

A new kinetic walk and percolation perimeters

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We introduce the smart kinetic walk (SKW), a new kinetic-walk model which is in a different universality class from other such models. The SKW is strictly self-avoiding, yet is never forced to terminate, because it never starts down a path which would lead to its being trapped. We show that a ring-forming version of the model in two dimensions traces out the external perimeter of critical percolation clusters. Using previous results on these perimeters, we find that the SKW fractal dimension is $D_{\text{SKW}} \approx 1.75$. The equivalence between the walk and percolation perimeters leads to a scaling form for the number of N -step rings. Finally, we see that the walk with a bias to turn to the left more often than to the right (or vice versa) traces out the perimeter of clusters that are not at the percolation threshold. This implies a maximum ring size depending upon the strength of the bias.

There has been considerable interest in recently introduced “kinetic-growth” models of geometric structure, as distinguished from more traditional “equilibrium” models. Equilibrium models such as percolation,¹ lattice animals, and the self-avoiding walk² (SAW) are defined by an ensemble of possible objects with statistical weights determined by simple properties of the object. Thus, field-theoretic solutions have been found for many of these models.³ On the other hand, kinetic-growth models⁴ such as diffusion-limited aggregation, kinetic gelation, and certain kinetic-walk models involve explicit construction of the objects step by step, with a probability associated with each step. Therefore, the total weight of an object is determined by the history of its construction.

This distinction between kinetic and equilibrium models is not a strict one. For example, the normal random walk can be viewed in both ways: as the path of a (drunk) traveler who takes N steps, each in an arbitrary direction, or as the set of all N -link chain configurations, each given an equal weight. However, the so-called self-avoiding walk, a model for linear polymers² with excluded-volume interactions, seems to be most naturally described as an equilibrium problem: It considers the set of all N -link *nonintersecting* chain configurations, with each given equal weight.

There are a number of possible kinetic-walk models which incorporate a self-avoiding constraint.⁵ Amit *et al.*⁶ introduced the “true” self-avoiding walk (TSAW), which considers the path of a traveler who avoids his previous path if possible, but when he becomes trapped he will step on his previous path in order to continue. On the other hand, Majid *et al.*^{7(a)} very recently discussed the kinetic-growth walk (KGW), which differs from the TSAW in that a trapped walker terminates his walk rather than revisiting any site. Thus, the KGW is strictly self-avoiding, unlike the TSAW. In this paper we study a new model, the “smart” kinetic walk (SKW). In our model the walk is strictly self-avoiding, but it is never forced to terminate because it never starts down a route which would lead to a trapping situation.

It appears that these three kinetic-walk models are all

in a different universality class than the “equilibrium” SAW, and also that they each define their own universality class.^{7(b)} For example, in two dimensions the fractal dimensions D of the various models are all different. The fractal dimension is defined by $N \sim R^D$, where N is the number of steps and R is the (average) size of the resulting paths. For the SAW,⁸ $D_{\text{SAW}} = \frac{4}{3}$, while the true SAW is at its upper critical dimension (above which the self-avoiding constraint is irrelevant) and $D_{\text{TSAW}} = 2$. Computer studies^{7(a)} of the KGW give $D_{\text{KGW}} \approx 1.5$, and by relating our SKW to the external perimeter of percolation clusters we shall find $D_{\text{SKW}} \approx 1.75$.

These results for the fractal dimensions are suggested by noting that the TSAW can be expected to be the most “dense” since it intersects itself. Moreover, the SAW weighs all configurations equally, while the SKW and KGW tend to give a greater weight to a walk which approaches itself so that the self-avoidance and “smartness” constraint come to bear. The reason that the SKW is more dense than the KGW is again because the SKW weighs more heavily configurations which come close where the “smartness” becomes relevant; this point will be discussed more fully below.

