Distribution of sizes of erased loops for loop-erased random walks

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We study the distribution of sizes of erased loops for loop-erased random walks on regular and fractal lattices. We show that for arbitrary graphs the probability P(l) of generating a loop of perimeter l is expressible in terms of the probability $P_{st}(l)$ of forming a loop of perimeter l when a bond is added to a random spanning tree on the same graph by the simple relation $P(l) = P_{st}(l)/l$. On d-dimensional hypercubical lattices, P(l) varies as $l^{-\sigma}$ for large l, where $\sigma = 1 + 2/z$ for 1 < d < 4, where z is the fractal dimension of the loop-erased walks on the graph. On recursively constructed fractals with $\tilde{d} < 2$ this relation is modified to $\sigma = 1 + 2\bar{d}/(d\bar{z})$, where \bar{d} is the Hausdorff and \tilde{d} is the spectral dimension of the fractal. [S1063-651X(97)51003-8]

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The loop-erased random walk (LERW) is a simpler variant of the well-known self-avoiding walk (SAW) problem, which retains the no self-intersection property of SAWs, but is closer to the ordinary random walk problem. In this paper, we study the distribution of sizes of erased loops for LERWs on arbitrary graphs and relate it to the distribution of sizes of loops formed when a bond is added to a random spanning tree on the same graph. In the themodynamic limit this distribution has a power law tail, and we express the exponent in terms of the fractal dimension of the chemical paths on spanning trees. We also show how this relation is modified for deterministic fractals.

In spite of the fact that the LERW model is somewhat more tractable analytically than the SAW problem, the number of papers devoted to this problem has remained rather small. The model was defined by Lawler [1], who called it the loop-erased self-avoiding walk (LESAW). This terminology is somewhat inappropriate, and we prefer to use the term LERW in this paper [2]. Lawler showed that for space dimensionality d>4, the large length scale properties of the LERWs are the same as those of simple random walks. Thus, if r_n is the end-to-end distance of an *n* step LERW and we define the exponent ν such that $\langle r_n^2 \rangle \sim n^{2\nu}$, then ν has the value 1/2 in d>4. For d<4, Lawler derived the rigorous bound that $\nu \ge$ the flory value 3/(d+2) for SAW [3]. From numerical simulations, Guttman and Bursill [4] obtained the $\nu = 0.800 \pm 0.003$ in two dimensions values and $\nu = 0.616 \pm 0.004$ in three dimensions. The corresponding values for SAWS are $\nu = 0.750$ and $\nu = 0.59 \pm 0.004$ in two and three dimensions, respectively. This shows that LERW and SAW are in different universality classes. Guttman and Bursill conjectured $\nu = 4/5$ in two dimensions (see, however, [5]). This was proved by Majumdar [6] by relating the LERW problem to that of random spanning trees and showing that the fractal dimension of LERWs is the same as that of chemical paths in random spanning trees. In two dimensions the latter is known using the equivalence of spanning trees to the $q \rightarrow 0$ limit of the q-state Potts model from conformal field theory [7].

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Bounds on the expected number of erased steps have been obtained by Lawler [8], and it was found that in ≤ 4 dimensions the fraction of steps remaining unerased $\rightarrow 0$ as the number of steps $N \rightarrow \infty$. Duplantier obtained exact exponents for the behavior of the probability that *k* LERWs of length *n* starting at neighboring points do not intersect and also the winding number distribution of a LERW [9]. Lawler has also shown [10] that the LERW is equivalent to the Laplacian random walk model studied by Lyklema and Evertsz [11].

Our interest in this paper is the distribution of sizes of erased loops for the LERW problem. The corresponding question for the totally random walks is the well-known Polya problem [12]. For SAWs the problem is also the well-studied question of enumeration of polymer rings [13]. A similar problem is encountered in the context of the self-organized Eulerian walkers model and has been studied recently by Shcherbakov *et al.* [14]. We show that the probability P(l) that an erased loop has perimeter l, equals $P_{st}(l)/l$ where $P_{st}(l)$ is the probability that a loop of perimeter l is formed when a bond is added to a random spanning tree. For large l, P(l) and $P_{st}(l)$ are expected to show power law behaviors, say $P(l) \sim l^{-\sigma}$ and $P_{st}(l) \sim l^{-\tau}$. Then our result implies that

$$\sigma = \tau + 1 \,. \tag{1}$$

We give scaling arguments to derive the exponent σ in terms of the fractal dimension z of chemical paths on random spanning trees. For deterministic fractals, this expression is modified, and also involves the ratio of Hausdorff and spectral dimensions of the fractal. As a simple illustrative example we consider the Sierpinski gasket, and calculate the exponents z and τ directly from first principles.

