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LETTER TO THE EDITOR

Reflecting and absorbing boundary conditions on the tail of the Laplacian random walk

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Abstract. We introduce a new version of the Laplacian random walk (LRW) for which the tail of the trajectory acts like a hard wall for incoming diffusing particles. We show how to implement these reflecting boundary conditions through the use of a modified discrete Laplace equation. From an exact enumeration on the square lattice we find that reflecting boundary conditions on the tail of the trajectory give rise to a denser fractal compared with the recently studied Laplacian random walk with absorbing boundary conditions.

Recently we have introduced a one-parameter (η) family of indefinitely growing and strictly self-avoiding random walks, the so-called Laplacian random walk (LRW) (Lyklema and Evertsz 1986, Lyklema *et al* 1986). For this walk the one-step jump probabilities p_i at site i are related to the solution of the discrete Laplace equation with boundary conditions $\Phi(\text{trajectory}) = 0$ and $\Phi(r = R_c) = 1$. Here $r = R_c$ is a $(d-1)$-dimensional sphere centred on the origin of the walk. More precisely, the probability to jump to a nearest neighbour (NN) of the growing tip is taken to be proportional to the gradient of the potential Φ in that direction. With $\Phi(\text{tip}) = 0$ this gradient is equal to the potential at the NN site. This can be generalised by choosing a power-law dependence with exponent η, $p_i \propto \Phi_i^\eta$. This model is essentially a linearised version of the stochastic model for dielectric breakdown as introduced by Niemeyer *et al* (1984) and Pietronero and Wiesmann (1984). For $\eta = 0$ the LRW reduces to the indefinitely growing self-avoiding walk (IGSAW, Kremer and Lyklema (1985a, b)). This walk is a fractal, whereas the $\eta = 0$ limit of the dielectric breakdown problem reduces to a compact object, the Eden model (Pietronero and Wiesmann 1984, Richardson 1973).

In this letter we study the influence of reflecting-tail boundary conditions on the asymptotic properties of the walk. Tail sites are the already occupied sites of the LRW, except for the growing tip. In our previous study of the LRW we solved the discrete Laplace equation on the square lattice

$$\Phi_i = \frac{1}{4} \sum_{\text{NN}} \Phi_j \qquad (1)$$

iteratively with the above described boundary conditions. An alternative way to solve this equation is to consider it as a stationary random walk problem with a source at

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infinity and sinks on the lattice sites of the trajectory (Pietronero and Wiesmann 1984b). For the LRW, random walkers only stick at the growing tip of the trajectory, the walkers which reach the tail of the trajectory disappearing without leaving a trace. This clearly is a process with absorbing boundary conditions and we therefore add an 'a' to the acronym (LRWa). For a physical aggregation process this may not be the appropriate situation. Another possibility is to choose reflecting boundary conditions (LRWr) on the tail of the trajectory. In this case the random walkers are bounced back to the previously visited site if they hit the tail. This model seems more realistic because no diffusing particles disappear. Clearly this choice is not available for the branching dielectric breakdown problem where all sites are potential growth sites. However, an intermediate model which allows for this possibility, and thus having only a limited number of growth sites, can easily be defined. To study the effect of reflecting boundary conditions one has to solve a slightly modified Laplace equation. The $\eta = 1$ version of this walk has been studied independently by Debierre and Turban (1986) and Bradley and Kung (1986). Both groups have performed Monte Carlo simulations, using techniques developed for the simulation of DLA (Witten and Sander 1983, Meakin 1983). As will be discussed later, our results do not agree with theirs because of the finite lattice size effects of their Monte Carlo simulation.

To study the LRWr we have to solve the following equation (Evertsz and Lyklema 1986):

$$\Phi_i = \frac{1}{z} \sum_{\mathrm{NN}}' \Phi_j. \tag{2}$$

The prime denotes that the sum only runs over NN sites which are not occupied by the tail and z equals the number of NN sites. The boundary conditions are now $\Phi(r = R_c) = 1$ and $\Phi(\mathrm{tip}) = 0$. The boundary conditions on the tail are not of importance. However for practical purposes one can again take $\Phi(\mathrm{trajectory}) = 0$ and omit the prime in equation (2). The only difference from the absorbing case is then the normalisation z, which equals the coordination number minus the number of tail sites. Similar to the LRWa, the jump probabilities p_i in the LRWr are defined as

$$p_i = \Phi_i^\eta \left(\sum_{\mathrm{NN}} \Phi_j^\eta \right)^{-1}. \tag{3}$$

For $\eta > 0$ we have a repulsive walk compared with the IGSAW. As for the LRWa, one can also define this model for negative η. Together with the LRWa ($\eta < 0$) this will be discussed elsewhere (Evertsz and Lyklema 1986).