We have found that Kremer and Lyklema⁹ have independently introduced a model, their smart growing self-avoiding walk, which is apparently equivalent to our SKW model. They have studied the walk on the square lattice by explicit enumeration of the walks up to $N = 22$ steps, and find $R \sim N^{\nu_{\text{SKW}}}$ with $\nu_{\text{SKW}} = 0.57 \pm 0.01$. The resulting value for the fractal dimension, $D \equiv (\nu_{\text{SKW}})^{-1} = 1.75$ is in excellent agreement with our result.

We believe in “universality” for this problem, in that the large-distance behavior, such as the fractal dimension, should be independent of the particular choice of two-dimensional lattice. Considering the honeycomb lattice, we shall show that the SKW is equivalent to the external perimeter of clusters of the triangular site-percolation problem at criticality. Thus, this apparently kinetic problem is, in fact, isomorphic to an aspect of the (equilibrium) percolation problem. (However, we have not

developed a field-theoretic formulation of the problem.) Despite the fact that many of the two-dimensional percolation critical exponents are known exactly,¹⁰ the behavior of the external perimeter is known only from computer simulations.^{11,12} In Ref. 13, the present authors discuss a continuum percolation model which percolates at zero area fraction of conductor, in which the perimeters of percolation clusters play a major role.

A recent study by Ziff *et al.*¹⁴ bears a number of similarities to our work here. He has introduced an algorithm for constructing the perimeter of clusters of the two-dimensional square site-percolation problem. His algorithm creates (on the square lattice) a “kind of two-sided self-avoiding walk” which is a realization of a perimeter of a cluster. Since the walk of Ziff *et al.* and our SKW are both realizations of the external perimeter of percolation clusters in two dimensions, we believe that at large-distance scales the walks are equivalent. However, the simple nature of the SKW is not apparent at short distances for the walk as constructed by Ziff on the square lattice, both because of the nature of the lattice and because his walk is defined on the lattice on which the percolation clusters sit, while ours (see below) is defined on the dual lattice. We shall discuss the case of the square lattice using our approach somewhat more below.

We now more carefully define the SKW and show its equivalence to percolation perimeters in two dimensions. We then use known scaling laws for the percolation problem to derive relations for the number of rings constructed from SKW’s, and we briefly discuss the case when the percolation problem is not critical ($p \neq p_c$) and the problem on a square lattice.

The rules which define the SKW model are as follows: At each time interval the walker steps with equal probability to one of the allowed sites. An allowed site is, in general, a nearest-neighbor site which has not been visited previously. In addition, trapping sites are disallowed, where a trapping site is one from which there is no allowed path to infinity, so that the traveler would eventually be forced to terminate or step on a previously occupied site. A variation of the rule, which forms rings, shall be important below: The origin from which the walker starts is an allowed site, and a trapping site is one from which there is no path to the origin.

We believe that the fractal dimension of large walks will be the same for both of these versions of the SKW, much as the fractal dimension of the SAW and the self-avoiding ring problem are the same.^{2,15} Far from the origin of the walk, the requirements that the traveler can return to the origin and that he can go to infinity are essentially equivalent.

Note that in spatial dimension $d = 1$ the self-avoidance constraint forces the walk to be a simple line ($D_{\text{SKW}} = 1$) and the “smartness” is never applicable. For $d = 2$ local information is sufficient for the walk to be “smart.” As illustrated schematically in Fig. 1(a), when the traveler approaches his previous path he can use the local configuration plus knowledge of the direction of the old path to determine which way to turn to avoid being trapped. The direction of the old path can be provided by arrows on the steps, or can be inferred from the coloring of the two sides

