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## LETTER TO THE EDITOR

**Precise critical exponents for the basic contact process**

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**Abstract.** We calculated some of the critical exponents of the directed percolation universality class through exact numerical diagonalizations of the master operator of the one-dimensional basic contact process. Perusal of the power method together with finite-size scaling allowed us to achieve a high degree of accuracy in our estimates with relatively little computational effort. A simple reasoning leading to the appropriate choice of the microscopic time scale for time-dependent simulations of Markov chains within the so-called quantum chain formulation is discussed. Our approach is applicable to any stochastic process with a finite number of absorbing states.

In its original formulation [1, 2], the so-called directed percolation (DP) conjecture stated that all continuous phase transitions about a single absorbing state in single-component systems with a scalar order parameter are in the DP universality class of critical behaviour [3]. In this form the conjecture has been confirmed in a host of model systems, amongst others the basic contact process [4, 5], Schlögl's models for autocatalytic chemical reactions [1, 2, 6], and a phenomenological classical field theory of high-energy hadronic collision processes [7–10]. Further investigation revealed that the DP universality class is robust enough to accommodate more general models, with more than a single component [11–14] as well as with multiple, in some cases infinitely many absorbing states [15–17]. Even some nonequilibrium growth models without absorbing states were found to share some of the DP exponents [18–20]. For recent reviews, see [21, 22].

The basic contact process (CP) [4, 5] may be viewed as a model for the spread of an epidemic amongst individuals living in a  $d$ -dimensional orchard. In this process, a healthy individual  $\emptyset$  becomes infected at a rate proportional to the number of its infected neighbours, whilst an infected individual  $X$  becomes healthy at unit rate. Pictorially, in one dimension it is defined by the elementary processes  $X\emptyset\emptyset \xrightarrow{\lambda} XX\emptyset$ ,  $\emptyset\emptyset X \xrightarrow{\lambda} \emptyset XX$ ,  $X\emptyset X \xrightarrow{2\lambda} XXX$ , and  $X \xrightarrow{1} \emptyset$ . As  $\lambda$  increases from zero, the basic CP suffers an extinction–survival phase transition in all dimensions, the upper critical dimension being  $d^* = 4$ . There is not an exact evaluation of the critical points  $\lambda^*$  for  $d < d^*$  to date, but there are some narrow bounds: in one dimension it is known that  $1.539 < \lambda^* < 1.942$  [23].

In this letter we were concerned with the accurate determination of the critical point and some of the critical exponents of the one-dimensional basic CP through exact numerical diagonalizations of its master operator. Our method is based on the standard matrix power method [24] applied to a discrete-time version of the continuous-time Markov chain, taking advantage of the presence of an absorbing state. Combined with finite-size scaling [25] and modern extrapolation techniques [26], the method allowed for a high degree of numerical

accuracy within quite reasonable computational efforts. Successful attempts at the application of phenomenological renormalization group ideas to directed problems on the lattice dates back at least to the work of Kinzel and Yeomans [3], and have from time to time reappeared in the literature with varied levels of sophistication [27]. The application of the ‘quantum chain formulation’ of Markov chains on the lattice [28] to study time-dependent properties, however, remained scarce; for a recent example, see [29]. In this work we provide a simple reasoning leading to the appropriate choice of the microscopic time scale for simulations that should be of value to anyone interested in similar calculations.

