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Random walks on random systems: Eigenspectrum of large Markov matrices

Hisao Nakanishi, Sonali Mukherjee, and Norman H. Fuchs
Department of Physics, Purdue University, West Lafayette, Indiana 47907
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We study the eigenvalue spectrum of the hopping transition probability matrix W for the random walk in randomly diluted clusters, both in critical and weak dilution. We obtain the relations between the spectrum in the limit where the eigenvalue $|\lambda| \to 1$ and the long-time behavior of the velocity autocorrelation function and mean probability of the random walk to return to the starting point after t steps by scaling and by numerical diagonalization of W.

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The random-walk problem is encountered in many physically interesting situations, including transport phenomena such as electrical conduction [1], the Brownian motion of a tagged particle in fluid [2], and the conformational statistics of macromolecular chains [3, 4]. Particularly interesting in this connection is the case where the random walk is constrained to a disordered medium, e.g., electrical conduction in a random mixture of good and poor conductors [5], fluid flow through a porous medium, or information flow through randomly flawed network.

On the one hand, the random walk confined to a critically disordered medium (a *fractal* [6]) executes *anomalous diffusion* [7], and on the other hand, if the disorder is weak, a *long-time tail* appears in the velocity autocorrelation function as for the so-called Lorentz gas [8, 9]. In the past, these different regimes were studied mostly separately using rather different approaches and techniques. In this Rapid Communication, we focus on some quantities that are ideally suited for studying the two regimes from a unified point of view. The key is the spectral properties of some Markov matrices [10] that describe the disorder and kinetics of the particular problem at hand.

We model a disordered medium in the simplest possible way using a randomly site-diluted lattice in two and three dimensions. If each site is removed as inaccessible to the random walker with an independent probability $1-p$, then the remaining sites of the lattice can be grouped into connected components (defining *connection* through nearest-neighbor bonds between remaining sites) called *clusters*, using the terminology of the percolation problem [11]. For p greater than the percolation threshold p_c, there will be one indefinitely large cluster (in addition to finite ones); this cluster will be used as the model disordered medium in which to study the random walk that hops from a site to one of its nearest neighbors at each time step. At $p = p_c$, the infinite cluster is *incipient* in that it is just at the point of breaking up into many finite clusters.

First, the transition probability matrix W is constructed where the element W_{ij} is simply the probability for the random walker to jump from site j to site i in a given time step. The size of the matrix is $S \times S$ (S being the cluster size); an infinite cluster may be effectively represented either by a truncated large cluster or by using periodic boundary conditions. W is random since a nonzero entry corresponds to a nearest-neighbor connection in a randomly created percolation cluster, and it is a *Markov* matrix [10] since the sum of the elements (each of which is non-negative) in each column is exactly 1. The kinetics of the random walk is represented in the hopping probability W_{ij}. In this Rapid Communication, we are mostly interested in the *blind-ant* [12] kinetics in which all off-diagonal nonzero elements $W_{ij} = 1/z$ (where z is the full coordination number of the lattice) and where the remaining diagonal elements are such that each column adds up to 1.

Since W contains all the information on the geometry of the cluster and the kinetics of the random walk, we expect to be able to extract any information on the behavior of the random walk at a discrete time t from the properties of this matrix. One way to obtain the behavior of, say, the velocity autocorrelation function would be to calculate the expectation values of W^t in suitable states explicitly [13–15]. However, more insight is provided by looking for the relationship between the intrinsic spectral properties of W and that of the random walk described by W.

For the Markov matrix W satisfying the detailed balance condition when applied to a positive-definite stationary state, all eigenvalues λ are real [16] and between -1 and 1. As we will explicitly determine, the density $n(\lambda)$ of the eigenvalues has a power-law behavior in terms of $|\ln|\lambda||$ in the limit of $|\lambda| \to 1$, and this behavior can be related directly to a physical quantity in the time domain [17].