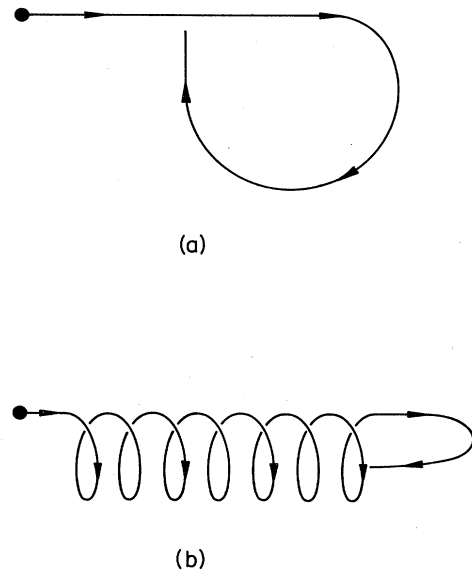


FIG. 1. (a) Schematic view of a two-dimensional situation in which the traveler must be “smart” and turn to the left rather than to the right. (b) Three-dimensional case in which the traveler must be “smart.” He may enter the tube only if he can escape at the other end. The travelers start at the dots and walk in the direction of the arrows.

of the path defined by occupied and vacant sites of the percolation problem. For $d > 2$, nonlocal information is required in order to avoid traps; consider the $d = 3$ example illustrated in Fig. 1(b), where local information will not suffice to determine whether the other end of the “tube” is open or closed, and thus whether the traveler may enter the tube or not. However, at each step a search of only finite length is required to determine the allowed moves, so that the walk is well defined even for $d > 2$.

In Fig. 2 we show a number of examples of smart kinetic walks on a honeycomb lattice with their associated weights. The model can be generalized to other lattices in a transparent way, and we expect by universality that re-

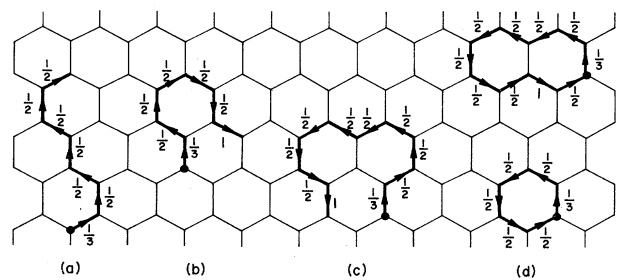


FIG. 2. Examples of smart kinetic walks on the honeycomb lattice. The walk starts at the site with the large dot and the weight of each step is indicated. The total weights of the walks are (a) $\frac{1}{3}(\frac{1}{2})^6$, (b) $\frac{1}{3}(\frac{1}{2})^5$, (c) $\frac{1}{3}(\frac{1}{2})^8$, and (d) $\frac{1}{3}(\frac{1}{2})^8$ and $\frac{1}{3}(\frac{1}{2})^5$. Panel (d) illustrates two rings formed by the ring-forming version of the SKW.

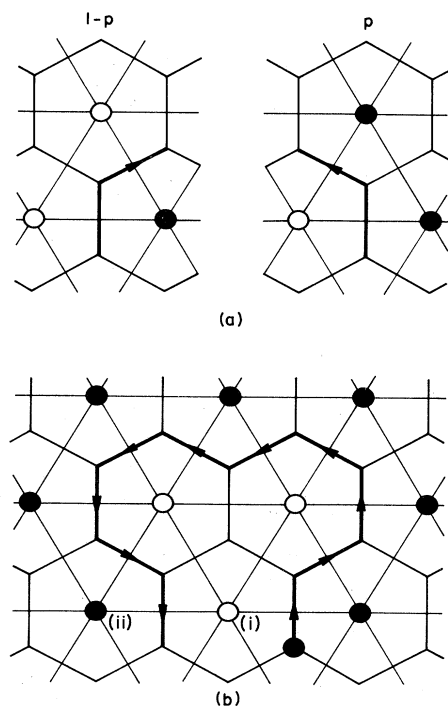


FIG. 3. Equivalence between the SKW and percolation perimeters. We show the site-percolation problem on the triangular lattice, where solid and open circles indicate occupied or vacant sites, respectively. The perimeter of the percolation cluster, and the equivalent SKW, are defined on the dual honeycomb lattice. (a) The two basic steps, to the right and to the left, are determined by the occupation of the upper site. Thus, they have weights $1-p$ and p , respectively, where p is the probability that a site is occupied. (b) Example of a walk which displays the "smartness" constraint, and the corresponding percolation site occupations. The occupation of the site labeled (ii) was chosen at random and was found to be occupied, which determined the second-to-last step of the random walk. The final step was then automatically determined, because site (i) was previously determined to be vacant.

sults for the critical behavior (such as the fractal dimension of large walks) will be independent of the detailed lattice structure.

