Finite size analysis of eigenvalue spectrum for random walks on a critical percolation cluster in four dimensions

2000 J. Phys. A: Math. Gen. 33 2943

(http://iopscience.iop.org/0305-4470/33/15/303)

J. Phys. A: Math. Gen. **33** (2000) 2943–2950. Printed in the UK PII: S0305-4470(00)08320-7

Finite size analysis of eigenvalue spectrum for random walks on a critical percolation cluster in four dimensions

Sang Bub Lee† and Hisao Nakanishi‡

† Department of Physics, Kyungpook National University, Taegu, 702-701, Korea
‡ Department of Physics, Purdue University, W Lafayette, IN 47906, USA

Received 25 September 1999

Abstract. We study by Markov chain analysis the random walks on a critical percolation cluster embedded in a four-dimensional hypercubic lattice. We calculate the number of dominant eigenvalues of the transition probability matrix and estimate the spectral and fractal dimensions d_s and d_w of random walks from the eigenvalues and their distribution. The estimates of d_s and d_w obtained from the data for a given size S of the percolation cluster exhibit some S dependence. Extrapolating the results to $S \to \infty$ limit, we obtain $d_s = 1.330 \pm 0.010$ close to the previous result by other methods and a new result $d_w = 4.50 \pm 0.15$. These values are also confirmed by direct Monte Carlo simulations of random walks on a percolation cluster.

The random walk (RW) has served well as a model for the Brownian motion of particles, such as electrons in metal and colloidal particles in solution [1,2]. As the number of steps t gets larger, the rms displacement R_t normally increases as $R_t \propto t^{1/2}$, where the proportionality constant is related to the diffusion coefficient. On the other hand, percolation models, both lattice and continuum, play an important role in describing real materials, including the polyfunctional condensation of monomers, the hydrogen bond network in liquid water, the crosslinking of polymers, and the two-component disordered media [3–5].

The RW on a critical percolation network is naturally used to describe the elastic and transport properties in self-similar porous media [1,2,6]. The rms displacement of such RWs at t timesteps is known to exhibit an anomalous behaviour, given as $R_t \sim t^{1/d_w}$, with the fractal dimension of RWs d_w greater than 2.

Recently, the critical behaviour of such RWs was studied by a technique called Markov chain analysis, in which the probability $P(t)$ that a walker returns to the starting point and the velocity autocorrelation function $\langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(0) \rangle$ after t timesteps are related to the eigenvalue spectrum of the transition probability matrix $\boldsymbol{W}$ of RW [7,8]. The matrix $\boldsymbol{W}$ is defined with its ijth element equal to the probability that a particle at a site j hops to a site i in the next timestep. The matrix element W_{ij} depends on the type of RW model, such as the blind ant or the myopic ant model [9]. The blind ant moves to one of the occupied nearest neighbour sites in one timestep with equal probability of $\frac{1}{z}$ (z being the coordination number of the underlying lattice) and it remains at the same site with the probability equal to $(z - z_i)/z$ (z_i being the number of occupied nearest neighbour sites of the site i). On the other hand, the myopic ant never stays at the same site but always moves to one of the nearest neighbour occupied sites with equal probability $\frac{1}{z_i}$ at each timestep. In both cases, each element of the matrix $\boldsymbol{W}$ is equal to or greater than zero and the sum of all elements in each column is equal to 1, i.e. $\boldsymbol{W}$ is a Markov matrix.

0305-4470/00/152943+08$30.00

In the long-time limit, $P(t)$ and $\langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(0) \rangle$ are expected to obey the following power laws:

$$P(t) \sim t^{-d_s/2} \tag{1}$$

$$\langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(0) \rangle \sim t^{2/d_w - 2} \tag{2}$$

d_s being the spectral dimension of the underlying fractal substrate. For a standard diffusive behaviour on a regular lattice, d_s is equal to the spatial dimensionality d, while on a fractal it is generally different from d.