To see this in a simple way, consider for integer time step t,

$$\mathrm{Tr}\, W^t \equiv P(t)S = \sum_{\lambda} \lambda^t. \qquad (1)$$

The quantity $P(t)$ is simply the mean probability of the random walk to return to the starting point in t steps, if the initial distribution is uniform over the cluster. For large t, only λ near ±1 contribute significantly to $P(t)$. For a blind ant in general and for a myopic ant (which avoids attempting to step into vacant sites) in media that are *not* bipartite (i.e., that do not decompose into two equivalent sublattices connected by nearest-neighbor bonds), the spectrum for $\lambda < 0$ is relatively insignificant (no $\lambda = -1$ and no buildup near -1). For a myopic ant on a bipartite cluster, the spectrum is symmetric about $\lambda = 0$. Thus, the right-hand side of Eq.(1) can be replaced by $\sum_{\lambda\approx1}\lambda^t$ for the long time behavior. Then, upon inverse Laplace transforming Eq.(1), we obtain for small ω

$$\frac{1}{2\pi i}\int_\Gamma dz\, e^{\omega z}\mathrm{Tr}\, W^z \approx \sum_{\lambda\approx1}\frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{i(\omega-|\ln\lambda|)t} \tag{2}$$

$$= \sum_{\lambda\approx1}\delta(\omega-|\ln\lambda|), \tag{3}$$

where (1) has been continued analytically to the complex plane and Γ is along the imaginary axis.

The quantity on the right is the density of the eigenvalues Λ in the space of $\omega \equiv |\ln\Lambda|$, and for Λ near 1, it is essentially equal to $n(\Lambda)$. Since $P(t)$ has in general an asymptotic power-law decay in time [12], Eqs.(1)–(3) then imply that $P(t)$ corresponds to the Laplace transform of $n(\lambda)$ in the variable $|\ln\lambda|$ (for large t, and thus for $\lambda \to 1$). Thus the following scaling relation between the leading power laws is obtained:

$$n(\lambda) \sim |\ln\lambda|^x \Longleftrightarrow P(t) \sim t^{-x-1}. \tag{4}$$

Let us note that the Laplace connection between $P(t)$ and $n(\lambda)$ is a direct analog of the technique known as the equation-of-motion method, used, e.g., in the calculation of the electron density of states for oxides with defects [18]. In that case, the trace is applied to the time evolution operator $e^{-iHt/\hbar}$, giving the density of states for the quantum-mechanical system with random defects.

Moreover, when we note the equivalence [19] between the diffusion and the lattice vibration problems, it becomes clear that, for p_c, the relationship discussed above is essentially the same as that discussed by Alexander and Orbach [20] in introducing the so-called *fracton* regime of the fractal lattice vibrations. Thus the fracton density of states corresponds to the density of the eigenvalues of W at p_c, and the verification of Eq.(4) by the explicit calculation of $n(\lambda)$ amounts to verifying the underlying assumption in the fracton problem that the equivalence works even for the (randomly) diluted geometry. Above p_c, the analogous correspondence is between the phonon density of states and the eigenvalue density of W.

Returning to the random walk, since the long-time behavior of $P(t)$ is the same for both blind and myopic ants, the eigenvalue density $n(\lambda)$ must also behave in the same way as $\lambda \to 1$. At critical dilution $p = p_c$, $P(t) \sim t^{-d_s/2}$ (where d_s is the spectral dimension of the percolation problem), resulting in $n(\lambda) \sim |\ln\lambda|^{d_s/2-1}$. For weak dilution ($p > p_c$), we have the usual Lorentz-gas regime with asymptotically diffusive behavior $P(t) \sim t^{-d/2}$, which leads to $n(\lambda) \sim |\ln\lambda|^{d/2-1}$. Note that this implies the saturation of eigenvalue density for $d = 2$ and indeed a power-law decrease for $d = 3$ as $\lambda \to 1$. It is interesting to note that the study of the crossover from the anomalous diffusion to Lorentz gas regimes corresponds to that from the fracton-to-phonon regimes in the lattice vibration problem [21]. In Table I, the values of x are summarized for $d = 2$ and 3.

These results have been checked by calculating $n(\lambda)$ using a numerical method to approximately diagonalize the matrix W. In this method [16, 22], a relatively small square matrix of typically 300 rows is first constructed from the much larger matrix W (of typically several thousand to 15 000 rows). Then this smaller matrix is exactly diagonalized. This corresponds to obtaining approximate eigenvalues λ and eigenvectors v_λ in the sense that $(W - \lambda I)v_\lambda$ is only orthogonal to the basis vectors of the subspace chosen. In this way, about 200 of the largest eigenvalues and their eigenvectors are determined to six digit accuracy.

