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

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

R Mark Bradley†, David Kung†, Jean-Marc Debierre‡ and Loïc Turban‡

† IBM T J Watson Research Center, PO Box 218, Yorktown Heights, NY 10598, USA
‡ Université de Nancy I, BP 239, F 54506 Vandoeuvre les Nancy, France

Abstract. In a recent letter Lyklema and Evertsz found a value of ν for the $\eta = 1$ Laplacian random walk which differs from the value we obtained for the diffusion-limited self-avoiding walk (DLSAW). We show that this results from different boundary conditions at the ends of these chains and not from a failing in our Monte Carlo studies of the DLSAW.

Recently we introduced a new self-avoiding walk (SAW) which grows without terminating as a model of the diffusion-limited growth of linear polymers (Debierre and Turban 1986, Bradley and Kung 1986). In this model—which is known as the diffusion-limited SAW (DLSAW)—bifunctional monomers diffuse to the growing tip of a polymer chain from faraway and adhere to the chain once a nearest-neighbour site of the tip has been reached. Once a monomer has adhered to the polymer, it moves no further. Our finite-size Monte Carlo studies yielded comparable values for the radius of gyration exponent on the square lattice: $\nu = 0.79 \pm 0.01$ (Debierre and Turban 1986) and $\nu = 0.774 \pm 0.006$ (Bradley and Kung 1986).

In a recent letter, Lyklema and Evertsz (1986) obtain the value $\nu = 0.67$ for the Laplacian random walk with reflecting boundary conditions (LRWr) with $\eta = 1$. Lyklema and Evertsz assume that the LRWr with $\eta = 1$ and the DLSAW are in the same universality class, and attribute the difference in the values of ν found in the DLSAW and the LRWr to finite-size effects in our studies of the DLSAW.

In this comment we show that in fact there is an important distinction between the boundary conditions at the tip of the chain in the DLSAW and the LRWr. It is this difference in boundary conditions which leads to the observed difference in the values of ν, not any failing in our Monte Carlo work on the DLSAW.

To see that the DLSAW and the LRWr are not the same, consider the example shown in figure 1. In the DLSAW, a diffusing monomer is released far from the chain. Two monomers cannot occupy the same site, and as the diffusing monomer moves it weights each of its unoccupied nearest-neighbour sites equally. The monomer adheres to the chain once it reaches a nearest-neighbour site of the tip, and so can only adhere at A or B§. In the LRWr, on the other hand, non-interacting random walkers are released at infinity and diffuse until they move onto the tip site and are absorbed. If a particle

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§ This is the limit of absolute adhesion ($\alpha = 1$) in Bradley and Kung (1986).
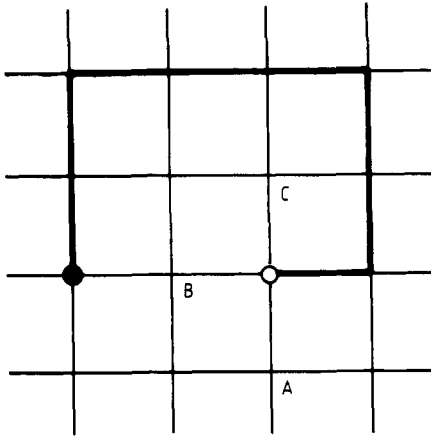
Figure 1. A conformation on the square lattice. The polymer is shown as a bold line, and the root and tip are shown as a closed and open circle, respectively.

is released at infinity each time one is absorbed, in the steady state the density of diffusers at r, $n(r)$, is given by

$$n(r) = \frac{1}{z - k'} \sum_{r'} n(r'). \tag{1}$$

Here z is the coordination number, k' is the number of occupied nearest-neighbour sites of r excluding the tip and the sum runs over the unoccupied nearest-neighbour sites r'. The density is subject to the normalisation condition $\sum n(r) = $ constant. Once the $n(r)$ have been determined, the probability of growth at an unoccupied nearest-neighbour site of the tip, r, is taken to be

$$\frac{n(r)}{\sum_{r'} n(r')}$$

where the sum runs over the unoccupied nearest-neighbour sites of the tip. In our example, it is easy to show that the probability of growth at C is $\frac{1}{3}$ that of growth at B and hence the former is non-zero. Therefore the growth probabilities are not the same in the DLSAW and the LRWr with $\eta = 1$ and there is no reason to assume that they share the same exponent ν. In fact, our example shows that there is a greater probability for the tip of the chain to enter a cul de sac in the LRWr, so we would expect the value of ν for the LRWr to be smaller than that found in the DLSAW. This is borne out by the numerical studies of the two models.

We have also obtained Monte Carlo evidence that the difference in boundary conditions at the tip of the polymer leads to the observed difference in scaling behaviour. It is convenient to first note that although the LRWr (as introduced by Lyklema and Evertsz) is formed by weighting the sites adjacent to the tip according to the solution of the steady-state diffusion equation, the same SAW can be constructed by releasing a monomer at infinity and allowing it to diffuse until it adheres to the tip, then releasing another monomer which diffuses until joining the polymer, and so on. In this new formulation of the LRWr, a nearest-neighbour site of the current position of the diffusing monomer is chosen at random at each time step. If this site is occupied by a polymer site other than the tip, the monomer remains where it is until the next time step. If the site is the tip, the monomer adheres to the polymer at its present position and

another monomer is released far from the polymer. Finally, if the chosen site is unoccupied, the monomer moves there and continues to diffuse. The monomer there-fore moves in exactly the same way as in the DLSAW except when it is at a nearest-neighbour site of the tip: having reached one of these sites, the diffuser in the LRWr need not adhere.

