a) The triangular lattice. This case has already been studied in the literature, at least under equivalent forms (Weinrib and Trugman 1985). The generators take here their

simplest structure. Only two generators can be constructed, completely defined by two successive dressed steps $G_i = \{e_{n-1}, e_n\}$,

The arrows are on the honeycomb dual lattice and the walker can either turn right or left with an angle $(e_{n-1}, e_n) = 2\pi m/3$ with $m = \pm\frac{1}{2}$. The application of a new generator G_1 or G_2 at time $n+1$ consists only, if the place is free, in adding a black or a white particle. If black particles are added with probability p, it is known (Ziff *et al* 1984) that the walker generates the perimeters of percolation clusters at a concentration p for the triangular lattice with first-neighbour connection. At each step one can associate with each value of m an increase in the number δN_{fA} of black points and δN_{fB} of white points. Then for the triangular lattice

$$m = \tfrac{1}{2} \qquad \begin{cases} \delta N_{fA} = 1 \\ \delta N_{fB} = 0 \end{cases}$$

$$m = -\tfrac{1}{2} \qquad \begin{cases} \delta N_{fA} = 0 \\ \delta N_{fB} = 1. \end{cases}$$

Now when the walker progresses the added site A (black) or B (white) is either a new site or an already created one. In the last case the walker is not free to walk right or left: the walk is intrinsically self-avoiding. Moreover it is quite easy to show that a DSAW never finishes abruptly like in an ordinary self-avoiding walk. We always obtain closed loops which delimit finite clusters. Nevertheless it is possible to build in a systematic way an infinite walk using an additional constraint similar to that used by Weinrib and Trugman (1985) or Kremer and Lyklema (1985).

(b) The square lattice. Here the different possible sets of two successive generators must correspond to the four possibilities (figure 2) of putting black and white particles on the upper corners of a square (the lower side is always e_{n-1} and always has a white particle on the left and a black on the right).

One sees in this case that the definition of a generator G must be completed. A generator defined only with two successive steps is not sufficient for the square lattice as one corner is undetermined and this may correspond to a different evolution of the walk.

Moreover on each polygon of the lattice we have to consider all the possible connections between the sites (first- and second-neighbour connections in the square lattice case). The generators are then the set of two successive steps on which connections between identical particles have been added. These connections avoid indetermination.

For the square lattice the four possibilities of setting black and white particles on the two remaining corners lead to five distinct possible generators shown on the right in figure 2. The generators drawn in figure 2(b) contain second-neighbour connections

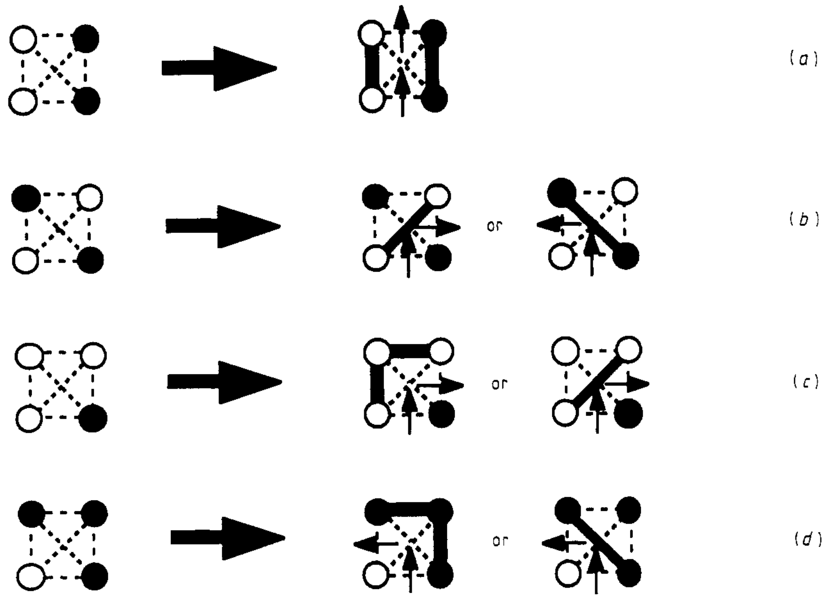


Figure 2. On a square lattice, two dressed steps are not sufficient to completely define the generators. In this figure we show on the left the different occupations of the corners of a square by black and white particles and the possible (first- and second-) neighbour connections (broken lines) between these corners. All the corresponding possible generators are represented on the right-hand side.