The square-lattice results in Fig. 1(a) have been obtained for the percolating cluster formed on a 100×100 grid with periodic boundary conditions averaging over 750, 1000, and 400 clusters for $p = 0.593$ ($\approx p_c$), 0.75, and 0.90, respectively, all for the blind ant. The particular fit line shown at p_c has a slope of -0.357, while the lines to guide the eye for $p = 0.75$,0.90 have a slope of about 0.027,0.052, respectively. The corresponding slope for the myopic ant at p_c is nearly the same (0.37 ± 0.01) as for the blind ant, as expected, but the data are not shown to avoid overcrowding in the figure [23]. The simple cubic lattice results in Fig. 1(b) have been obtained for the blind ant on the 30^3 grid with periodic boundaries averaging over 449 and 100 clusters for $p = 0.312(\approx p_c)$ and 0.50, respectively. The fit line shown here at p_c has a slope of -0.35 and the line to guide the eye for $p = 0.50$ has a slope of about 0.44. Again the corresponding slope for the myopic ant at p_c is also about -0.35, as it should be, but those data are not shown [23].

The agreement with the scaling predictions is excellent at p_c for both the square lattice and the simple cubic lattice. For $p > p_c$ only qualitative agreement may be concluded. Clearly, the density $n(\lambda)$ does *not* build up as $\lambda \to 1$, as it does for p_c, but the oscillations (*not* statistical fluctuations) are much too great to accurately fit for a power law.

It was recently pointed out [16] that the long-time behavior of the envelope of the *oscillating* velocity autocorrelation function for the myopic ant on the bipartite cluster at p_c can be related to the $\lambda \to -1$ behavior of a certain function $\pi(\lambda)$:

$$\pi(\lambda) \sim |\ln|\lambda||^y \Longleftrightarrow |\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle| \sim t^{-y-1}, \tag{5}$$

with $y = d_s/2 - 1$ for this case. The function $\pi(\lambda)$ is

TABLE I. Exponent x for $n(\lambda)$. Estimates at p_c are for the blind ant, and numerical values for d_s are from Ref. [12].

d	This work ($p = p_c$)	$d_s/2 - 1$ ($p = p_c$)	$d/2 - 1$ ($p > p_c$)
2	-0.35 ± 0.01	-0.347 ± 0.013	0
3	-0.35 ± 0.01	-0.336 ± 0.003	$\frac{1}{2}$

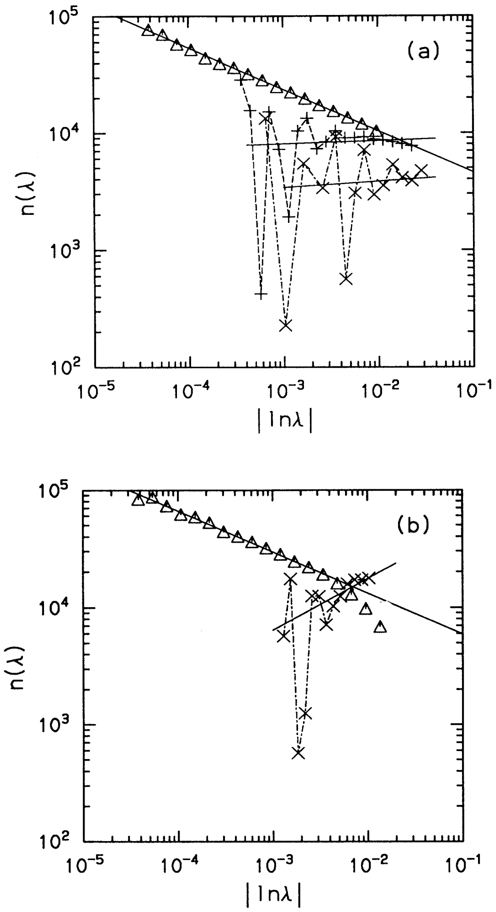

FIG. 1. Density $n(\lambda)$ of the eigenvalues of the Markov matrix W for the blind ant on the spanning percolation cluster is shown in (a) for the square and in (b) for the simple cubic lattice. In (a) symbols Δ, $+$, and $\times$ correspond to $p = 0.593$, 0.75, and 0.90, respectively, and in (b) Δ and $\times$ correspond to $p = 0.312$ and 0.50, respectively.

given by

$$\pi(\lambda) \equiv n(\lambda) a_\lambda (\lambda - 1)^2, \tag{6}$$

where a_λ are coefficients determined when the stationary initial distribution is expanded in terms of the eigenvectors of W [13, 16].