Consider an N step simple random walk $\omega = [\omega(0), \omega(1), \ldots, \omega(N)]$, where $\omega(k)$ is the position of the random walker on the lattice after k steps. Let j be the smallest value such that $\omega(j) = \omega(i)$ for $0 \le i \le j \le N$. We then obtain a new walk, $\overline{\omega} = [\omega(0), \omega(1), \ldots, \omega(i), \omega(j+1), \ldots, \omega(N)]$, by deleting all steps between i and j. This process, corresponding to the removal of loops

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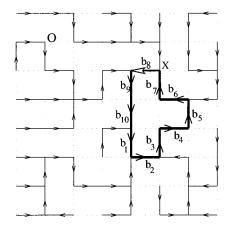


FIG. 1. A spanning tree T_N with the end point of walk at X. The loop \mathcal{L} (shown in bold) of ten directed bonds is formed if the bond b_8 , denoted by the white arrow, is added to T_N . In this case there is a directed path from the origin O to the head of b_8 .

from ω in chronological order, is repeated until a *j* can no longer be found. The resulting walk is a LERW of length $n \leq N$.

Consider a LERW, on a *d*-dimensional hypercubical L^d torus, formed from an *N* step simple random walk by erasing loops. We define P(l,N,L) to be the probability that the (N+1)th step results in erasing a loop of perimeter *l*. Let

$$P(l) = \lim_{L \to \infty} \lim_{N \to \infty} P(l, N, L).$$
(2)

Consider the random walk starting at *O*. After *N* steps of the walk, we consider the directed tree that is formed using last exit bonds from all the sites visited by the walk, except the end point of the walk. This is called the last exit tree T_N after *N* steps. For $N \ge L^d$, all sites of the lattice are visited at least once, and T_N is a spanning tree. It was proved by Broder [15] that in the steady state all such spanning trees occur with equal probability. The LERW after *N* steps is just the directed path from *O* to the end point of the walk along T_N .

Now, consider a particular loop \mathcal{L} of l directed bonds b_1, b_2, \ldots, b_l (see Fig. 1). Let $P(\mathcal{L}, b_j)$ be the probability that the (N+1)th step of the walk will result in formation of the loop \mathcal{L} in the LERW problem, with the (N+1)th step being along the bond b_j . This occurs if and only if (i) the (N+1)th step forms the loop \mathcal{L} on T_N , with b_j as the last step, (ii) there is a directed path in T_N from O to the head site of b_j , which does not include any bonds in \mathcal{L} .

Let $P_{st}(\mathcal{L}, b_j)$ denote the probability that (i) occurs. This probability is easy to compute using the break-collapse method [16], which collapses loop \mathcal{L} to a single point. Hence, it is easy to to see that $P_{st}(\mathcal{L}, b_j)$ is the same for all *j* from 1 to *l*. Thus,

$$P_{st}(\mathcal{L}, b_j) = P_{st}(\mathcal{L})/l, \qquad (3)$$

where $P_{st}(\mathcal{L})$ denotes the probability that loop \mathcal{L} is formed on T_N , whatever the position of the last step. To calculate $P(\mathcal{L}, b_i)$, we have to multiply $P_{st}(\mathcal{L}, b_i)$ by the conditional probability $P(O|\mathcal{L}, b_j)$ that (ii) occurs given that loop \mathcal{L} is formed on the spanning tree with b_j as the last bond. Thus, we have

$$P(\mathcal{L}, b_j) = P_{st}(\mathcal{L}, b_j) \cdot P(O|\mathcal{L}, b_j).$$
(4)

As for any spanning tree T_N with end point of walk on \mathcal{L} , the directed path from O must lead to one of the sites in the loop \mathcal{L} , we must have

$$\sum_{j=1}^{l} P(O|\mathcal{L}, b_j) = 1.$$
 (5)

Summing Eq. (4) over j from 1 to l, and using Eq. (5) we get

$$\sum_{j=1}^{l} P(\mathcal{L}, b_j) = P_{st}(\mathcal{L})/l.$$
(6)

Finally, we sum over different shapes and positions of loop \mathcal{L} having the same perimeter *l*, to get

$$P(l) = P_{st}(l)/l.$$
⁽⁷⁾

In deriving this result we have used the fact that the $N \rightarrow \infty$ limit is taken before the $L \rightarrow \infty$ limit. It seems reasonable that the order of limits in definition (1) can be interchanged without affecting the value P(l). However, our proof uses the spanning tree property, and hence needs modification if the $L \rightarrow \infty$ limit is taken before the $N \rightarrow \infty$ limit.