The two walks of Figs. 2(a) and 2(b) have different weights even though they have the same number of steps; this is due to the kinetic nature of the model and is in contrast to the equal weighting of all legal configurations in the usual SAW model. In Fig. 2(b) the traveler has stepped away with probability unity from revisiting a previously visited site.

Figure 2(c) shows the first walk for which the smartness of the traveler is relevant. Here the traveler has stepped away with probability unity to avoid a path which would eventually lead to his being trapped. This behavior is different from that of the KGW model, which could enter the trap, but would then be eliminated at the next step. Thus, the KGW weight of Fig. 2(c) would be $\frac{1}{3}(\frac{1}{2})$.⁹ Finally, in Fig. 2(d) we show examples of comp-

leted rings formed by the ring-forming version of the SKW model.

We have illustrated the SKW on the honeycomb lattice because it is for this lattice that there is an equivalence¹⁶ between the walk and the external perimeter of clusters of the site-percolation problem at its percolation threshold. (The case of a noncritical percolation problem and the associated walks will be briefly discussed later.) This equivalence is only exact for the ring-forming version of the walk which always maintains an allowed path to the origin. However, as discussed above, we believe that the distinction between the two versions is immaterial for the fractal dimension of large walks.

With the percolation problem defined on a triangular lattice, we define the perimeter of a cluster to be bonds of the dual (honeycomb) lattice which separate occupied from unoccupied sites (see Fig. 3). Now we imagine building up the edge of a percolation cluster in a stepwise fashion by choosing the occupations of the sites which determine the perimeter as we go along.¹⁷ The resulting rules for growth of the perimeter are exactly those of the SKW model. At each step a decision is made as to whether a single site is occupied (with probability p) or vacant (with probability $1-p$). This decision exactly determines whether the perimeter turns left or right at that step. For triangular site percolation, the critical probability is $p_c = \frac{1}{2}$, and so, in general, the walk turns left or right with an equal probability of $\frac{1}{2}$. Moreover, as demonstrated in the example of Fig. 3, when the perimeter approaches itself it realizes the self-avoidance and smartness character of the walk because the occupation of sites has previously been determined, so that the traveler steps with unit probability. Because the perimeter separates occupied from vacant sites, by its very nature it cannot cross or enter a trap which would force it to eventually cross.

With probability one, every perimeter will eventually close. If it closes one way it encloses occupied sites, while if it closes the other it encloses vacant sites. However, for triangular site percolation, $p_c = \frac{1}{2}$, so that occupied clusters and what we have labeled "vacant" clusters are both critical. It is convenient to redefine an *internal* perimeter of an occupied cluster to be, instead, the *external* perimeter of a vacant cluster. Then the set of all clusters (occupied and vacant) is in one-to-one correspondence with the set of all perimeters, with each cluster associated with its *external* perimeter.

In this way the SKW on a honeycomb lattice traces out the external perimeters of critical percolation clusters. Considering a configuration of occupied and vacant sites in the percolation ensemble, we must choose a perimeter site at random as the origin of the SKW. The traveler then proceeds to follow that perimeter. Thus, the average spatial extent of an N -step SKW ring is the same as the average extent of a percolation perimeter of length N , so that the fractal dimension of the SKW is identical to the fractal dimension of the external perimeters of critical percolation clusters. Because we can choose any of the N sites of a particular perimeter as the origin of the walk, a given perimeter in the percolation ensemble corresponds to N distinct walks. Thus, below, we can relate the num-

ber of N -step rings produced per walk to known percolation scaling behavior.