This was shown assuming that the spectrum near $\lambda = -1$ dominates the autocorrelation in the long-time limit and therefore that the Laplace transform type relationship exists between the leading behavior of $\pi(\lambda)$ (as $\lambda \to -1$) and that of the velocity autocorrelation function (as $t \to \infty$). Although it was discussed only for the myopic ant problem at p_c, such a relation can in fact be generalized.

For example, for a blind ant, $n(\lambda)$ builds up anomalously at p_c as $\lambda \to 1$ as discussed above, and the resulting power-law behavior of $\pi(\lambda)$ dominates the autocorrelation in the long-time limit. Thus, in this case, the velocity autocorrelation does *not* oscillate in sign (rather, always negative, representing the *cage effect*), and the

TABLE II. Exponent y for $\pi(\lambda)$ of the blind ant. Numerical values for d_w from Ref. [12].

d	This work ($p = p_c$)	$1 - 2/d_w$ ($p = p_c$)	$d/2$ ($p > p_c$)
2	0.30 ± 0.01	0.30 ± 0.01	1
3	0.46 ± 0.01	0.46 ± 0.03	$\frac{3}{2}$

anomalous diffusion exponent $y = 1 - 2/d_w$ applies in Eq.(5) [12, 13]. Similarly, for $p > p_c$, where the velocity autocorrelation decays as $t^{-d/2-1}$, we would expect $\pi(\lambda) \sim |\ln\lambda|^{d/2}$. In Table II we summarize the values of y for the blind ant. Even for the myopic ant on a bipartite cluster, the center line through the oscillating autocorrelation function behaves much like the autocorrelation for the blind ant, and the eigenvalue spectrum near $\lambda = 1$ is very similar to that of the blind ant.

Plotted in Fig. 2 are the numerical results obtained by the same approximate diagonalization of the matrix W as for $n(\lambda)$. The number of clusters used for averaging is 400, 250, and 200 for $p = 0.593$, 0.75, and 0.90, respectively for the square lattice in (a), and 199 and 100 for $p = 0.312$ and 0.50, respectively for the simple cubic lattice in (b). Otherwise the parameters of these data are

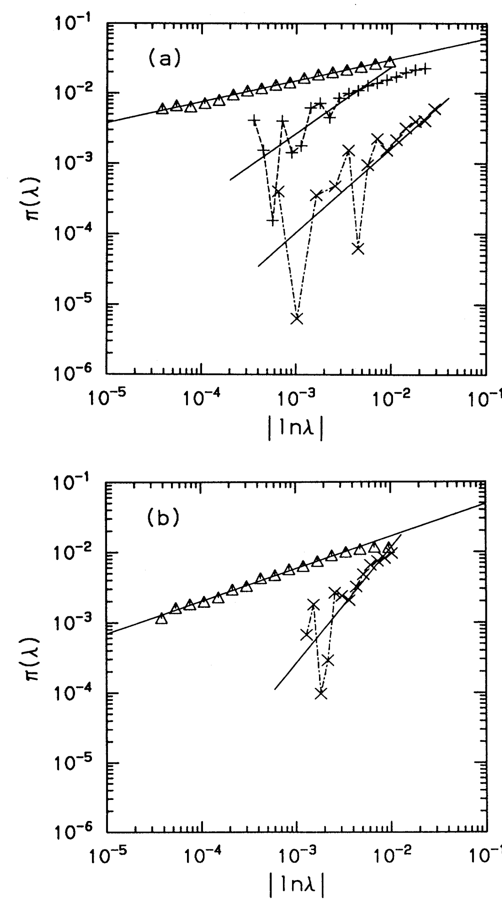

FIG. 2. The function $\pi(\lambda)$ corresponding to each of the cases in Fig.1 is shown. Symbols correspond to the same cases.

the same as for Fig. 1. In (a) the best-fit line for p_c has a slope of 0.30 and the lines drawn to guide the eye for $p = 0.75,0.90$ have a slope of about 0.95,1.2 respectively. In (b) the best-fit line for p_c has a slope of 0.46, while that for $p = 0.50$ has a slope of 1.65.

Clearly, the discussion above for Eq.(5) is consistent with the data. Furthermore, we can see that the crossover from p_c to above p_c progresses as $\pi(\lambda)$ in the region of λ close to 1 first breaks away from the p_c result, and then the newly formed region of the Lorentz gas regime increases in size as p is raised further. This is accompanied by the overall decrease of π, as the velocity autocorrelation is much smaller for the Lorentz gas regime than for the anomalous diffusion regime.

