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Transfer-matrix methods and results for directed percolation

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For directed percolation, the second nontrivial eigenvalue of the transfer matrix is shown to have its maximum at p_c. Using this, we obtain for $(1+1)$-dimensional directed site percolation $p_c = 0.706\,522 \pm 0.000\,005$, which agrees within 10^{-3} with other results, but is nevertheless significantly (in terms of quoted uncertainties) different from them. We also relate other quantities to the transfer-matrix spectrum and eigenfunctions.

I. INTRODUCTION

This paper has two principal themes. First we give relations between the spectrum and eigenfunctions of the transfer matrix and quantities of physical interest. Secondly, we use these relations to obtain numerical results for $(1+1)$-dimensional directed site and bond percolation. These results turn out to be in significant disagreement with previously published[1] work, work that we would otherwise have considered extremely reliable. Because of the potential seriousness of the issues raised we also supply details of numerical checks that we have made.

II. NOTATION

Sites are labeled (x,t), with both labels integer valued. Let A_{xt} and B_{xt} be a collection of independent $\{0,1\}$-valued random variables with $\langle A_{xt}\rangle = \langle B_{xt}\rangle = p$ for all x,t with fixed p, $0 \le p \le 1$. For directed bond percolation (DBP) the A's and B's are directed bond occupation variables with A_{xt} connecting (x,t) to $(x,t+1)$ and B_{xt} connecting (x,t) to $(x+1,t+1)$. For directed site percolation (DSP) A_{xt} is site occupation. Define an auxiliary set of $\{0,1\}$-valued variables $\mu(x,t)$ called "wetness," which for DBP satisfy

$$\mu(x,t+1) = B_{x-1,t}\mu(x-1,t) + A_{xt}\mu(x,t) - B_{x-1,t}A_{xt}\mu(x-1,t)\mu(x,t) . \quad (1)$$

This equation is a Boolean OR for simultaneous wetness and bond occupation in either of the precursors of site $(x,t+1)$. For $\{0,1\}$-valued x and y it is convenient to define

$$g(x,y) \equiv x + y - xy = (x \text{ OR } y) . \quad (2)$$

For DSP the evolution law corresponding to (1) is

$$\mu(x,t+1) = A_{xt}\, g(\mu(x,t),\mu(x+1,t)) . \quad (3)$$

Let μ be an N-vector of 0's and 1's and let $\mu(t) = (\mu(1,t), \mu(2,t), \ldots, \mu(N,t))$. Let $\psi(\mu,t) = \text{Prob}(\mu(t) = \mu \,|\, \mu(0) = \mu^{(0)})$ where the implicit dependence of ψ on $\mu^{(0)}$ has been suppressed. It follows that

$$\psi(\mu,t+1) = \sum_{\eta} W(\mu,\eta)\psi(\eta,t) , \quad (4)$$

where $W(\mu,\eta) = \text{Prob}(\mu(t+1) = \mu \,|\, \mu(t) = \eta)$ is the transition or transfer matrix. Equations (1) and (3) imply

$$W(\mu,\eta) = \prod_{j=1}^{N} (\mu_j\beta_j + \bar{\mu}_j\bar{\beta}_j) , \quad (5)$$

with $\bar{x} \equiv 1 - x$, μ_j is defined as the jth component of μ,

$$\beta_j = p^{1-\alpha} g(p^{\alpha}\eta_j, p^{\alpha}\eta_{j+1}) , \quad (6)$$

and $\alpha = 1$ for DBP, $\alpha = 0$ for DSP. Proofs of this and many of our subsequent assertions may be found in Ref. 2. In the space direction we take periodic boundary conditions.

For numerical work we make two significant reductions in the size of W. First, we restrict attention to translationally invariant eigenfunctions. Secondly, for DSP the evolution of the vector $\gamma(\mu) \equiv [g(\mu_1,\mu_2), g(\mu_2,\mu_3), \ldots, g(\mu_N,\mu_1)]$ is essentially the same as that of μ itself. Therefore for questions of relevance to percolation it is sufficient to study the reduced transfer matrix

$$T(\delta,\delta') = \text{Prob}(\gamma(\mu) = \delta \,|\, \gamma(\eta) = \delta') , \quad (7)$$

where in (7) η and μ are dummy variables. [The transition probability depends *only* on $\gamma(\eta)$, not η.] Defining $G(\delta) = \{\mu \,|\, \gamma(\mu) = \delta\}$, it follows that

$$T(\delta,\delta') = \sum_{\mu \in G(\delta)} \prod_{x=1}^{N} (\mu_x\phi_x + \bar{\mu}_x\bar{\phi}_x) , \quad (8)$$

with $\phi_x = p\delta'_x$.