The 'Faraday screening' effect is also present in equation (2) as can be seen from figure 1(a). For this example equation (2) becomes

$$\begin{aligned} \Phi_1 &= \tfrac{1}{2}(\Phi_2 + \Phi_{\mathrm{tip}}) \\ \Phi_2 &= \Phi_1 \end{aligned} \tag{4}$$

with the solution $\Phi_1 = \Phi_2 = 0$. Thus the walk cannot enter the cage. It can easily be seen that this property holds for cages of arbitrary size and for any dimension. So the LRWr is also truly kinetic and strictly self-avoiding. For $\eta = 0$ this walk reduces to the IGSAW (Kremer and Lyklema 1985a, b). Note that the trajectories of both the LRWa, LRWr and IGSAW are the same. However, the asymptotic behaviours are not identical because of the different weight distributions.

For the reflecting boundary conditions one again expects an η dependence of the asymptotic behaviour of the mean square end-to-end distance, but we expect it to

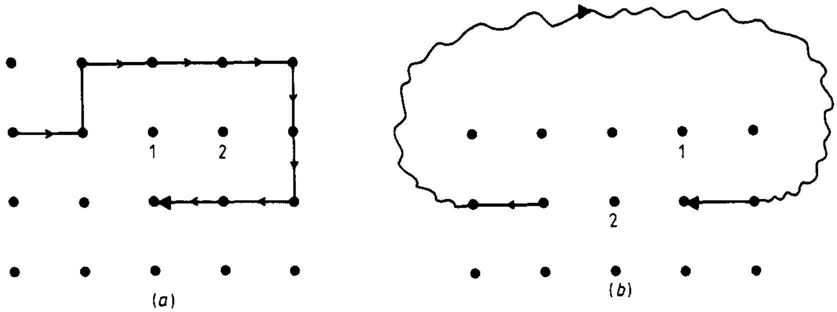

Figure 1. Possible trajectories of the LRW. The numbering is arbitrary. See the text for an explanation.

differ from that of the LRWa. Intuitively this can be understood from figure 1(*b*). Here the growing tip is at the entrance of a cage of arbitrary size. If a random walker enters the cage through site 2 (note that sticking occurs only when the walker's next step is to the tip) then the probability to reach site 1 some time later is larger for the LRWr than for the LRWa because in the latter case the walker can disappear in a sink. Therefore the LRWr will choose the inside direction (site 1) with a higher probability than the LRWa. This is true for cages of all sizes and in this sense it is a 'long-range effect'. Thus we expect that this effect of the tail of the walk gives a higher probability to denser trajectories and possibly results in smaller $\nu(\eta)$ values as compared with the absorbing boundary conditions.

To check this prediction we have performed an 18-step exact enumeration for the LRWr on the square lattice. The radius of the outer circle is $R_c = 36$ and the Laplace equation is solved by iterating equation (2). The program is vectorisable and it needed approximately 20 h CPU time on the Cray X-MP in Jülich. We have calculated the mean square end-to-end distance $\langle R^2(N)\rangle$ as a function of the step number and for 25 different η values. This quantity behaves asymptotically like a power law $\langle R^2(N)\rangle \propto N^{2\nu(\eta)}$. The analysis necessary to calculate the exponent $\nu(\eta)$ is the same as for the LRWa (Lyklema and Evertsz 1986). In figure 2 we show the effective exponent $\nu(N, \eta)$ plotted against $1/N$. The behaviour is similar to that of the LRWa. For large η values the effective exponent $\nu(N)$ increases with N and in the limit $\eta \to \infty$ we find $\nu(\eta) \to 1$. For small η values the effective exponent decreases with N. The crossover occurs at $\nu \sim 0.73$ as for the LRWa but now for $\eta \sim 1.5$. For $\eta = 0$ we recover the IGSAW value $\nu = 0.567$. This behaviour suggests the possibility of a multicritical phenomenon. However as for the LRWa there are no competing effects in our dynamics and thus a multicritical point at $\nu \sim 0.73$ appears improbable. We thus conclude that for these boundary conditions also the critical index ν varies continuously with the parameter η. The difference between the absorbing and reflecting boundary conditions for the whole η range is shown in figure 3 as a function of η. We indeed see the expected behaviour, the $\nu(\eta)$ values of the LRWr are always smaller than the corresponding values for the LRWa. For instance, for the linear equivalent of DLA, i.e. $\eta = 1$, we find $\nu(\text{LRWa}) = 0.80$ and $\nu(\text{LRWr}) = 0.67$. The fractal dimensions are 1.25 and 1.49 respectively, to be compared with $D = 1.70$ for DLA. This is also clear, because a branching structure fills space more completely and therefore it has a higher fractal dimension.

At this point we want to discuss the results of Debierre and Turban (1986) and Bradley and Kung (1986), who studied the $\eta = 1$ case. These authors find, from a Monte Carlo simulation on the square lattice, ν values of 0.79 (respectively 0.77), to

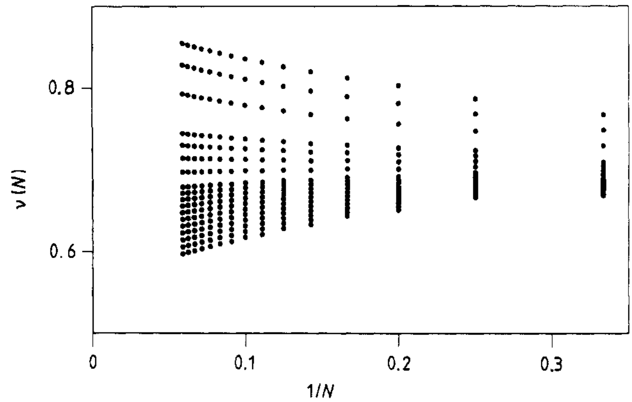

Figure 2. Plot of the effective exponent $\nu(N)$ against $1/N$ on the square lattice. The η values are from top to bottom: 5.0, 4.0, 3.0, 2.0, 1.75, 1.5, 1.25, 1.0, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2, 0.1 and 0.