The starting point of our approach is the master equation on the lattice. Let  $\Lambda \subset \mathbb{Z}$  be a one-dimensional lattice of  $|\Lambda| = L$  sites with periodic boundary conditions. To each site  $\ell \in \Lambda$  we attach a random variable  $n_\ell$  taking values in a finite set  $\omega = \{0, 1, \dots, N-1\} \subset \mathbb{N}$ , the state of the whole lattice being given by  $\mathbf{n} = (n_1, n_2, \dots, n_L) \in \Omega = \omega^\Lambda$ . In the basic CP sites can only be healthy or infected, thence  $N = 2$ . Given positive real numbers  $\Gamma(\tilde{\mathbf{n}}, \mathbf{n})$  denoting the rates at which the collision  $\mathbf{n} \rightarrow \tilde{\mathbf{n}}$  occurs, the master equation governing the time evolution of the probability  $P(\mathbf{n}, t)$  of realization of the configuration  $\mathbf{n}$  at instant  $t$  reads

$$\frac{d}{dt}P(\mathbf{n}, t) = \sum_{\tilde{\mathbf{n}}} [\Gamma(\mathbf{n}, \tilde{\mathbf{n}})P(\tilde{\mathbf{n}}, t) - \Gamma(\tilde{\mathbf{n}}, \mathbf{n})P(\mathbf{n}, t)]. \quad (1)$$

We now introduce vector spaces in the description of the above equation. To do this we turn  $\omega$  into  $\mathbb{C}^N$  and write

$$|P(t)\rangle = \sum_{\mathbf{n}} P(\mathbf{n}, t)|\mathbf{n}\rangle \quad (2)$$

for the generating vector of the probabilities  $P(\mathbf{n}, t) = \langle \mathbf{n} | P(t) \rangle$ , with  $\{|\mathbf{n}\rangle\}$  the orthonormal basis diagonal in the occupation number representation. We are in this way providing the space of generating functions with a Hilbert space structure. We then rewrite equation (1) as

$$\frac{d}{dt}|P(t)\rangle = -H|P(t)\rangle \quad (3)$$

where  $H$  is given by

$$H = \sum_{\tilde{\mathbf{n}}} \sum_{\mathbf{n}} H(\tilde{\mathbf{n}}, \mathbf{n})|\tilde{\mathbf{n}}\rangle\langle \mathbf{n}| \quad (4)$$

with  $H(\tilde{\mathbf{n}}, \mathbf{n}) = -\Gamma(\tilde{\mathbf{n}}, \mathbf{n})$  and  $H(\mathbf{n}, \mathbf{n}) = \sum_{\tilde{\mathbf{n}} \neq \mathbf{n}} \Gamma(\tilde{\mathbf{n}}, \mathbf{n})$ .  $H$  is but the infinitesimal generator of the Markov semigroup  $U(t) = \exp(-tH)$  of the continuous-time Markov chain  $\{\mathbf{n}(t), t \geq 0\}$  defined by the set of rates  $\Gamma(\tilde{\mathbf{n}}, \mathbf{n})$ . The spectrum of  $H$  lies in the complex right half-plane, and since  $H$  is a real matrix, its eigenvalues are either real or come in complex conjugate pairs. The steady state of  $H$  has eigenvalue zero, and for finite systems it is, up to symmetry degeneracies, unique. If we realize the algebra of operators of  $\Omega$  in terms of spin  $S$  Pauli matrices [28], the master operator  $H$  of the basic CP can be seen to be equivalent to a spin  $S = \frac{1}{2}$ , three-body non-Hermitian quantum chain.

The lowest gap  $E^{(1)} - E^{(0)} = E^{(1)}$  in the spectrum of  $H$  may be used to perform a finite-size scaling analysis in the same way as one does in equilibrium problems [25]. Let us briefly review some formulae. Around the critical point  $\lambda \gtrsim \lambda^*$ , the correlation lengths of the infinite system behave like

$$\xi_{\parallel} \propto \xi_{\perp}^z \propto (\lambda - \lambda^*)^{-\nu_{\parallel}} \propto (\lambda - \lambda^*)^{-\nu_{\perp}z} \quad (5)$$

where  $\xi_{\parallel}$  and  $\xi_{\perp}$  are the correlation lengths, respectively, in the time and space directions,  $\nu_{\parallel}$  and  $\nu_{\perp}$  are the corresponding critical exponents, and  $z = \nu_{\parallel}/\nu_{\perp}$  is the dynamic critical exponent. Notice that in the interacting particle systems literature it is more usual to find  $z$