and are again found in figure 2(c) (second-neighbour connection between white particles) and figure 2(d) (second-neighbour connection between black particles). The upper corner which is not connected is then free (black or white) when the DSAW grows.

These five generators give all the possible DSAW on a square lattice. In figure 3(a) the only three generators of perimeters needed in the case of the percolation problem of black A particles with first-neighbour connection ('A' lattice) are represented at the bottom of the drawing. The white particles ('B' lattice) are connected via first and second neighbours. 'A' and 'B' lattices form a *matching pair* (see Sykes and Essam 1964). The corresponding percolation problem is shown above the set of generators. In figure 3(b) we have represented the *same* distribution of particles but now associated with the set of generators with first-neighbour connection between white 'B' particles and first and second between black 'A' particles.

If we now choose all the five generators (figure 3(c)) a difficulty appears when we are faced with case (b) in figure 2 which shows two conflicting possibilities. Hence let p_2 be the probability that the connection is second neighbour between the black 'A' particles (and $1-p_2$ between the white). Then the set of generators again corresponds to a percolation problem with a statistical second-neighbour connection.

The percolation threshold varies continuously from $p_{cA} \simeq 0.5928$ when $p_2 = 0$ to $p_{cB} = 1 - p_{cA} \simeq 0.4072$ when $p_2 = 1$ (a relation which has no reason to be linear in p_2). The lattice pair $\{A, B\}$ may be called a statistical matching pair. We can also consider this case as a site-bond percolation problem with a critical line of percolation thresholds. The set of generators is symmetrical with respect to the permutation (A, B) only when $p_2 = \frac{1}{2}$. In this case $\{A, B\}$ may be called a statistical self-matching pair and its percolation threshold is at $p_c = \frac{1}{2}$.