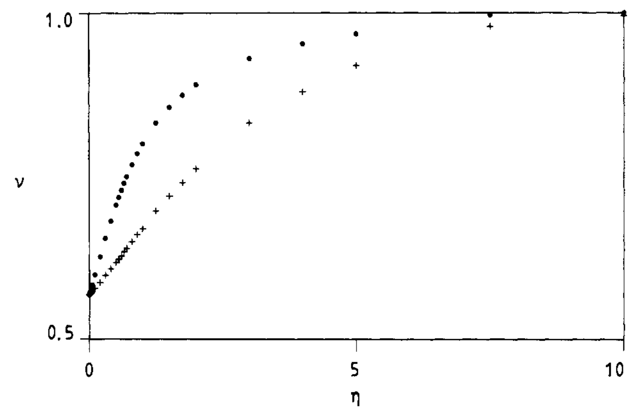

Figure 3. Plot of the estimated asymptotic ν values against η. The dots give the values for the LRWa, the crosses are the LRWr results.

be compared with our result $\nu(\text{LRWa}) = 0.80$ and $\nu(\text{LRWr}) = 0.67$. Both groups use reflecting boundary conditions in their simulation and thus their results disagree strongly with our value 0.67. Thus the conclusion of Debierre and Turban, that they find good agreement with our LRWa result, is not valid.

In an attempt to understand the discrepancy we have studied the influence of the finite lattice size effects. In practice, in a computer calculation one solves the discrete Laplace equation with boundary conditions $\Phi = 0$ on the walk and $\Phi = 1$ on a hypersphere with radius R_c. We have performed a few exact enumerations of length $N \leqslant 14$ with different values for R_c, e.g. 11, 15, 36, 56. In figure 4 we show the results. A clear finite-size effect is observed. This is due to the fact that for a dimininising R_c, the potential at growth sites close to R_c increases faster than at growth sites on a larger distance from R_c. Thus for decreasing R_c one expects that stretched configurations have a higher probability. Indeed for the smallest R_c value the effective exponents $\nu(N)$ extrapolate to a value larger than 0.75. The two larger R_c values give indistinguishable results on this scale. Thus in our calculation we have used $R_c = 36$. This value

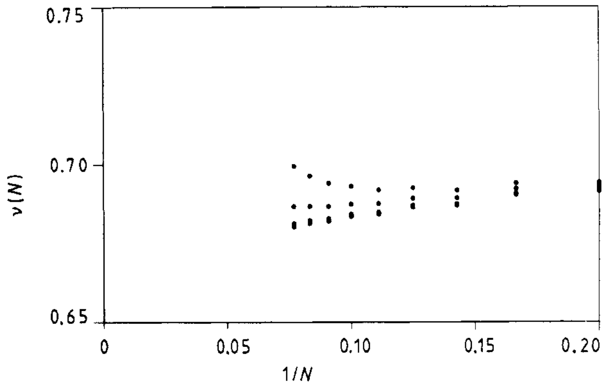

Figure 4. Plot of the effective exponent $\nu(N)$ against $1/N$ for different size lattices. The $\nu(N)$ are calculated on a lattice with radius $R_c = 11$, 15, 36, 56 (from top to bottom).

is smaller than the $R_c = 50$ value which was used for the LRWa enumeration. We expect that this will introduce a systematic error of ~0.001 for the higher η values. In their Monte Carlo study of the LRWr ($\eta = 1$) both Debierre and Turban, and Bradley and Kung, have used a variable R_c, namely only two times the actual length of the walk. As can be seen from our results, this is certainly not large enough to obtain the correct solution of the Laplace equation with $R_c \to \infty$. The slow convergence to the asymptotic solution is caused by the long-range behaviour of the Green function of the Laplace operator ($\ln r$ and $1/r$ for two and three dimensions respectively). Preliminary results of an enumeration in three dimensions ($N \leq 13$) show the same effect. Here the result of Bradley and Kung is also too large.

In summary we have shown the implications of different boundary conditions on the tail of the walk. This results in two different versions of the Laplacian random walk, one in which the tail of the trajectory acts like a hard wall (LRWr) and the other in which it acts like a sink (LRWa) for incoming diffusing particles. We have shown that the LRWr also has a continuously varying correlation length exponent ν. The value of $\nu(\eta)$ for the LRWr is always smaller than the corresponding value for the LRWa. Therefore the LRWr is a much denser object than the LRWa.

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