III. FEATURES AND USE OF THE TRANSFER MATRIX

Shown in Fig. 1 are eigenvalues for DSP with $N = 7$. In previous work[3] the changing curvature of $\lambda_1(p)$ has been used to locate the percolation threshold p_c. We will argue

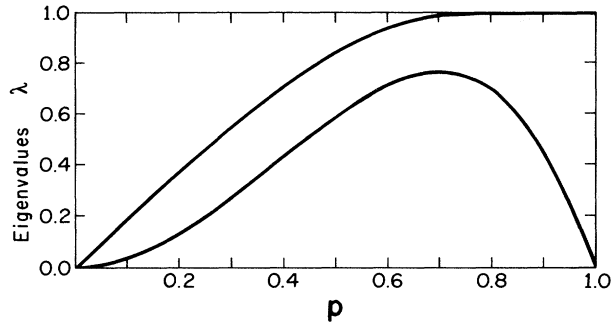

FIG. 1. Two largest nontrivial eigenvalues of the transfer matrix for seven-site DSP as a function of p.

that $p^*(N) \equiv p_2^{(N)}$, the location of the maximum in $\lambda_2(p)$, converges to p_c. [Numerically, for DSP, $p^*(N)$ converges exponentially fast to a number within 0.001 of published values of p_c, but which nevertheless differs significantly from those values.] Other features of transfer-matrix eigenvalues and eigenvectors will be related to physical quantities.

Let $\theta(t) = \text{Prob}(\mu_t \neq v \mid \mu_0 = s)$, where $s = (1,0,\ldots)$ (which represents "single"), $v = (0,\ldots)$ (which represents "vacuum"), and the N dependence is suppressed. By (4), $\theta(t) = \sum_{\mu \neq v} W^t(\mu, s)$. We assume[4] a spectral representation for W

$$W = \sum_{\alpha=0}^{2^N-1} \lambda_\alpha \psi_\alpha^R \psi_\alpha^{L\dagger}, \tag{9}$$

where right (R) and left (L) eigenvectors of W are distinguished. The eigenvalue $\lambda_0(p) \equiv 1$ is guaranteed by the stochastic property of W. We take $\psi_0^L(\mu) = 1$ for all μ and it follows that $\psi_0^R(\mu) = \delta_{\mu v}$. This eliminates $\alpha = 0$ when (9) is used for $\theta(t)$ and we have

$$\theta(t) = \sum_{\mu \neq v} \sum_{\alpha \geq 1} \lambda_\alpha^t \psi_\alpha^R(\mu) \psi_\alpha^{L*}(s). \tag{10}$$

It is useful to define W', coinciding with W except for the removal of the row and column labeled by v. Although W' is not stochastic, it is non-negative and, unlike W, it is irreducible (see Thm. 8, Chap. 5, Ref. 5). It follows that there is only one eigenvalue of maximum modulus, that it is positive and that its eigenvector is positive. Aside from λ_0, the spectra of W and W' coincide and the eigenvectors are simply related. Denoting eigenvectors of W' by ϕ we have for the right eigenvectors of W,

$$\psi_\alpha^R(\mu) = \left(-\sum_{\eta \neq v} W_{v\eta} \phi_\alpha^R(\mu)/(1-\lambda_\alpha),\ \phi_\alpha^R(\mu) \right).$$

It is convenient to take $\sum_\mu \phi_1^R(\mu) = 1$ [which implies $\psi_1^R(v) = -1$].

Except at p_c, λ_1 is found to be finitely (as $N \to \infty$) separated from λ_2 and we have, for large t,

$$\theta(t) \sim \lambda_1^t \psi_1^L(s). \tag{11}$$

For $p < p_c$, $\lambda_1^{(N)}(p)$ is bounded away from 1 (for $N \to \infty$) and relating $\theta(t)$ to the normal percolation concepts we have $\xi_\parallel(p) = 1/[-\ln\lambda_1(p)]$.