It is known [7,8] that $P(t)$ and $\langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(0) \rangle$ in the long-time limit are the Laplace transforms of the density of the eigenvalues $n(\lambda)$ and the quantity $\pi(\lambda) = n(\lambda) a_\lambda S(\lambda - 1)^2$ which scale, respectively, as

$$n(\lambda) \sim |\ln \lambda|^{d_s/2 - 1} \tag{3}$$

and

$$\pi(\lambda) \sim |\ln \lambda|^{1 - 2/d_w} \tag{4}$$

S and a_λ being, respectively, the size of the underlying cluster and the expansion coefficient of the position autocorrelation function to a power series of λ. Thus, equations (3) and (4) can be used to determine d_s and d_w from the eigenvalues and eigenvectors of the transition probability matrix in the region of the spectrum near $\lambda = 1$.

Based on this idea, researchers in [8,10–12] have studied the static and dynamic properties of various fractal substrates. They obtained on critical percolation clusters $d_s/2 - 1 = -0.35 \pm 0.01$ in both two (2D) and three dimensions (3D), $1 - 2/d_w = 0.30 \pm 0.01$ in 2D, and 0.46 ± 0.03 in 3D, for the range of the system sizes they used. These values correspond to, respectively, $d_s = 1.30 \pm 0.02$, $d_w = 2.86 \pm 0.04$, and $d_w = 3.70 \pm 0.07$. When compared with earlier estimates using other methods [9, 13], these Markov chain estimates were very close to the earlier ones in 2D, while in 3D the estimate of d_s was somewhat smaller, though that of d_w was close.

In this paper, we explicitly show by basically the same work in 4D that the estimates of d_s and d_w for a finite system depend on the size of the underlying clusters, and that careful finite size analysis should be undertaken to extract the correct values. Since the finite size effect alters the matrix elements W_{ij} near the edges, some eigenvalues will also be altered accordingly. Although the previous results in 2D and 3D reported negligible finite size effects (except when finite size scaling analyses of the very edge of the spectrum were performed), it is unclear whether or not the finite size effects in this method are generally small even for higher dimensions. We will see later that our data indeed indicate that the estimates of the powers in equations (3) and (4) depend substantially upon the size of the underlying clusters. We calculate both d_s and d_w, for the sake of cross-checking, by an alternative method of Monte Carlo simulation for RWs on a hypercubic lattice of 50^4 sites and find that results are in excellent agreement with those of the Markov chain analysis. It should be emphasized that, to the best of our knowledge, our estimate of d_w is new and no comparable estimate has been reported before now, although the upper and lower bounds were given in the review [2]. The spectral dimension d_s is also confirmed by an estimate using the subdominant eigenvalues.

The infinite percolation cluster at percolation threshold is generated using the breadth-first search algorithm. The known value of the percolation threshold $p_c = 0.197$ [3,14] was used for this purpose. (We also confirmed this value by Monte Carlo renormalization calculations [15] coupled with the finite size scaling analysis.) Once the desired cluster is obtained, we construct the matrix $\boldsymbol{W}$ from the number of occupied neighbouring sites, using the blind ant rule. We then calculate number of dominant eigenvalues using the Arnoldi–Saad algorithm [16], the