It has been proved,¹⁸ in general, that for a percolation cluster the total perimeter (external and internal) is proportional to the number of sites of the cluster, and thus the fractal dimension of the *total* perimeter is the same as that of the cluster, D_c . However, in two dimensions it appears that for large critical clusters the external perimeter is a vanishing amount of the total perimeter, and that its fractal dimension D_p is less than that of the cluster.

Despite the fact that many of the critical exponents are believed to be known exactly¹⁰ for $d=2$ percolation, there is relatively little known about the fractal dimension of the external perimeter. With computer studies, Leath and Reich¹¹ have measured the way that the length of the perimeter of a cluster (which we identify with N the number of steps of a SKW ring) scales with the cluster area s , finding

$$N \sim s^x, \quad (1)$$

with $x=0.93 \pm 0.02$. Noting that $N \sim L^{D_p}$ and $s \sim L^{D_c}$, where L measures the spatial extent of the cluster, we see that $x = D_p/D_c$. Thus $D_p \approx 1.76$, where we have used the exact¹⁰ $D_c = \frac{91}{48}$. More recently, Voss,¹² who calls the external perimeter the "hull," has measured $D_p = 1.75 \pm 0.02$. Thus we find the fractal dimension of the SKW,

$$D_{\text{SKW}} \equiv D_p \approx 1.75. \quad (2)$$

This result is in good agreement with the above-mentioned computer series of Kremer and Lyklema⁹ for the SKW on a square lattice: They find $D_{\text{SKW}} \approx (0.57)^{-1} = 1.75$.

Improved computer simulations for percolation will give D_p , and hence D_{SKW} , more accurately. Alternatively, improved values for D_p may be obtained if, as seems likely, the SKW proves to be easier to study than the percolation problem.

We now derive a scaling relation for \tilde{n}_N , the number of N -step rings produced per walk.¹⁹ For percolation at its critical point the number of clusters (per unit area) with s sites scales¹ as

$$n_s \sim s^{-\tau}, \quad (3)$$

with $\tau = \frac{187}{91}$ in two dimensions. Because of the one-to-one correspondence between a cluster and its external perimeter, and the (N -to-one) correspondence between SKW loops and external perimeters, we find

$$\tilde{n}_N \sim N n_s \frac{ds}{dN} \sim N^{-(\tau-1)/x} \sim N^{-1.14}, \quad (4)$$

where we have used Eqs. (1) and (3).

Up to this point we have only considered the case that the percolation problem is at its percolation threshold: $p = p_c = \frac{1}{2}$ for triangular site percolation. If $p \neq p_c$ there is a correlation length

$$\xi \sim |p - p_c|^{-\nu} \quad (5)$$

(with $\nu = \frac{4}{3}$ in two dimensions¹⁰) which sets the scale of the largest finite cluster. Clusters which are smaller than

ξ but still large compared to the lattice spacing are similar to the critical clusters which occur at $p = p_c$, while finite clusters larger than ξ are exponentially rare. There will be an infinite cluster of "occupied" or "vacant" sites if $p > p_c$ or $p < p_c$, respectively. However, the infinite cluster will not be relevant for the walks because it has no *external* perimeter. Instead, the walks will trace out the edges of the smaller clusters, some of which correspond to holes in the infinite cluster.