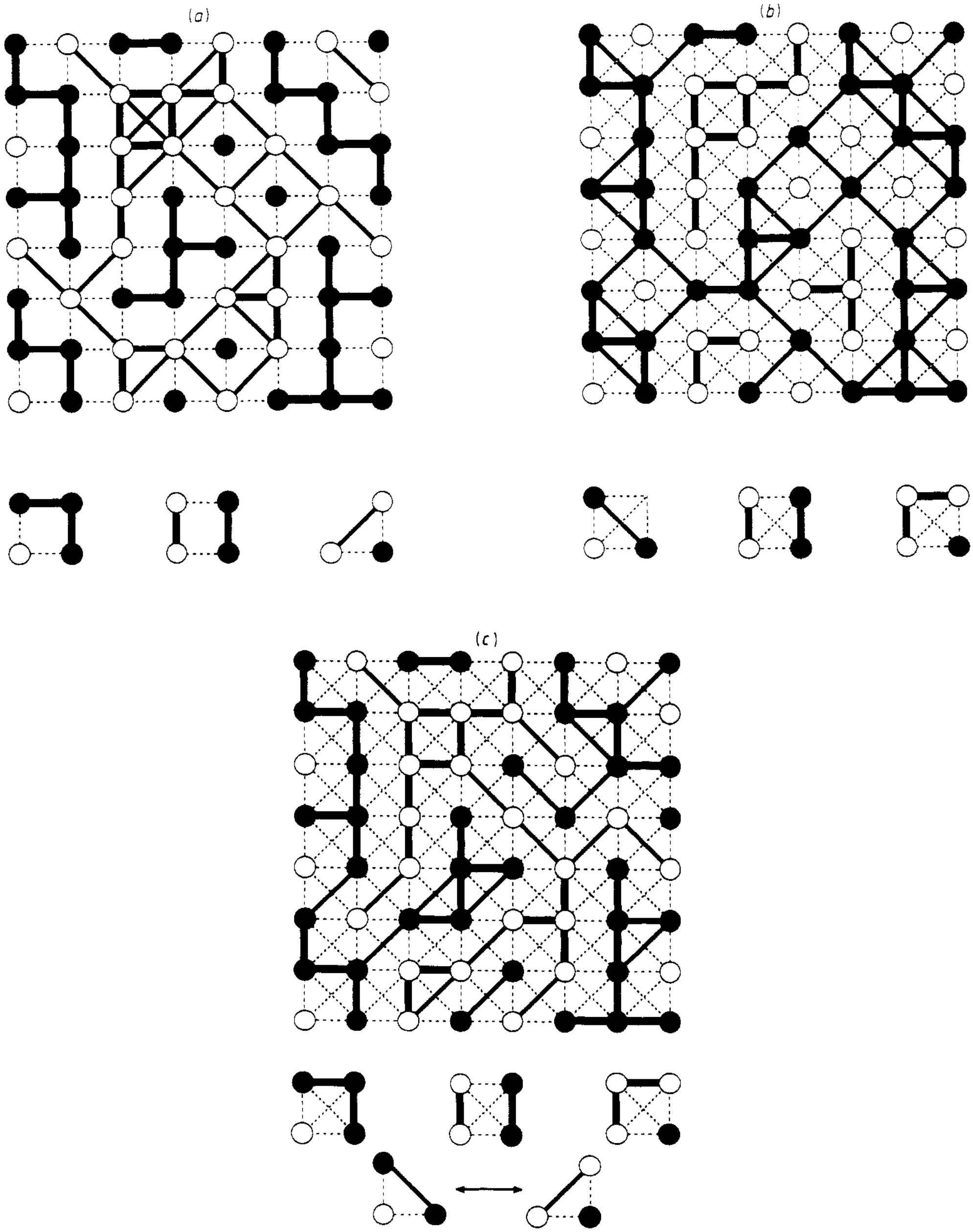


Figure 3. On these lattice structures as in all the following, any admitted connection between the black particles have been indicated with a broken line. On all figures associated with the percolation problem we have chosen for comparison the same distribution of black and white particles. (*a*) shows the first-neighbour connection square lattice, with at the bottom the set of perimeter generators. (*b*) shows the first- and second-neighbour case. (*c*) shows the case where second-neighbour connection is admitted for both black and white particles. A conflict appears which leads to choose some generators at random.

It is in fact possible to choose the generators in a manner depending on more complicated underlying connections of the lattice. Figures 4(a) and (b) show two examples of self-matching pairs, for which the set of generators is symmetrical. The first figure (a) represents the lattice site problem isomorphic to the bond problem ($p_c^{\text{bond}} = \frac{1}{2}$), while ($b$) represents the fully triangulated lattice.

If we keep in the generator set only the two generators with first-neighbour connection (figure 5(a)), it is no longer possible to consider them as perimeter generators. In other words the associated DSAW do not correspond to a percolation problem (figure 5(b)) due to the strong correlation between neighbouring sites generated by the walk.

However, if the generators are those with second-neighbour connections the DSAW is not associated with site percolation (figure 6a)), but with two identical bond percolations (figure 6(b)) on two imbricated independent square lattices, for which indeed $p_c^{\text{bond}} = \frac{1}{2}$.

(c) Other lattices. The same ideas can be applied to other 2D lattices. For a regular lattice structure, the rotation angle between two successive steps $(\boldsymbol{e}_{n-1}, \boldsymbol{e}_n)$ may be written in a general compact form

$$(\boldsymbol{e}_{n-1}, \boldsymbol{e}_n) = 2\pi m/(2S+2) \qquad m \in \{-S, S\}$$

where $2S+2$ is the number of faces of the elementary polygon,

$$2S+2 = \begin{cases} 3 & \text{for the triangular lattice} \\ 4 & \text{for the square lattice} \\ 6 & \text{for the hexagonal lattice.} \end{cases}$$

For instance, for the honeycomb lattice the generators with first-neighbour connection between the black sites can be classified according to table 1.