defined as  $z = 2v_{\perp}/v_{\parallel}$ . For finite systems of size  $L$ , according to the usual finite-size scaling assumptions [25] we expect

$$\xi_{\parallel,L}^{-1} = L^{-z_L} \Phi(|\lambda - \lambda_L^*| L^{1/v_{\perp,L}}) \tag{6}$$

where  $z_L$  and  $v_{\perp,L}$  are the finite versions of  $z$  and  $v_{\perp}$  and  $\Phi(x)$  is a scaling function with  $\Phi(x \gg 1) \sim x^{\nu_{\parallel}}$ . On general grounds one expects  $\lim_{L \rightarrow \infty} \lambda_L^*, z_L, v_{\perp,L} = \lambda^*, z, v_{\perp}$ . From equations (5) and (6) we obtain

$$\frac{\ln[\xi_{\parallel,L}(\lambda_L^*)/\xi_{\parallel,L'}(\lambda_L^*)]}{\ln(L/L')} = \frac{\ln[\xi_{\parallel,L''}(\lambda_L^*)/\xi_{\parallel,L}(\lambda_L^*)]}{\ln(L''/L)} = z_L \tag{7}$$

which through the comparison of three different system sizes  $L' < L < L''$  furnishes simultaneously  $\lambda_L^*$  and  $z_L$ . According to equation (6), the exponent  $v_{\perp,L}$  may be calculated through  $v_{\perp,L}^{-1} = z_L + \frac{1}{2}(\zeta_{L',L} + \zeta_{L,L''})$ , where

$$\zeta_{M,N} = \frac{\ln[(\partial \xi_{\parallel,N}^{-1}/\partial \lambda)/(\partial \xi_{\parallel,M}^{-1}/\partial \lambda)]}{\ln(N/M)} \tag{8}$$

with the derivatives calculated at  $\lambda = \lambda_L^*$ . Of course,  $\xi_{\parallel,L}^{-1} = \text{Re}\{E_L^{(1)}\}$ .

Several possibilities exist to proceed with the calculation of the gaps. When  $H$  is a symmetric matrix, Lanczos diagonalization becomes the method of choice. For stochastic processes, however,  $H$  is in general nonsymmetric, and although there exist nonsymmetric variations of the Lanczos algorithm, they are either much more memory demanding or are intrinsically unstable [24]. Since we are interested in only one very precise eigenvalue, we choose to work with the power method, which requires only matrix-by-vector multiplications that can be carried out using high precision data types.

In order to apply the power method, we first define the matrix  $T = 1 - \tau H$ . This matrix should be viewed as the time evolution operator of a discrete-time Markov chain whose transitions take place at intervals  $\tau$ . For  $T$  to be a stochastic matrix, its elements ought to satisfy  $0 \leq T(\tilde{n}, n) \leq 1$  and  $\sum_{\tilde{n}} T(\tilde{n}, n) = 1$ . This last condition is always satisfied, simply because  $\sum_{\tilde{n}} H(\tilde{n}, n) = 0$ . The first condition, however, demands that  $\tau^{-1} \geq \max\{|H(\tilde{n}, n)|\} = \max\{H(n, n)\}$ . Since we will calculate the eigenvalues of  $T$  by an iterative procedure, convergence will occur at a maximal rate if we choose  $\tau$  as large as possible, and we take  $\tau^{-1} = 1.01 \times \max\{H(n, n)\}$ . It is not advisable to take  $\tau^{-1} = \max\{H(n, n)\}$  because this will zero some elements in the diagonal of  $T$ , thus introducing cycles in an otherwise acyclic Markov chain. The spectrum of  $T$  lies in the unit circle, with the steady state corresponding to the eigenvalue one. Notice that the spectra of  $H$  and  $T$  appear in reverse order. The above choice of the microscopic time scale  $\tau$  for the discrete-time Markov chain is equivalent to the requirement that the probability of two transitions taking place in time  $\tau$  is negligible, of  $o(\tau)$ . This makes the approximation  $U(\tau) = \exp(-\tau H) \simeq 1 - \tau H$  to the Markov semigroup exact in what regards the dynamics, i.e., it preserves stochasticity, and the time-evolved vectors  $|P(t + \tau)\rangle = \exp(-\tau H)|P(t)\rangle$  and  $|P(t + \tau)\rangle = (1 - \tau H)|P(t)\rangle$  coincide up to  $o(\tau)$ .