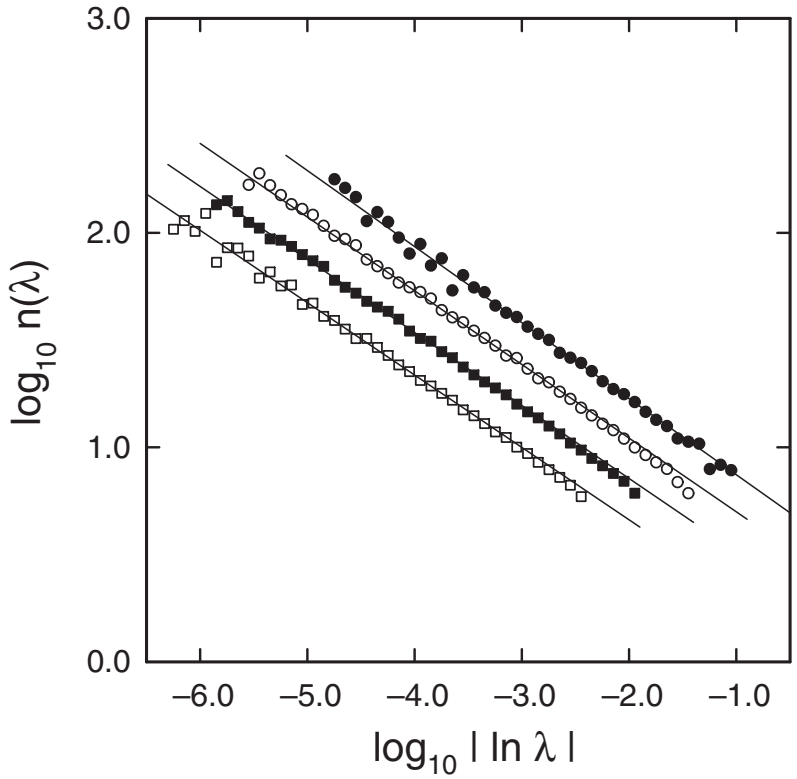

Figure 1. Plot of $10^{\alpha}n(\lambda)$ against the $|\ln\lambda|$ on a double common logarithmic scale for various sizes of cluster: from below, $S = 15\,000$ ($\alpha = 0$), $S = 8000$ ($\alpha = 0.2$), $S = 3000$ ($\alpha = 0.4$), and $S = 1000$ ($\alpha = 0.6$).

details of which were described in [8]. Since in this paper we are interested in the extent to which the estimates of d_s and d_w are dependent on the size of cluster S, we analyse our data for various values of S, ranging from $S = 500$ to $S = 15\,000$.

Shown in figure 1 is $n(\lambda)$ versus $|\ln\lambda|$, plotted on a double common logarithmic scale, for selected values of S. Data from below are for $S = 15\,000$, 8000, 3000, and 1000, shifted vertically by amounts of, respectively, 0, 0.2, 0.4, and 0.6, to avoid overcrowding of the data points. The solid line on each set of data is the regression fit obtained from at least two decades of $|\ln\lambda|$ in the large eigenvalue region near $\lambda = 1$, which corresponds to the asymptotic limit of $t \gg 1$ for RWs. However, the choice of the fitting region for the power-law behaviour is more or less subjective, implying that slightly different regions yield different powers. The fitting region was, thus, selected as an interval for which the linear regression coefficient is optimal (closest to 1), and the variation of the slopes was included in the error. As the size of cluster increases, the absolute slope of the regression fit gradually decreases, indicating that the finite size affects the distribution of the eigenvalues. The estimated slopes vary from -0.355 (for $S = 1000$) to as large as -0.338 (for $S = 15\,000$). This implies that a naive estimate of d_s from the data for any given size system gives the wrong result, and that the correct value should be obtained in the $S \to \infty$ limit.

In order to visualize how the estimates of the slope vary as S increases, we plot in figure 2 the slope against S^{-1}. If one estimates d_s with the data for $S = 15\,000$, it would be about

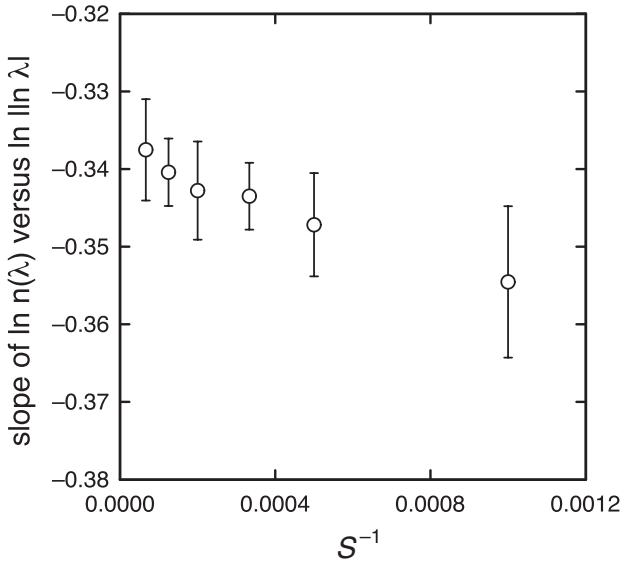

Figure 2. Plot of the slopes obtained from the regression fits of double common logarithmic plots of $n(\lambda)$ versus $|\ln\lambda|$ against the inverse of the size of cluster.