Table 1. Increase in the number of black (A) and white (B) particles at each step on the honeycomb lattice for the different possible directions of the walk.

m	2	1	0	-1	-2
δN_{fA}	4	3	2	1	0
δN_{fB}	0	1	1	1	1

For the Kagomé lattice (figure 7) the ten generators are simple combinations of triangular and honeycomb generators. These kinds of frontier-generating walk have been used by Ziff and Sapoval (1986) to check the efficiency of determining the percolation threshold by the gradient method (Rosso *et al* 1985).

3. The 3D case: dressed self-avoiding surfaces

The above considerations can be generalised to three dimensions. The dressed self-avoiding surfaces (DSAS) are built with plaquettes sitting on the dual graph of the lattice considered. Each plaquette can be oriented with a normal vector which will then be dressed with a white particle on one extremity and a black on the other (figure 8). The DSAS separates the white particle region from the black one. As we no longer

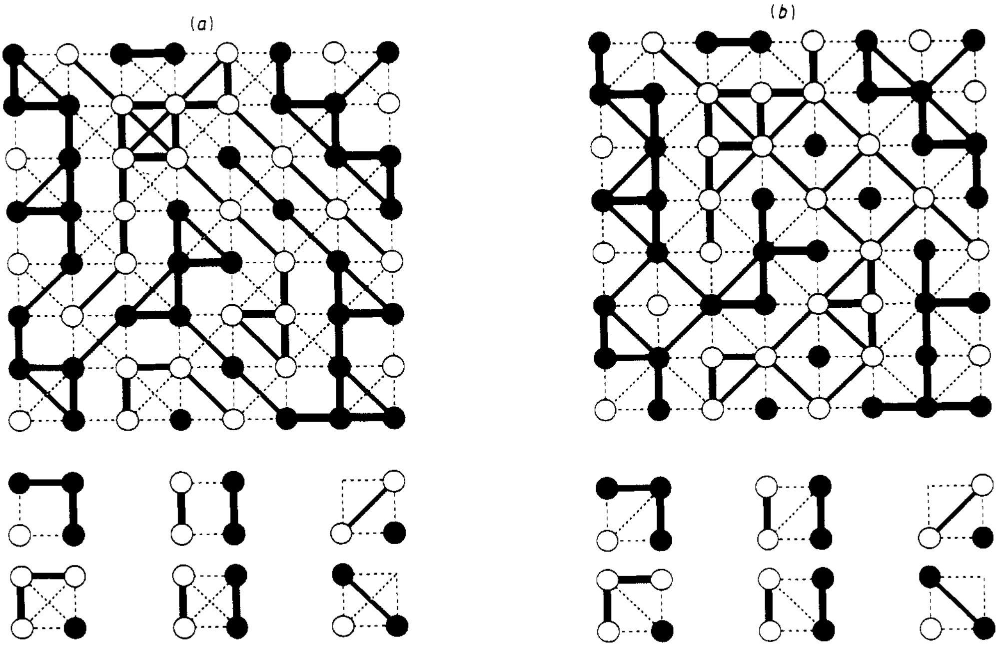


Figure 4. In these two cases of self-matching lattices, the connections differ from one square to the other. This leads to generators which must fit with the underlying connections of the lattice and along the walk these connections changes. This explains the higher number of generators. (*a*) represents the lattice site problem isomorphic to the bond problem. (*b*) represents the fully triangulated lattice.