On a square lattice it is easy to calculate $P_{st}(l)$ exactly for small values of l [17]. We thus find P(2)=0.25, $P(4)\approx 0.03681$, and $P(6)\approx 0.01034$. We have done Monte Carlo simulations and verified these figures to very high accuracy. In two dimensions, $\tau=8/5$ [17], and this implies that $\sigma=13/5$ for d=2. This is also in good agreement with our simulations.

For $d \leq 4$, the number of steps of the random walk of *N* steps that are still not erased is a negligible fraction of *N* [8]. Then the expected number of erased steps per step of the random walk is

$$\sum_{l=2}^{\infty} lP(l) = 1 \text{ for } d \leq 4.$$
(8)

For d>4, there is a finite probability that a bond of the random walk which is generating the LERW will not be erased at any future time. Let this probability be called P_{∞} . Then for d>4, the average length of loop erased walk for a random walk of N steps increases as NP_{∞} . Since the average length erased is $N\sum_{l=2}^{\infty} lP(l)$, this implies that

$$\sum_{l=2}^{\infty} lP(l) = 1 - P_{\infty}.$$
 (9)

Thus, by using our relation between the LERWs and spanning trees, we are led to the interesting and paradoxical result that P_{∞} can be thought of as the probability that adding a bond at random to a random spanning tree will not form a loop of finite perimeter, and this is nonzero if the dimension d of the space in which the spanning tree is embedded is greater than 4. This result clearly depends on the fact that the

thermodynamic limit of large system size is taken *before* the limit $\ell \to \infty$ in the summation. For finite lattices, adding a bond to a spanning tree must lead to the formation of a loop.

We now present a scaling argument to determine σ in terms of the fractal dimension of the LERW $(z=1/\nu)$. Let n(l,N) = no. of loops of length *l* generated when the random walk is of *N* steps. The typical excursion of a random walk of *N* steps *R* varies as $N^{1/2}$.

For 1 < d < 4, the linear size of the largest loop that is generated is expected to be of the order of *R*. Since $l \sim R^z$ the perimeter of the largest loop $\sim N^{z/2}$. For large *N*, n(l,N) grows as NP(l). From finite size scaling theory, we expect that for large *l* and *N*, n(l,N) satisfies the scaling form

$$n(l,N) \sim \frac{N}{l^{\sigma}} f\left(\frac{l}{N^{z/2}}\right),\tag{10}$$

where f(x) is a scaling function. For the cumulative distribution (no. of loops of size $\ge l$)

$$c(l,N) \sim \frac{N}{l^{\sigma-1}} g\left(\frac{l}{N^{z/2}}\right). \tag{11}$$

The scaling function g(x) is assumed to be finite at small x and decay rapidly for large x, i.e., for l larger than the cutoff length $N^{z/2}$. For $l = kN^{z/2}$, where k is a finite constant of order 1 we must have c(l) of order 1. This gives

$$\sigma = 1 + \frac{2}{z}.$$
 (12)

In one dimension, the scaling argument given above breaks down. On a linear chain, the erased loops can only be of size l=2. On more complicated but linear graphs, such as ladders, we can have loops of arbitrarily large values of l, but P(l) decays exponentially with l, and the size of the largest loop generated does not scale as R, as assumed in the scaling argument. For d>4, the LERW is approximately a random walk and $\sigma=d/2$.

Note that the scaling relation Eq. (12) does not involve the dimension of space *d* explicitly, but still is valid only for *d* less than the the upper critical dimension 4. It is interesting to ask how this relation needs to be modified to remain valid for noninteger values of *d*. We confine our arguments to recursively defined fractals, which are explicitly constructed spaces having a noninteger *d*.

The scaling argument above is easily extended to work for deterministic fractals. In this case, for a random walk of *N* steps, $R \sim N^{\tilde{d}/2\tilde{d}}$ (for $\tilde{d} \leq 2$), where \tilde{d} and \tilde{d} are the spectral and Hausdorff dimensions of the fractal. Repeating the above argument, we then obtain

$$\sigma = 1 + \frac{2\overline{d}}{z\overline{d}} \quad \text{for } \quad \widetilde{d} \le 2. \tag{13}$$

Calculation of the chemical distance exponent z for spanning trees is quite straightforward for simple deterministic fractals of finite ramification index. Since this calculation has not appeared so far in the literature we describe it briefly below for the Sierpinski gasket (SG). The exact renormalization equations for spanning trees on the SG may be deduced

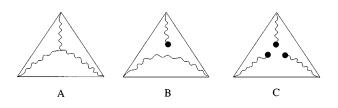


FIG. 2. Diagrams representing the generating functions for spanning trees on the Sierpinski gasket.