The equivalence between these two formulations of the LRWr is easily understood. In the new formulation, the probability that the diffusing monomer adheres at a particular nearest-neighbour site of the tip can be computed by releasing a large number of non-interacting walkers at infinity. At each time step, each walker randomly chooses one of the nearest-neighbour sites of its current position r. If this site is occupied by a polymer site other than the tip, the walker temporarily remains at r. If the site is unoccupied, the walker moves there. Lastly, if the chosen site is the tip, the walker is discarded and the tally of particles which would have adhered at r is increased by one. Another walker is then released at infinity. The single monomer in our formulation of the LRWr adheres at a site with probability proportional to the tally for this site. Clearly, in the steady state the density of diffusers satisfies equation (1), and the tally at each nearest-neighbour site of the tip is proportional to the value of n there. This is precisely Lyklema and Evertsz's formulation of the LRWr.

Having established this equivalence, we were able to perform a finite-size Monte Carlo study of the LRWr simply by changing the boundary condition at the tip in the program of Bradley and Kung. (Debierre and Turban's program could equally well have been employed.) We constructed 10 000 chains of length $N = 32$ on the square lattice using precisely the same variable discard radius used in Bradley and Kung (1986) and Debierre and Turban (1986). The finite-size scaling analysis was performed following Bradley and Kung (1986), and we refer the reader to this reference for details. Figure 2 shows our results for $\nu(N)$ for the LRWr. Also displayed are the values of $\nu(N)$ obtained by constructing 10 000 DLSAW of length 32 (Bradley and Kung 1986). It is immediately obvious that the values of ν obtained by extrapolating these data to $N = \infty$ are quite different, even though the simulations differed only in
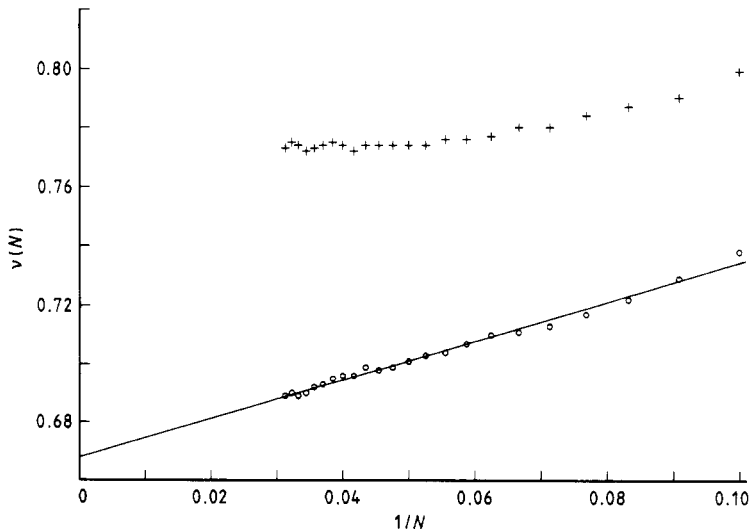

Figure 2. Plot of $\nu(N)$ against N^{-1} for the LRWr with $\eta = 1$ (open circles) and the DLSAW (crosses). The full line is the least-squares fit to the form (2).

the choice of boundary conditions at the polymer tip. Moreover, a least-squares fit to the first two terms in the expansion

$$\nu(N) \equiv \tfrac{1}{2} \ln[\langle R^2(N+1)\rangle / \langle R^2(N)\rangle] / \ln[(N+1)/N]$$

$$= \nu - \tfrac{1}{2} BN^{-1} - \tfrac{1}{2} \Delta CN^{-\Delta} + \ldots \tag{2}$$

yielded the value $\nu = 0.668 \pm 0.001$ for the LRWr with $\eta = 1$, in good agreement with Lyklema and Evertsz's result $\nu = 0.67$. These observations show conclusively that our value of ν for the DLSAW differs from Lyklema and Evertsz's result for the LRWr with $\eta = 1$ because the boundary conditions at the tip are not the same in the two models.

Finally, note that although Lyklema and Evertsz studied the effect of using different lattice sizes, their lattice size was held fixed during polymer growth. This makes a comparison with our work difficult because in our calculations the radius R_c at which a diffuser was discarded was varied as the polymer grew—we took R_c to be twice the distance from the seed to the furthest point in the chain. In Bradley and Kung it had a maximum value of the order of 24 lattice spacings; in Debierre and Turban it was larger still. Referring to figure 4 of Lyklema and Evertsz (1986), we see that for $R_c \sim 24$ the extrapolated value of ν could not possibly be as high as 0.8.

We conclude that finite-size effects in our Monte Carlo studies of the DLSAW cannot explain why the value of ν differs from that found in the LRWr, as contended by Lyklema and Evertsz. On the contrary, the DLSAW and the LRWr are in different universality classes because the way in which diffusing monomers adhere to the tip of the growing polymer differs in these two models: in the LRWr the monomers need not adhere to the chain once a nearest-neighbour site of the tip has been reached. This is in striking contrast to the situation in diffusion-limited aggregation, where the probability of adhesion on contact is believed to be irrelevant (Witten and Sander 1983, Meakin 1983a, b, Strenski and Bradley 1985).

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