1.325, which is already close to the earlier estimate [13]. From the trend, one can expect that the slope for an infinite cluster would yield a slightly larger value. A simple eyeball extrapolation fit indicates that the data appear to converge to a value of -0.335 ± 0.010. The corresponding value of d_s would be $d_s = 1.330 \pm 0.010$, which is consistent with the earlier estimate $d_s = 1.328 \pm 0.006$ [2, 13].

Our observation that the Markov chain estimates of d_s and d_w show non-negligible finite size effects in 4D percolation is in contrast to the results of the previous works for 2D and 3D percolation. Whether a more careful analysis of size dependence would expose similar finite size effects (and allow for better exponent estimates) even in 2D and 3D remains to be seen.

The plot of $\pi(\lambda)$ is qualitatively similar to those of the earlier works in low dimensions. The slope estimated from the plot of $\pi(\lambda)$ against $\ln\lambda$ on a double logarithmic scale is presented in figure 3. Apparently, the slope increases as the size of cluster increases, again indicating that the estimate of d_w for a finite size system gives the wrong result. If one estimates the exponent d_w from the slope for a given size system, one would get $d_w \simeq 3.99$ for $S = 1000$ and $d_w \simeq 4.40$ for $S = 15\,000$. However, from the figure, it is clear that the correct value of d_w would be even larger than the latter. The intercept on the ordinate, i.e. the slope in the infinite system limit, is obtained by a simple eyeball fit as 0.55 ± 0.01, yielding $d_w = 4.50 \pm 0.15$.

The subdominant eigenvalue λ_2 is known to be related to the cluster size S as [8]

$$|\ln\lambda_2| \sim S^{-2/d_s} \sim S^{-d_w/d_f} \tag{5}$$

from which one can also estimate d_s. Figure 4 is the plot of $|\ln\lambda_2|$ against S; the symbols are the logarithmic average of the eigenvalues and the solid line is the regression fit. The slope of the fit is 1.5071 ± 0.0037, which yields $d_s = 1.327 \pm 0.004$. This value is very close to our earlier estimate. Since this analysis is based on finite size scaling, it is clear that the spectrum edge shows finite size effect.

The spectral and fractal dimensions of RWs can also be obtained alternatively by direct measurement of $P(t)$ and R_t. For the consistency check, we generated RWs on an 'incipient'

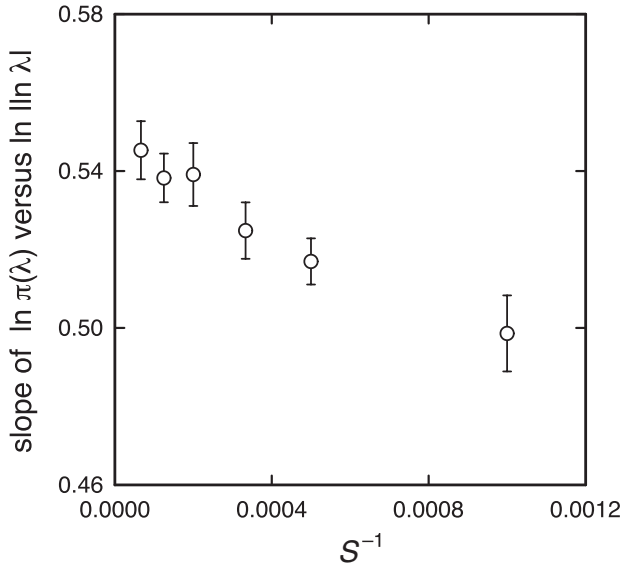

Figure 3. Plot of the slopes obtained from the regression fits of double common logarithmic plots of $\pi(\lambda)$ versus $|\ln\lambda|$ against the inverse of the size of cluster.