The construction of the matrix  $T$  presented above together with the appropriate choices of  $\tau$  with the purpose of studying time-dependent properties of stochastic processes is well known in queueing theory, where with some minor refinements it is called the method of uniformization [30].

In the basic CP in finite volume, the steady state is given by the unique absorbing state  $|0\rangle = |0, 0, \dots, 0\rangle$ . This *a priori* knowledge of the steady state of the process makes it possible to calculate the second largest eigenvalue of  $T$ , that corresponding to the gap of  $H$ ,

by simply orthogonalizing the iterated vector of the power method against the steady state at every iteration. We thus end up with an implementation of the power method that reads

$$|P(m+1)\rangle = (T - |\mathbf{0}\rangle\langle\mathbf{0}|)|P(m)\rangle \quad (9)$$

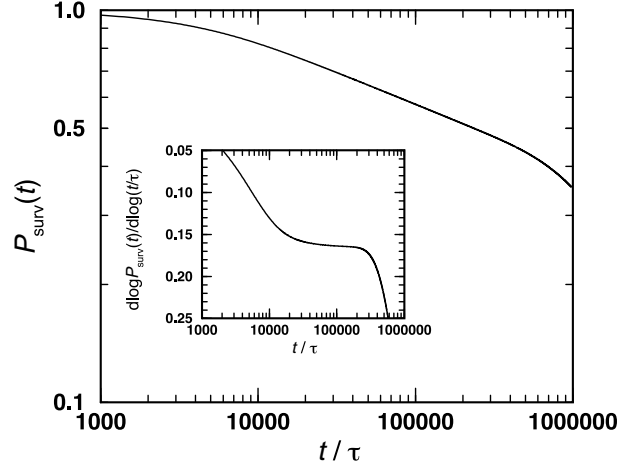
with  $m$  in units of  $\tau$ . We expect that after enough successive applications of the above relation it reaches a fixed point  $E^*|P^*\rangle = T|P^*\rangle$  where  $E^* = \langle P^*|T|P^*\rangle / \langle P^*|P^*\rangle = 1 - \tau E^{(1)}$  and  $|P^*\rangle$  is a linear combination of one-particle states. The advantage of dealing with an absorbing state in contrast to, e.g., a numerically determined steady state, is that the former is usually a ‘pure’ state, as is our case, or a rather simple combination of states with known coefficients, e.g. white noise, a fact that both minimizes the inevitable numerical round-off errors and saves computer time, turning the calculations more reliable and fast. In our calculations, we consider an eigenvalue to have converged if it coincides more than 64 times with its predecessors in more than one part in  $2^{112} \simeq 5.2 \times 10^{33}$ .

The complete characterization of the DP universality class requires, besides  $z$  and  $\nu_\perp$ , one more exponent to be calculated, the other exponents following from well known hyperscaling relations [9, 15, 21]. One calculable exponent is  $\delta$ , defined through the asymptotic behaviour of the survival probability at the critical point  $\lambda^*$  as

$$P_{\text{surv}}(t) = \sum_{n \neq \mathbf{0}} P(n, t) = 1 - P(\mathbf{0}, t) \stackrel{t \rightarrow \infty}{\propto} t^{-\delta} (1 + at^{-\delta'} + \dots). \quad (10)$$