For $p > p_c$, $\lambda_1(p) \sim 1 - e^{-N/\xi^*}$. There is reason to believe[6] $\xi^* = \xi_\perp$. For ordinary (nondirected) percolation above p_c, ξ characterizes large clusters that are *not* part of the infinite cluster. Similarly, for directed percolation with $p > p_c$ we take $\xi_\parallel$ to govern the survival time of clusters that do not last indefinitely. However, care must be exercised since for finite N every cluster dies on a time scale of order $1/(1-\lambda_1) \sim e^{N/\xi_\perp}$. For deriving $\xi_\parallel$ this scale is to be thought of as infinite and we define $\xi_\parallel$ in terms of t such that $1 \ll t \ll 1/(1-\lambda_1)$. On this scale, Eq. (11) shows that $\psi_1^L(s)$ is just the usual percolation probability—giving a handle on this quantity that is conceptually independent of Monte Carlo or series extrapolation. The quantity $\xi_\parallel$ is thus defined by the asymptotic relation

$$e^{-t/\xi_\parallel} \sim \bar{\theta}(t) \equiv \text{Prob}(\mu_t \neq v \mid \mu_0 = s,\ \mu_{t'} = v) \tag{12}$$

for $1 \ll t \ll t' \ll 1/(1-\lambda_1)$. [For any particular $p(\neq p_c)$, there is a lower bound on N such that these inequalities are satisfied.] A series of manipulations based on the spectral expansion of W shows that[7]

$$\bar{\theta} = \lambda_2^t \sum_{\beta \geq 2} \left(\frac{\lambda_\beta}{\lambda_2} \right)^t \psi_\beta^{L*}(s) \sum_{\mu \neq v} \psi_\beta^R(\mu)/[1 - \psi_1^L(s)]. \tag{13}$$

Note that t' does not appear in (13). Thus $\xi_\parallel(p) \to \infty$ for $p \searrow p_c$, requires that $\max_p \lambda_2^{(N)}(p) \to 1$ as $N \to \infty$ and that *the location of this maximum tends to* p_c. If we further assume that (13) is in fact dominated by λ_2^t, we have (for $N \to \infty$)

$$\xi_\parallel = 1/[-\ln\lambda_2(p)],\ p > p_c. \tag{14}$$

Another result of general interest is

$$\text{Prob}(\mu(t) = \mu \mid \mu(0) = s \text{ and } \mu(t') \neq v \text{ for } t' \gg t) \sim \psi_1^R(\mu) \psi_1^{L*}(\mu), \tag{15}$$

showing that $\psi_1^R(\mu)\psi_1^L(\mu)$ plays the role of probability measure for instantaneous configurations within the "infinite" cluster.

IV. NUMERICAL TECHNIQUES

To study the problem numerically we first generate the transfer matrices for strips of finite width N. Because of the translational symmetry, the number of basis vectors for the W' matrix is greater than or equal to $1 + (2^N - 2)/N$ (equality holds for prime N). For the T matrix, the number of basis vectors is further reduced. (In fact, it grows asymptotically like a^N/N with $a \simeq 1.75$.) Thus for small n one can work out the transfer-matrix elements by hand. These elements are polynomials in p, given by Eqs. (5)–(7). When N is not small, it is fairly straightforward to program the process of writing down the polynomial matrix elements.

We then diagonalize the transfer matrices and find the eigenvalues $\lambda_i(p)$. We have used MATLAB.[8] for the numerical diagonalization. For present purposes, we are only concerned with $\lambda_2(p)$. The quantity $p_2^N \equiv p^*(N)$ is the value of p for which $\lambda_2^{(N)}(p)$ is maximum. As shown above [Eq. (14) and discussion preceding it], $p^*(N) \to p_c$ as $N \to \infty$. It can also be shown that $1 - \lambda_2^{(N)}(p^*) \sim 1/N^x$, where $x = \nu_\parallel/\nu_\perp$, the ratio of the critical exponents for the longitudinal and the perpendicular correlation lengths. We used these two relations to estimate p_c

and x for DSP and DBP.

We tested our numerical work with a variety of internal checks. The W' matrices for DBP for up to $N=7$ and the T matrices for DSP up to $N=9$ were worked out by hand. After mechanizing the generation of the matrix elements these matrices were reproduced and extended up to $N=10$ (107 basis vectors) for DBP and $N=12$ (76 basis vectors) for DSP. Another test consisted in using the W' matrices for DBP to generate W' matrices for DSP, using $\alpha=0$ rather than $\alpha=1$ in Eq. (6). The results thus obtained for DSP were in perfect agreement with those from the T matrices, derived independently. Finally, we worked out the transfer matrix for $N=3$ without using the vector space reduction due to translational invariance. The values for λ_1 and λ_2 were in perfect agreement with those of the reduced W' and T for the equivalent N.