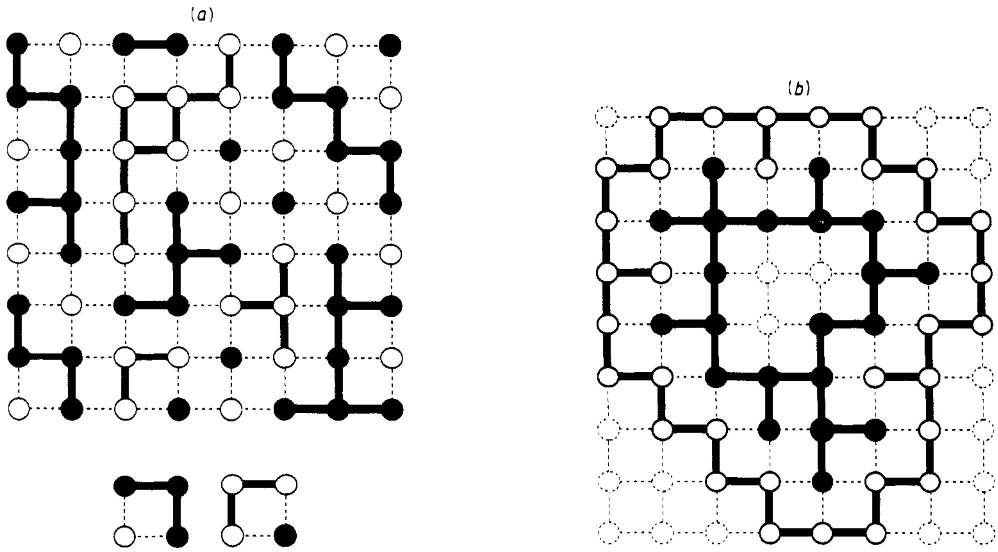


Figure 5. In (*a*) the distribution of points is at random, identical to the preceding examples, but here with first-neighbour connections between both black and white particles. The corresponding generators are inadequate to generate cluster perimeters of this system. In contrast they generate DSAW shown in (*b*), which clearly do not correspond to a random distribution of particles.

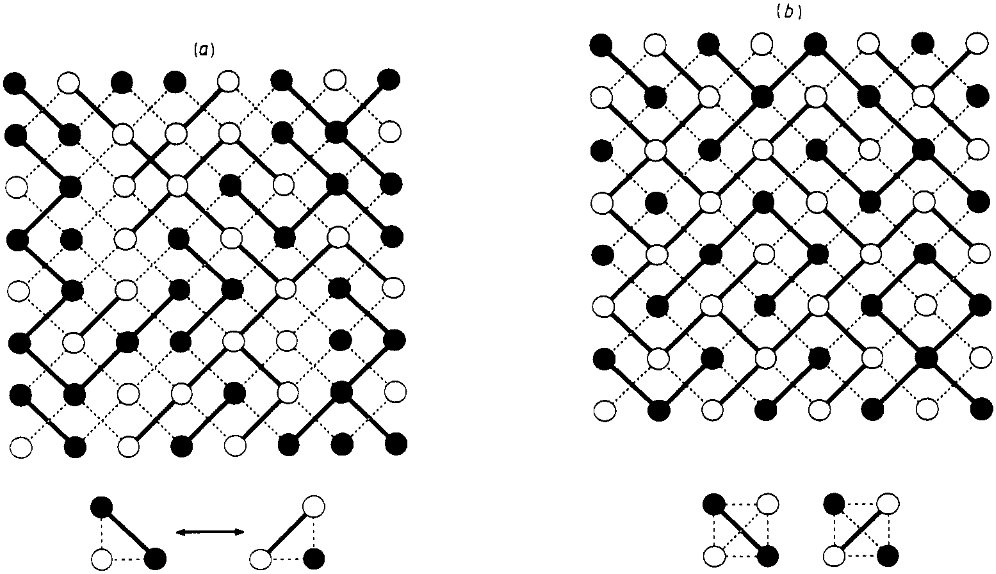


Figure 6. This figure is drawn in the same spirit as figure 5. (*a*) shows the random distribution, while we can see in (*b*) that the perimeters correspond to a double bond-percolation problem.

have a walk we cannot define a simple set of generators and we must proceed by successive addition of dressed plaquettes.