A logarithmic plot of  $P_{\text{surv}}(t)$  versus  $t$  for an infinite system should be a straight line at large  $t$ , the slope of which is  $\delta$ . The correction exponent  $\delta'$  seems to be given by  $\delta' = 1$  [21, 31]. For finite systems, however, the spectrum always has a gap, and the survival probability ultimately enters a regime of exponential decay ruled by the finite gap. In order to follow the time evolution of the process before it gets trapped into an absorbing state, we take a small  $\tau$  in the definition of  $T$  and successively calculate  $|P(m+1)\rangle = T|P(m)\rangle$ . We choose  $\tau^{-1} = 1000 \times \max\{H(n, n)\}$ . The initial state was given by  $|P(0)\rangle = |\mathbf{1}\rangle = |1, 0, \dots, 0\rangle$ , the state with a single particle located at the origin. A plot of  $P_{\text{surv}}(t)$  versus  $t$  for a system of  $L = 16$  sites is shown in figure 1. From that figure we clearly see that after an initial transient in which the highest ‘modes’ are washed out, the curve enters a regime of almost pure algebraic decay until the gap in the spectrum manifests itself and we begin to observe the expected late times exponential behaviour. This is more clearly appreciated in the inset of figure 1, which shows the derivative of  $\log P_{\text{surv}}(t)$  with respect to  $\log t$ , that is the instantaneous value of  $\delta_L$ .

Our results for  $\lambda^*$ ,  $z$ ,  $\nu_\perp$  and  $\delta$  are summarized in table 1. The  $L = \infty$  values in this table were obtained through the Bulirsch–Stoer (BST) extrapolation scheme [26], with  $\omega_{\text{BST}}$  the free parameter of the algorithm chosen so as to minimize the difference between the penultimate entries in the BST extrapolation tableaux. The derivatives in equation (8) were calculated with a nine points symmetric difference formula with an  $O(h^9)$  error using steps of  $h = 10^{-9}$  [32], whilst the values of  $\delta$  were obtained through linear regression fits to  $\log P_{\text{surv}}(t)$  in the region of algebraic decay of  $P_{\text{surv}}(t)$  (typically through 100 data points, with points separated by a time interval  $\Delta t = 100\tau$ ). The numbers in table 1 confirm that the basic CP belongs to the DP universality class of critical behaviour with a high degree of accuracy. The uncertainties associated with the extrapolated numbers are mainly due to finite-size effects and corrections to scaling, as well as to the extrapolation procedure itself. Our numbers compare well with those obtained by other means, namely, high-temperature expansions on a closely related ‘reggeon quantum spin chain’ model [7], other finite-size scaling studies [27], time-dependent operator perturbation calculations [33], and extensive series expansions and differential approximants analyses [34]. The best values of  $z$ ,  $\nu_\perp$ , and  $\delta$  to date are given by  $z = 1.580745(10)$ ,  $\nu_\perp = 1.096854(4)$ , and  $\delta = 0.159464(6)$  [34]. Our estimate of  $\lambda^*$  is as precise as those



**Figure 1.** Survival probability at  $\lambda = \lambda_L^*$  for a system of  $L = 16$  sites. The inset shows the instantaneous value of the critical exponent  $\delta_L$ .

**Table 1.** Finite-size data and extrapolated values for the the critical point  $\lambda^*$  and the exponents  $z = \nu_{\parallel}/\nu_{\perp}$ ,  $\nu_{\perp}$  and  $\delta$  of the one-dimensional basic CP. The numbers between parentheses represent the estimated errors in the last digit of the data, whilst those data without an associated error are numerically precise to the figures shown.