V. NUMERICAL RESULTS

Our results for p^* and $1-\lambda_2^{(N)}(p^*)$ for DBP are summarized in Table I. For DSP, the $p^*(N)$ increase monotonically with N, beyond (but close to) the currently believed[1] percolation value of 0.705489. Plotting p^* as a function of $1/N$ and $1/N^2$ shows that the convergence of p^* to p_c is faster than either alternative. This led us to test for a possible exponential convergence of the form $p^*(N)\sim p_c - Ae^{-\alpha N}$, where A and α are constants. Our data for $N>7$ support this assumption, with $\alpha=0.50\pm0.01$ and $p_c=0.706522\pm0.000005$. If we further assume that $\alpha=\frac{1}{2}$, the error bars for A and p_c reduce, yielding $p_c=0.706518\pm0.000002$, but we cannot justify $\alpha=\frac{1}{2}$ other than by its aesthetic appeal.

The data for the percolation probability of DBP are less conclusive. In this case, $p^*(N)$ decreases monotonically with N but convergence to p_c is not as fast. Plots of $p^*(N)$ show that the convergence is faster than $1/N$ but slower than $1/N^2$ and definitely not exponential. For our largest $N=10$, p^* is still above the currently believed value of $p_c=0.644699$. However, a naive extrapolation according to the formula $p^*\sim p_c - A/N^\alpha$ (A and α are constants) is more consistent with $p_c=0.6450$, a value which is, again, slightly higher than that currently accepted. The shift in p_c, incidentally, would cause a significant shift in the exponents reported in Ref. 9.

To obtain the ratio $x=v_\parallel/v_\perp$, we plot $\ln[1-\lambda_2(p^*)]$ as a function of N. This should yield a curve with constant slope x. Instead, the slope of the curve increases slightly with N for DBP, and it decreases for DSP. Fortunately, the slopes seem to converge. For DBP, the convergence is faster than $1/N$ but slower than $1/N^2$. For DSP, the convergence is faster than $1/N^2$, but slower than $1/N^3$. In either case, we extrapolate the local slopes with a three-parameter fit of the form $x+A/N^\alpha$ (A and α are constants). We thus obtain $x=1.5879\pm0.0005$ for DBP, and $x=1.588\pm0.001$ for DSP. Although these results are in agreement with each other, as predicted from universality, they disagree with recent numerical work[1,3,10] and with the conjectured[1] values of the critical exponents for directed percolation, $x=\frac{26}{15}/\frac{79}{72}=1.5797\ldots$.

Finally we mention another numerical result of interest. For all values of p and sufficiently large N, some of the eigenvalues below λ_2 pick up an imaginary part. Because of the presence of larger eigenvalues (in norm) this does not imply a violation of the Markov condition, but it may be surprising. Complex eigenvalues were also reported in Ref. 10, where there were indications that the imaginary parts go to zero for $N\to\infty$.

VI. CONCLUSIONS

Various properties of directed percolation are related to eigenvalues and eigenfunctions of the transfer matrix. Interpreting directed percolation as a description of a stochastic process leads to corresponding associations with the master equation.

Of the general results we obtain, the relation of λ_2 to $\xi_\parallel$ for $p>p_c$ leads to surprising numerical consequences. It seems that for directed site percolation the location of the maximum of $\lambda_2(p)$ [which we call $p^*(N)$] converges exponentially fast to a number p^* which our theoretical considerations suggest should equal p_c. In fact it agrees with published values within 0.1%. However, at that level it does disagree, and since those published values (as well as our number) have a claimed 10^{-6} accuracy we are left with a significant and unexplained discrepancy. A change in the estimate of p_c at the 10^{-3} level also causes a shift in critical exponents.

TABLE I. Results for p^* and $1-\lambda_2^{(N)}(p^*)$ for DBP and DSP.

	DBP			DSP	
N	p^*	$1-\lambda_2(p^*)$	N	p^*	$1-\lambda_2(p^*)$
2	0.6886615	0.724838			
3	0.6718086	0.4939116	3	0.7034683	
4	0.6631806	0.3538142	4	0.7045147	0.5295724
5	0.6582834	0.2658667	5	0.7050803	0.3873086
6	0.6552337	0.2076364	6	0.7055862	0.2960564
7	0.6531959	0.1671856	7	0.7059299	0.2345034
8	0.6517590	0.137934	8	0.7061516	0.1910554
9	0.6507022	0.1160684	9	0.7062930	0.1591977
10	0.6498985	0.0992665	10	0.7063821	0.1350935
			11	0.7064368	0.1163748
			12	0.7064684	0.1015182

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