from the general recursion equations for the q-state Potts model in the limit $q \rightarrow 0$ [18]. However, for our purpose here, it is more convenient to use the recursion equations written down by Knezevic and Vannimenus (KV) [19] in the context of studying collapse transition of branched polymers on the SG. Only three of the six graphs studied by KV have no vacant sites, and thus only these have nonzero weights for the problem of spanning trees (with no other interactions). These correspond to the cases where all the three vertices of the rth order triangle are connected to each other using bonds within the tree, two are connected to each other and not to the third, and all three are unconnected (Fig. 2). Let these weights be called $A^{(r)}$, $B^{(r)}$, and $C^{(r)}$, respectively. By definition $A^{(r)}$ gives the number of spanning trees on the rth order gasket, $B^{(r)}$ gives the number of two-rooted trees with two vertices connected, and $C^{(r)}$ gives the number of three-rooted spanning trees with all vertices unconnected. From KV, or directly, the recursion equations for A, B, and C are easily written as

$$A^{(r+1)} = 6A^{(r)^2}B^{(r)},$$

$$B^{(r+1)} = 7A^{(r)}B^{(r)^2} + A^{(r)^2}C^{(r)},$$

$$C^{(r+1)} = 12A^{(r)}B^{(r)}C^{(r)} + 14B^{(r)^3}.$$

(14)

The initial values are given by $A^{(1)}=3$, $B^{(1)}=1$, $C^{(1)}=1$. We define a new variable $X^{(r)}=A^{(r)}C^{(r)}/B^{(r)^2}$. It is easy to see that $X^{(r)}$ satisfies the following recursion equation:

$$X^{(r+1)} = \frac{2X^{(r)} + 7/3}{49/36 + X^{(r)^2}/36 + 7X^{(r)}/18}.$$
 (15)

This equation has the fixed point $X^*=3$. Let l_a and l_b be the average lengths of the chemical paths connecting the lower two vertices of the *r*th order generating functions A and B, respectively. To find the recursions for l_a and l_b consider, for example, the graph of order (r+1) and type B shown in Fig. 3(a). The probability of this graph is $A^{(r)}B^{(r)^2}/B^{(r+1)}$

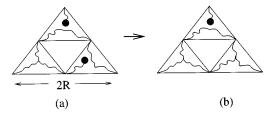


FIG. 3. Formation of a loop of perimeter of the order of R^z on addition of a bond.

 $= 1/(7 + X^*) = 1/10$. The length of the chemical path connecting the vertices is $l_a + 2l_b$. Thus, the contribution of this graph to $l_b^{(r+1)}$ is $(l_a + 2l_b)/10$. Summing up over all relevant graphs we get

$$l_{a}^{(r+1)} = 5l_{a}/3 + 2l_{b}/3,$$

$$l_{b}^{(r+1)} = 6l_{a}/5 + l_{b}.$$
 (16)

We thus obtain l_a , $l_b \sim \lambda^r$, $\lambda = (20 + \sqrt{205})/15$ being the largest eigenvalue in Eq. (16). Thus $l \sim R^z$, where *R* is the linear size of the gasket and $z = \ln \lambda / \ln 2$. Putting in the value of λ we get z = 1.1939...

We now find the exponent τ . We show in Fig. 3 how a loop of the order of R^z may be obtained by adding a bond so that the one of the lower order *B* type graph becomes an *A* type graph. Supposing there are R^β positions where we could have added the bond in order to get the loop. Then the probability of this event $\sim R^\beta/R^{\overline{d}}$. Hence, we obtain

$$R^{-z(\tau-1)} = R^{(\beta-\overline{d})}.$$
(17)

Thus, we can find τ if we can determine the exponent β , which gives the fractal dimension of the boundary between the two constituting subtrees of the *B* type graph. We note that R^{β} times $B^{(r)}$ gives the number of ways of getting an

A graph by the addition of a bond to a B graph with the added bond labeled. But for every resulting A graph the labeled bond could be anywhere on the backbone (path joining the three corner vertices) of length of order R^z . This gives us

$$B^{(r)}R^{\beta} = A^{(r)}R^{z}.$$
 (18)

Now we note that the resistance between two points on a lattice with unit resistances on all bonds is given by the ratio of number of two-rooted spanning trees, with roots at the two given points, to the number of single-rooted spanning trees. It follows then that the ratio B/A gives the resistance between the corner points of a triangle, which scales as R^{α} and so is related to the spectral dimension of the lattice. It can be shown easily that $\alpha = 2\overline{d}/\overline{d} - \overline{d}$. Thus from Eq. (18) we get

$$\beta = z - \alpha = z - 2\overline{d/d} + \overline{d}. \tag{19}$$

Using this in Eq. (17) we get

$$\tau = 2\overline{d}/z\overline{d} . \tag{20}$$

From Eq. (7) the LERW exponent $\sigma = \tau + 1$ and we verify the result Eq. (13) obtained by simple scaling arguments.

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