$L', L, L''$	$\lambda_L^*$	$z_L$	$\nu_{\perp, L}$	$\delta_L$
7, 8, 9	1.629 092 086 131	1.495 084 128 194	0.963 208 351 697	0.1657(2)
8, 9, 10	1.632 522 345 029	1.502 980 235 818	0.977 844 866 308	0.1656(2)
9, 10, 11	1.635 178 201 359	1.509 743 775 238	0.989 427 140 315	0.1654(2)
10, 11, 12	1.637 262 542 035	1.515 558 577 190	0.998 833 401 056	0.1653(2)
11, 12, 13	1.638 921 714 266	1.520 588 023 063	1.006 632 974 979	0.1651(2)
12, 13, 14	1.640 260 494 445	1.524 967 656 357	1.013 211 430 501	0.1649(2)
13, 14, 15	1.641 354 409 414	1.528 807 324 384	1.018 839 364 776	0.1647(1)
14, 15, 16	1.642 258 557 889	1.532 195 497 121	1.023 712 402 567	0.1645(1)
15, 16, 17	1.643 013 687 274	1.535 203 516 105	1.027 975 558 429	0.1644(1)
16, 17, 18	1.643 650 350 303	1.537 889 180 610	1.031 738 664 206	0.1643(1)
17, 18, 19	1.644 191 762 995	1.540 299 611 765	1.035 086 466 706	0.1641(1)
18, 19, 20	1.644 655 789 991	1.542 473 490 560	1.038 085 430 711	0.1640(1)
$L = \infty$	1.648 96(2)	1.580 77(2)	1.096 81(2)	0.162(2)
$[\omega_{\text{BST}}]$	[1.071]	[1.171]	[0.895]	[2.701]

available in the current literature on the basic CP [23, 33]. Although our determination of  $\delta$  is not as precise as that of  $z$  and  $\nu_{\perp}$ , it nevertheless is precise enough to discriminate amongst the universality classes that are likely to arise in systems with absorbing states [21]. An alternative to estimate  $\delta$  is to determine each  $\delta_L$  as the value of the derivative of the corresponding  $\log P_{\text{surv}}(t)$  with respect to  $\log t$  at its inflexion point, see figure 1. This provides a more ‘local’ determination of  $\delta_L$  than that obtained by fitting a straight line to  $\log P_{\text{surv}}(t) \times \log t$  over tens or hundreds of points, and may improve the final result once the uncertainties are correctly assessed. We intend to pursue this alternative in a future, more thorough study.

A remark about symmetries. In the calculation of the gaps of  $H$ , one can take advantage of any symmetries of the process to reduce  $H$  to block-diagonal form. The numerical

diagonalization is then performed in the sector of lowest gap with a considerable economy of computation. Internal symmetries, like  $U(1)$  and  $Z(N)$  symmetries, usually separate the dynamics into sectors corresponding to the closed classes of the stochastic process, with each block a stochastic transition matrix governing the dynamics within the given sector. Geometric symmetries, however, like translation and reflexion symmetries, generally lead to block operators that are not stochastic due to the occurrence of ‘artificial’ combinations of states. If one decides to make use of geometric symmetries, care should then be exercised in properly weighting the basis vectors in order to interpret the resulting symmetry-invariant  $|P(t)\rangle$  as a vector of probabilities. In this work we explored the translational invariance of the basic CP on a periodic lattice in order to achieve a reduction of order  $1/L$  on the size of the matrices we needed to diagonalize.

In summary, we have successfully applied the power method to the one-dimensional basic CP, and obtained accurate values for the critical point  $\lambda^*$  and the critical exponents  $z$  and  $\nu_{\perp}$ , together with a good estimate of the critical exponent  $\delta$ . The method is fast, yields accurate estimates for the critical point and some of the exponents, and is easily coded. Given that it took less than 500 h of CPU time (running at 300 MHz) to complete table 1, and that in the largest cases it took less than 21 Mb of memory to conduct the calculations, the method seems to be very competitive. Extension to processes with more than one absorbing state as well as in more than one dimension is immediate. It would be of interest to refine the calculations of  $\delta$  as well as to try to calculate other exponents by the same methods. In particular, it would be very interesting to establish relationships between dynamical exponents like  $\delta$  and the spectrum of  $H$ . We are currently pursuing these objectives, and intend to release our results soon.

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