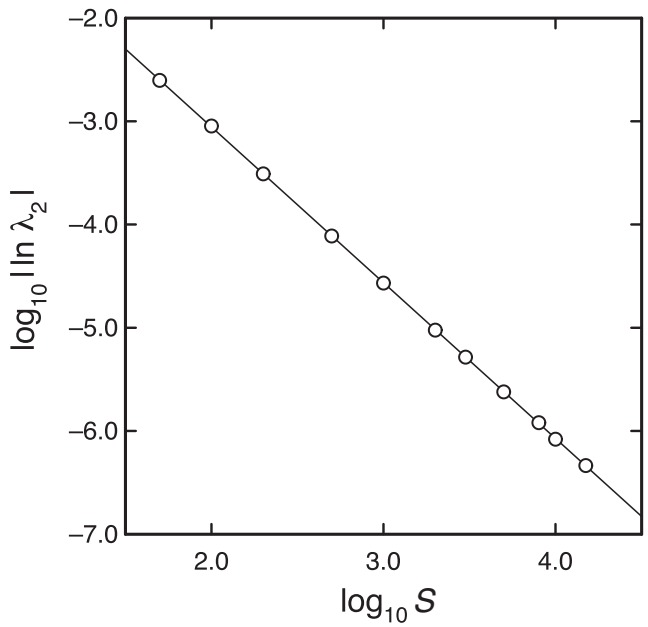

Figure 4. The subdominant eigenvalues plotted against the size S on a double common logarithmic scale. The size of error bar on each data is smaller than the size of symbol and the solid curve is the regression fit.

infinite network on a 50^4 hypercubic lattice using the blind ant rule. An infinite network in a given cell of side L is defined in two ways: (i) clusters which span along all coordinate directions and (ii) clusters which span along any (one or more) of the coordinate directions. In

both rules, the cluster must wrap the cell along the spanned coordinate direction(s) by periodic boundary conditions, so that RWs may extend further to the periodic images of the system without termination at the cell edges. We use $p_c = 0.1988$ in rule (i) and $p_c = 0.197$ in rule (ii). The slightly larger value is chosen in rule (i) to save computing time because there are fewer chances of sampling desired clusters in rule (i). A predetermined number of RWs are sampled, each from the randomly selected points, and the probability $P(t)$ and the mean square displacement are averaged over 2.5×10^4 walks on each realization and over 60 realizations.

The raw Monte Carlo data of $P(t)$ exhibited strong even–odd oscillations due to the characteristic of the underlying lattice structure. We averaged the data within every interval of $\Delta(\ln t) = 0.05$ to get rid of such oscillations and plotted the result on the average position in each interval. The linear regression fit for $100 \leqslant t \leqslant 50\,000$ yielded a good linear behaviour (not shown) with the slope -0.6647 ± 0.0009 which, accordingly, yielded $d_s = 1.329 \pm 0.002$. This value is in excellent agreement with our earlier estimate by eigenvalue spectrum and also with the estimate from the subdominant eigenvalues.

In order to estimate d_w from the data for rms displacement, one should plot, as for $P(t)$, R_t against t on a double logarithmic scale and estimate the asymptotic slope in the $t \to \infty$ limit. However, if the rms displacement exhibits nontrivial correction terms, as it turns out, estimation of d_w will not be as simple as for $P(t)$. Assuming nonanalytic correction terms in R_t, one can write

$$R_t = At^{1/d_w}(1 + Bt^{-s} + Ct^{-1} + \cdots). \tag{6}$$

In order to estimate the value of $1/d_w$, we define the effective value $d_{w,\mathrm{eff}}^{-1}(t)$, similar to $\nu_{\mathrm{eff}}(t)$ in [17], which results in, using equation (6),