In conclusion, we have presented the scaling relations between the properties of the spectrum of the Markov matrix W and the velocity autocorrelation and mean probability of the random walk to return to the starting point. These relations are confirmed numerically, which may be interpreted to verify the equivalence of the diffusion and vibration problems on the randomly constrained geometry.

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[1] See, e.g., *Random Walks and Their Applications in the Physical and Biological Sciences*, edited by Michael F. Shlesinger and Bruce J. West, AIP Conf. Proc. No. 109 (AIP, New York, 1984).

[2] For an introduction, see, e.g., R. K. Pathria, *Statistical Mechanics* (Pergamon, Oxford, 1977); for original descriptions, see P. Langevin, C. R. Acad. Sci. (Paris) **146**, 530 (1908); A. Einstein, *Investigations on the Theory of the Brownian Movement* (Dover, New York, 1956); M. Smoluchowski, Ann. Phys. **21**, 756 (1906).

[3] P. G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University, Ithaca, NY, 1979), and references therein.

[4] J. des Cloizeaux and G. Jannink, *Polymers in Solution: Their Modeling and Structure* (Oxford, New York, 1990), and references therein.

[5] See, e.g., J. P. Straley, in *Electrical and Optical Properties of Inhomogeneous Media*, edited by J. C. Garland and D. B. Tanner, AIP Conf. Proc. No. 40 (AIP, New York, 1978).

[6] B. Mandelbrot, *Fractal Geometry of Nature* (Freeman, San Francisco, 1982).

[7] Y. Gefen, A. Aharony, and S. Alexander, Phys. Rev. Lett. **50**, 77 (1983).

[8] B. J. Alder and W. E. Alley, J. Stat. Phys. **19**, 341 (1978); Physica A **121**, 523 (1983).

[9] M. H. Ernst and A. Weyland, Phys. Lett. **34A**, 39 (1971).

[10] See, e.g., N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).

[11] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, 2nd ed. (Taylor and Francis, London, 1992).

[12] S. Havlin, and D. Ben-Avraham, Adv. Phys. **36**, 695 (1987), and references therein.

[13] D. Jacobs and H. Nakanishi, Phys. Rev. A **41**, 706 (1990).

[14] I. Majid, D. Ben-Avraham, S. Havlin, and H. E. Stanley, Phys. Rev. B **30**, 1626 (1984).

[15] A. Giacometti, H. Nakanishi, A. Maritan, and N. H. Fuchs, J. Phys. A **25**, L461 (1992).

[16] N. H. Fuchs and H. Nakanishi, Phys. Rev. A **43**, 1721 (1991); similar (but smaller scale) calculations were also reported earlier in H. Nakanishi, Y. Meir, Y. Gefen, A. Aharony, and P. Schofield, J. Phys. A **20**, L153 (1987), but the scaling exponent was incorrectly interpreted.

[17] A. B. Harris, Y. Meir, and A. Aharony, Phys. Rev. B **36**, 8752 (1987) pointed out the same connection. We apply it at p_c and $p > p_c$ and evaluate $n(\lambda)$ explicitly in this work.

[18] J. W. Halley (private communication) and J. W. Halley and H. B. Shore, Phys. Rev. B **36**, 6640 (1987), and references therein.

[19] See, e.g., E. W. Montroll and B. J. West, in *Fluctuation Phenomena*, edited by E. W. Montroll and J. L. Lebowitz (North-Holland, Amsterdam, 1979).

[20] S. Alexander and R. Orbach, J. Phys. Lett. (Paris) **43**, 625 (1982).

[21] G. S. Grest and I. Webman, J. Phys. (Paris) **45**, L1155 (1984); K. Yakubo and T. Nakayama, Phys. Rev. B **36**, 8933 (1987).

[22] Y. Saad, Linear Algebra Appl. **34**, 269 (1980); see also W. E. Arnoldi, Quart. Appl. Math. **9**, 17 (1951).

[23] Although the main point of Ref. [16] was the calculation of a different quantity (i.e., the exponent associated with the envelope of an oscillating velocity autocorrelation), that work also mentioned some crude estimates for the exponent x of the myopic ant at p_c. Unfortunately, those values are significantly different from the ones calculated here. We attribute this to an incomplete analysis in [16] which failed to distinguish the asymptotic regime properly.