For the walks, the $p \neq p_c$ case translates into a bias for a given walk to step left more often than right, or vice versa [see Fig. 3(a)]. Thus, if $p < p_c$ the walks will tend to form clusters of "occupied" sites, while for $p > p_c$ they will tend to form clusters of "vacant" sites. Because of the bias, the walks will close more quickly than for the unbiased walk, forming smaller rings. The percolation equivalence gives the scale of the largest rings, which is the correlation length ξ . Walks smaller than ξ are essentially the same as unbiased walks and will have the fractal dimension D_{SKW} found above. Thus, the number of steps in the largest rings can be written as

$$N_{\text{max}} \sim \xi^{D_{\text{SKW}}} \sim |p - p_c|^{-\nu D_{\text{SKW}}}. \quad (6)$$

The scaling arguments leading to Eq. (4) can be easily generalized to the case $p \neq p_c$ in order to relate the distribution of ring sizes to the percolation-cluster-size distribution function. We find

$$\tilde{n}_N \sim N^{-(\tau-1)/x} F(|p - p_c| N^{\sigma/x}), \quad (7)$$

where the percolation scaling exponent $\sigma = \frac{36}{91}$ in two dimensions, and $F(z)$ falls off rapidly for large z . This implies, for example, that the average number of steps in a ring can be written as

$$\langle N \rangle \sim |p - p_c|^{-\psi}, \quad (8)$$

with $\psi = (1 - \tau + 2x)/\sigma \approx 2.0$. This result is in excellent agreement with the computer study of Ziff *et al.*¹⁴ of percolation perimeters which gave $\psi = 2.0 \pm 0.1$.

While we expect that the two types of SKW (which keep available an allowed path to the origin or to infinity) are essentially the same when there is no bias, we do not believe that this is the case when a bias is imposed. As just discussed, the biased ring-forming walk is equivalent to percolation perimeters with $p \neq p_c$. Thus there is a maximum ring size ξ , with smaller rings the same as unbiased ones. However, the walks formed by the model which requires a path to infinity will never terminate, and thus will have no maximum size. When small compared to ξ , these walks will be equivalent to the ring-forming walks and will have fractal dimension D_{SKW} . We expect that for larger walks there will be crossover to new behavior, in which the traveler basically spirals around a central core. It appears that this spiral will fill some finite fraction of space, and thus that the fractal dimension of large walks will be 2, the same as the spatial dimension.

It is tempting to apply the methods of this paper to the square lattice. Considering site percolation on the square lattice, we can define the perimeter²⁰ of clusters on the dual (also square) lattice exactly as for triangular site percolation. However, while the SKW is easily defined on

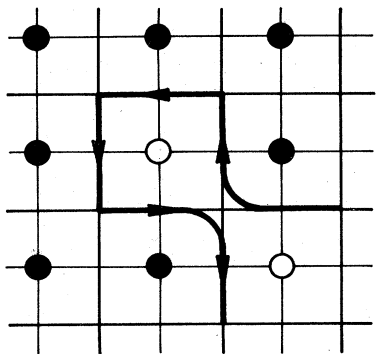


FIG. 4. Walk generated by the perimeter of square site-percolation clusters which self-intersects.

the square lattice, this walk is *not* generated by the percolation problem. Rather, due to the lack of symmetry between occupied and vacant sites at the percolation threshold $p_c \approx 0.59$, the percolation problem generates a

more complex walk, which may, in certain cases, self-intersect at single sites (see Fig. 4). Thus, while we believe that at large distances the SKW and the perimeter of percolation clusters are the same independent of the lattice, this equivalence is not manifest at short distances.

In summary, we have introduced a new kinetic-walk model which is in a distinct universality class from other such models. The smartness of the walker rarely comes to bear, yet it leads to new asymptotic behavior. We have related our kinetic problem to the equilibrium percolation problem, and thus identified the fractal dimension D_{SKW} . The equivalence to percolation implies a scaling relation for the number of N -step rings, and for the effect of a bias in the walk.

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¹⁷A similar approach was used in Ref. 11 to study entire clusters, and in Ref. 14 to study somewhat differently defined perimeters.

¹⁸See Ref. 1 and references therein.

¹⁹Similar scaling arguments are used in Ref. 13 to study a $p_c = 0$ percolation model.

²⁰To define this perimeter, one must state at the outset whether the perimeter is that of an occupied or vacant cluster. This ambiguity does not occur on the triangular lattice, in which the two perimeters are identical.