$$d_{w,\mathrm{eff}}^{-1}(t) = 1/d_w + at^{-s} + bt^{-1} + \cdots. \tag{7}$$

Shown in figure 5 is the $d_{w,\mathrm{eff}}^{-1}(t)$ plotted against t^{-1}; the circles are those obtained by rule (i) and the crosses by rule (ii). From the figure, it appears that there exists a strong nonanalytic correction term with $s < 1$. If this is indeed the case, then the plot of $d_{w,\mathrm{eff}}^{-1}(t)$ against t^{-s} is expected to exhibit linear behaviour in the $t \gg 1$ region. On this basis, we have chosen s as a parameter and plotted $d_{w,\mathrm{eff}}^{-1}(t)$ against t^{-s}. The best linear fits were obtained for $s = 0.27$ for the data from rule (i) and $s = 0.25$ for those from rule (ii), as shown in the inset of figure 5, and, from these, the value of $1/d_w$ was estimated to be 0.221 ± 0.001 and 0.213 ± 0.001 for rule (i) and rule (ii), respectively. Such a strong correction has not been reported before, as far as we are aware. It should be noted that the result by rule (i) is slightly larger than that by rule (ii), apparently due to the fact that the underlying clusters in (i) are more compact than those in (ii). The displacement of RWs on such compact clusters is generally enhanced, yielding a smaller estimate of d_w. We thus expect $1/d_w = 0.22 \pm 0.01$, which is again consistent with that by Markov chain analysis.

With our estimates of $d_s = 1.33 \pm 0.01$ and $d_w = 4.50 \pm 0.15$ for RWs, the fractal dimension of the underlying percolation cluster can be obtained, using the Alexander–Orbach scaling relation [18], as $d_F = d_s d_w/2 = 2.99 \pm 0.13$, which is consistent, within error bounds, with the known values [2, 19, 20].

In summary, we have calculated by Markov chain analysis the two exponents d_s and d_w of RWs on an infinite network of 4D percolation at the percolation threshold. Our results indicated that the power-law exponent of the density of eigenvalues for the transition probability matrix $\boldsymbol{W}$ as a function of $|\ln \lambda|$ decreases as the size of system increases. Extrapolating to an infinite system limit, it appeared to better agree with the previously available estimates than that obtained without the extrapolation.

Such a size dependence is caused by the incorrectly determined matrix elements of the occupied sites near the cluster edges. Since we employed the blind ant model and since the

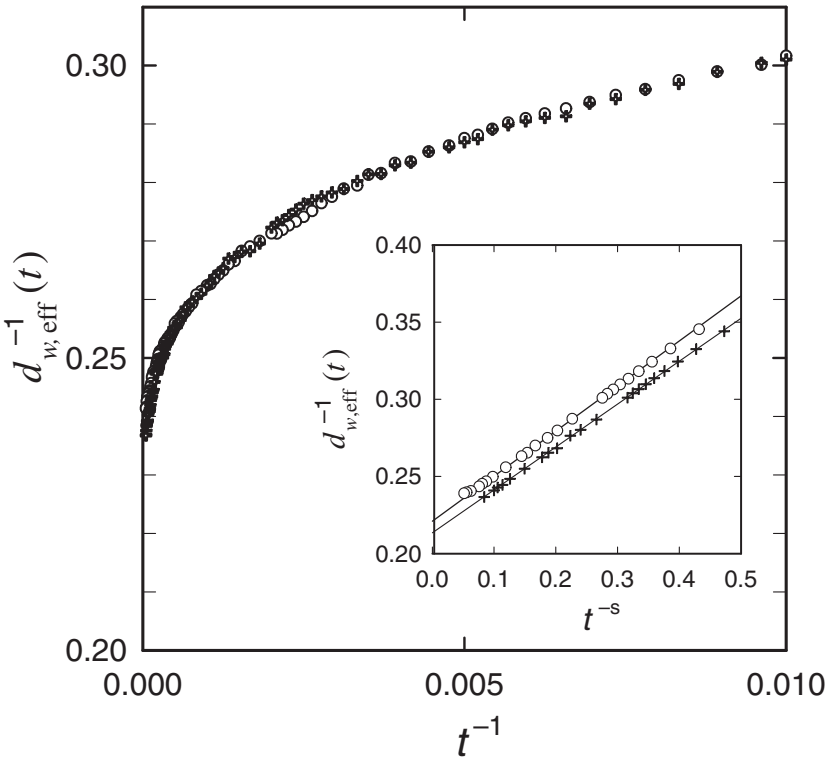

Figure 5. The effective exponent $d_{w,\mathrm{eff}}^{-1}(t)$ against t^{-1} for random walks on an infinite cluster. The circles are the data by rule (i) and the crosses by rule (ii) described in the text. The inset is the plot against t^{-s}, with $s = 0.27$ for circles and $s = 0.25$ for crosses.