Figure 9 shows the simple cubic lattice case. The lattice '*A*' has a first-neighbour connection between black particles while the '*B*' lattice needs first-, second- and third-neighbour connections between the white particles. To generate a DSAS one starts from a dressed plaquette (figure 8) which represents the seed. Addition of a second dressed plaquette will consist in adding a plaquette with one side in common with the seed (3×4 possibilities) or with one corner in common and two black first-neighour sites (2×4 possibilities). Hence, while the black sites are first neighbours, the white sites can be first or second (by addition of a plaquette with one common *side*) or third neighbours (by addition of a plaquette with one common *corner*), as is shown in figure 9. The three first cases in figure 9 are, in fact, very similar to the 2D case because all the particles remain in a plane. But this is no longer the case with the fourth case.

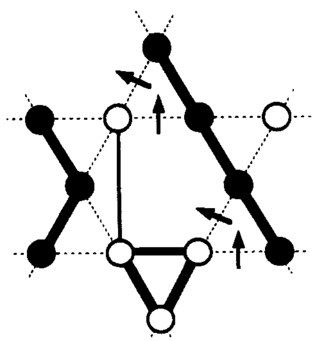


Figure 7. We have represented here only one of the possible generators for the Kagomé lattice.

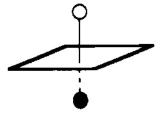


Figure 8. A dressed plaquette is the generalisation in three dimensions of the 2D dressed step. It separates interior and exterior of a 3D percolation cluster. For the simple cubic lattice the plaquette is a square.

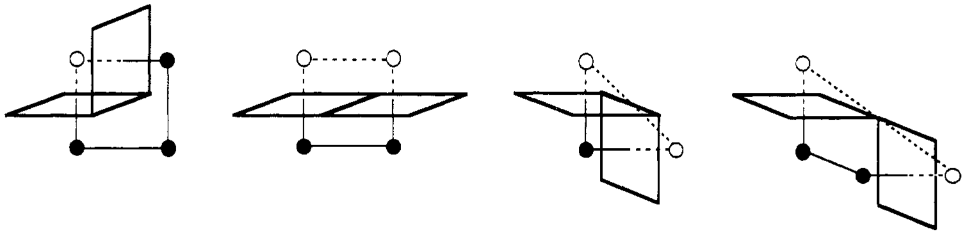


Figure 9. This figure shows the different possibilities of associating dressed plaquettes in the simple cubic lattice case.

New dressed plaquettes are added following one of the four possibilities in figure 9. In figure 10 we show addition as an example of three and five plaquettes.

The manner in which the dressed plaquettes are added is important in the DSAS case. One way is to consider the *perimeter* of the cluster formed with the plaquettes as the set of 'growth sides and corners' of the surface. If the plaquettes are added at random along the perimeter, the generated surface will certainly not be the hull of a percolation cluster (as it is in the case in Wilke *et al* (1985) and Kertész and Herrmann (1985)).

To be sure to generate a three-dimensional hull a possible way consists in filling first the growing *sides* and *corners* situated at the shortest distance from the seed generator. Independence in the occupation of different sites by black or white particles ensures that the hull correctly grows, as addition of dressed plaquettes can be done in any arbitrary order.

4. Conclusion

There are various motivations to consider dressed self-avoiding walks. One motivation is that it allows one to directly build up the external surface (or hull) of percolation clusters (Gouyet *et al* 1987). It is then related to the study of diffusion fronts of the

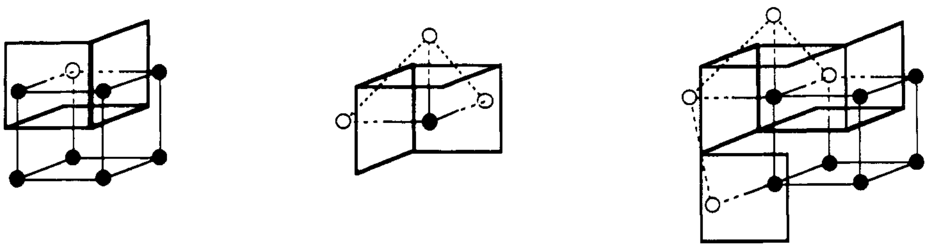


Figure 10. This shows some different simple combinations of dressed plaquettes.