undetermined sites neighbouring to the edge sites were treated as if they were unoccupied, the matrix elements of those sites would have varied if the clusters were extended beyond the desired size. The variation of the eigenvalues corresponding to those elements appear to have yielded the size effect in estimating d_s and d_w. One possible way to investigate how those elements affect the estimates of d_s and d_w would be to compare the results with those of direct Monte Carlo simulations of RWs on the same finite size clusters.

We have also studied, for corroboration, RWs on sufficiently large spanning clusters by direct Monte Carlo simulations and found that the spectral and fractal dimensions of the RWs were consistent with those of the Markov chain analysis. Considering these results, it appears that the Markov chain analysis is a viable alternative technique for studying RWs on disordered media as long as the finite size effect is carefully taken into account.

Acknowledgments

The major part of this work was done while SBL visited Purdue University. He acknowledges the hospitality of Purdue Physics Department. This work was supported by the Basic Science Research Institution (BSRI 1998-015-D00132) at Kyungpook National University and also by the Korean Science and Engineering Foundation under grant No 981-0207-029-2.

References

[1] See for example, Shlesinger M F and West B J (ed) 1984 *Random Walks and Their Applications in the Physical and Biological Sciences (AIP Conf. Proc. vol 109)* (New York: AIP)
[2] Havlin S and Ben-Avraham D 1987 *Adv. Phys.* **36** 695 and references therein
[3] Stauffer D and Aharony A 1992 *Introduction to Percolation Theory* (London: Taylor and Francis)
[4] Essam J W 1980 *Rep. Prog. Phys.* **43** 833
[5] Kirkpatrick S 1973 *Rev. Mod. Phys.* **45** 574
[6] Pfister G and Sher H 1978 *Adv. Phys.* **27** 747
[7] Fuchs N H and Nakanishi H 1991 *Phys. Rev.* A **43** 1721
[8] Nakanishi H, Mukherjee S and Fuchs N H 1993 *Phys. Rev.* E **47** R1463
see also Mukherjee S, Nakanishi H and Fuchs N H 1993 *Phys. Rev.* E **49** 5032
[9] Majid I, Ben-Avraham D, Havlin S and Stanley H E 1984 *Phys. Rev.* B **30** 1626
[10] Nakanishi H 1993 *Physica* A **196** 33
[11] Jacobs D J, Mukherjee S and Nakanishi H 1994 *J. Phys. A: Math. Gen.* **27** 4341
[12] Mukherjee S, Jacobs D J and Nakanishi H 1995 *J. Phys. A: Math. Gen.* **28** 291
[13] Rammal R, Angles d'Auriac J C and Benoit A 1984 *Phys. Rev.* B **30** 4087
[14] Ballesteros H G, Fernandez L A, Martin-Mayor V, Munoz Sudupe A, Parisi G and Ruiz-Lorenzo J J 1997 *Phys. Lett.* B **400** 346
[15] Reynolds P J, Stanley H E and Klein W 1980 *Phys. Rev.* B **21** 1223
[16] Saad Y 1980 *Linear Algebra Appl.* **34** 269
see also Arnoldi W E 1951 *Q. Appl. Math.* **9** 17
[17] Lam P M 1990 *J. Phys. A: Math. Gen.* **23** L831
[18] Alexander S and Orbach R 1982 *J. Physique Lett.* **43** L625
[19] Jan N, Hong D C and Stanley H E 1985 *J. Phys. A: Math. Gen.* **18** L935
[20] Grassberger P 1986 *J. Phys. A: Math. Gen.* **19** 1681