hard-core particle lattice gas (Sapoval *et al* 1985). A second very important motivation is that it gives the fastest (and the most accurate) way to determine numerically a percolation threshold (Rosso *et al* 1985, Ziff and Sapoval 1986). The DSAW is, in this case, generated with a vanishing gradient of probability. A third motivation is that it contains enough flexibility to allow quite general random walks (Gouyet *et al* 1987) which may be used in relation with polymer statistics. Last, but not least, the DSAW characterises the percolation problem in general, beyond the properties of the hull studied so far. Its extension to dressed self-avoiding surfaces appears to be very interesting. It will be the subject of further studies.

Acknowledgments

Fruitful remarks by T Gobron and M Rosso are greatly acknowledged.

Appendix 1. Relation with perimeters of the bond percolation problem

Up to now all studies on perimeters walks have been devoted to perimeters of clusters of the site percolation problem. What then are the equivalent walks for the bond percolation case?

In site percolation problems the perimeters are associated with walks on the dual lattice L^D and the corresponding A and B sites on L belong to matching pairs. In

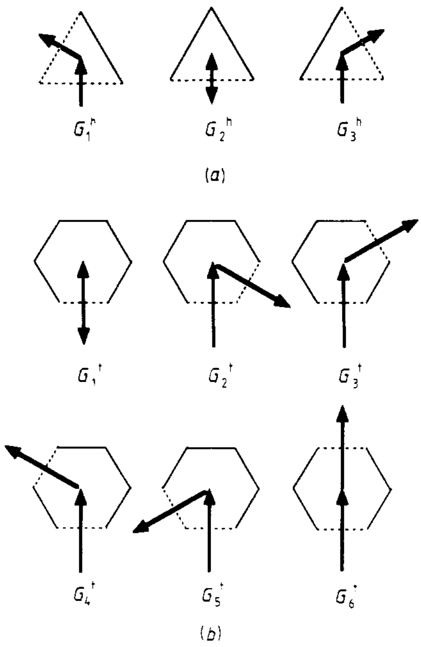


Figure 11. (*a*) The three dominos necessary to generate the cluster perimeters in the honeycomb bond percolation problem. The arrows follow the perimeter itself and a part of perimeter can be visited at most two times in two opposite directions. The second generator corresponds to the extremity of a dangling bond run over in both directions. (*b*) This is the dual problem of that (*a*). The six dominos generating perimeters of the triangular lattice.

bond percolation problems, the perimeters are generated as a domino game. The dominos are the polygons (P_n) of the L^D lattice and the perimeter generators are represented by two successive arrows $\boldsymbol{b}_{n-1}$ and $\boldsymbol{b}_n$ on lattice L.

Figure 11(a) represents the cluster perimeter generators of the bond percolation problem on the honeycomb lattice. Figure 11(b) represents the dual problem, i.e. the cluster perimeter generators of the bond percolation problem on the triangular lattice.

The growth rules are the following. The polygons are associated as in the site problem, $\{\boldsymbol{b}_0, \boldsymbol{b}_1\}, \ldots, \{\boldsymbol{b}_{n-1}, \boldsymbol{b}_n\}\{\boldsymbol{b}_n, \boldsymbol{b}_{n+1}\}, \ldots$, in such a way that each polygon side can at most wear two opposite bonds $\boldsymbol{b}_i$ and $\boldsymbol{b}_j = -\boldsymbol{b}_i$. Such a walk, a set of $\{\boldsymbol{b}_n\}$ vectors, is not strictly self-avoiding because a step can possibly be visited two times, but nevertheless belong to the same universality class. As in the site percolation case (Rosso *et al* 1985) if one considers the double frontier of the 'infinite' cluster in the gradient percolation problem, it is easy to show that this frontier is located at p_c and that the relation

$$p_c^{\text{bond}}(L) + p_c^{\text{bond}}(L^D) = 1$$

holds (Sykes and Essam 1964) and its fractal dimension is expected to be $d_H = \frac{7}{4}$. The bond percolation case in fact belongs to the general class of 'squig fractal constructions' defined a few years ago by Mandelbrot (1984), with the particular building rule we gave above.

It is interesting to show the correspondence with the site equivalent problem. For instance, we have shown in figure 4(a) the lattice site problem isomorphic to the bond problem on the square lattice. We show in figure 12 the corresponding bond problem.

Appendix 2. Approximate evaluation of the percolation threshold

An approximate calculation of p_c consists in supposing the DSAW as a pure random walk without self-avoidance and that at the percolation threshold there is an equal

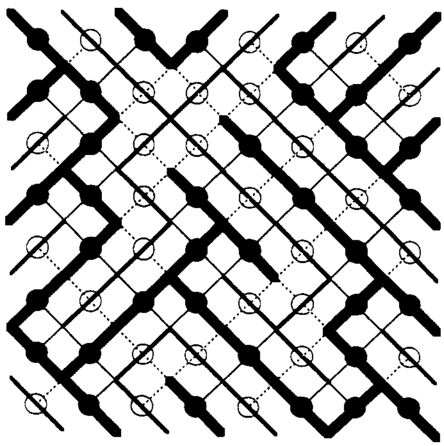


Figure 12. The bond percolation problem (here with the same distribution as in figure 4(a)) is related to four self-dual dominos (not represented). The two lattices L (---) and L^D (—) are the same so that $p_c = \frac{1}{2}$. The bonds (——) have been chosen at the same positions as the sites (●) in figure 4(a). The bonds (——) corresponding to the sites (○) are the bonds of the dual lattice L^D.

probability to turn right or left. This case is easily calculated and leads to the following equations:

for the triangular lattice $p_c^* = \frac{1}{2}$ and $p_c^* = 0.5$.

for the square lattice $p_c^{*2} + p_c^* = 1$ and $p_c^* = 0.618$.

for the honeycomb lattice $p_c^{*4} + p_c^{*3} + p_c^{*2} + p_c^* = 2$ and $p_c^* = 0.741$.

The deviation from the exact values increases with the asymmetry between the matching pairs and one shows that self-avoidance reduces this asymmetry.

An interesting remark, due to M Rosso, concerns the use of the ratio $N_{fA}/(N_{fA} + N_{fB})$ which we showed to converge to p_c when the length N of the walk goes to infinity. In this expression N_{fA} (N_{fB}) is the total number of A sites (B sites) on the walk after N steps. If the DSAW was a pure random walk, without constraints, the above ratio would be directly given by an average on the new sites created by a set of generators. This corresponds to replacing N_{fA} by $N'_{fA} = N\langle \delta N_{fA} \rangle$ (and equivalent relations for B). It is remarkable that the corresponding values give a quite good approximation of p_c.

Table 2.

	Triangular	Square	Honeycomb	Kagomé
$p_c^{\text{approx}} = N'_{fA}/(N'_{fA} + N'_{fB})$	$\frac{1}{2}$	$\frac{3}{5}$	$\frac{10}{14}$	$\frac{25}{38}$
p_c	$\frac{1}{2}$	0.5928 ...	0.698 ...	0.6527 ...
Difference	0	0.007	0.016	0.0052

The best approximate values are obtained with the last method. They are shown on table 2 and again self-avoidance reduces the asymmetry so that $p_c^{\text{approx}} \geqslant p_c$.

This means that, for simple lattices, p_c is approximated by $p_c^{\text{approx}} = (z+2)/(3z-2)$ where z is the coordination number. This expression is also valid in 1D ($z = 2, p_c = 1$) but not in 3D.

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