Perturbative series expansion for the gap of the evolution operator associated with the contact process

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The gap between the eigenvalues of the dominant and subdominant eigenvectors of the evolution operator associated with the contact process in one dimension is studied by perturbative series expansions in powers of the creation rate. The series expansion for the gap was computed with 49 coefficients. An analysis by Padé approximants allowed the determination of the critical creation rate and the time correlation critical exponent.

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I. INTRODUCTION

A major role in the theory of stochastic Markovian processes is played by the gap between the dominant and subdominant eigenvectors of the evolution operator. When the gap is nonzero, the time correlations decay exponentially with a characteristic length which is identified as the inverse of the gap. If the gap vanishes as one varies an external parameter, the dominant eigenvalue becomes degenerate and a continuous phase transition takes place. The characteristic length, or correlation length, then diverges at the transition point. The calculation of the gap requires the knowledge of both the dominant and subdominant eigenvectors of the evolution operator. However, in the case of a contact process [1–11], which concerns us here, this task is simplified because the dominant eigenvector is trivial. It is simply the state devoid of particles. The problem is thus reduced to the calculation of the subdominant eigenvector.

Our main purpose here is a study of the gap of the evolution operator associated with the contact process in an infinite lattice in the subcritical regime by means of a perturbative series expansion and Padé analysis [12,13]. Series expansions for the contact process and related models have been used not only to study the subcritical regime but also to study the supercritical regime [4–8,14–16]. Perturbative and time series expansions for the contact process have been computed for several quantities but not for the gap.

The contact process [1–11] is one of the simplest nonequilibrium interacting systems described by a continuous-time Markov process, that is, governed by a master equation. In the usual interpretation, the contact process describes an interacting-particle system in which particles are annihilated spontaneously and created catalytically on the sites of a regular lattice. The contact process in an infinite lattice exhibits a continuous phase transition from an absorbing state devoid of particles to an active state with a nonzero density of particles. Its critical behavior places the model in the directed percolation universality class [17,18].

In the contact process a particle is created on an empty site with rate λ times the fraction of nearest-neighbor occupied sites. If the neighboring sites are all empty no particle is created. A particle is annihilated with rate 1. If all particles are annihilated the system becomes trapped in the absorbing state devoid of particles. This will always happen in a finite lattice if we wait long enough, no matter what the transition rate is. This is so because the Perron-Frobenius theorem guarantees that the dominant eigenvalue is nondegenerate as long as the evolution operator is finite, which is the case of a finite system. In other words, the gap is always nonzero. However, in an infinite system the theorem no longer applies and the dominant eigenvalue may become degenerate. This indeed happens at a sufficiently high value of λ where a phase transition to an active state takes place. Above the critical point the system will not fall into the absorbing state and will remain in the active state.

We have developed a perturbative series expansion for the contact process by treating the catalytic creation of particles as a perturbation and the spontaneous annihilation of particles as the unperturbed evolution operator. An important simplification contained in the present method is the use of a vector representation, which we call the σ representation, defined by the eigenvectors of the unperturbed operator in the place of the usual occupation representation. A long series for the gap of the evolution operator associated with the one-dimensional contact process in powers of the creation rate was then obtained with 49 coefficients. A biased Padé analysis leads to the following results: for the critical creation rate $\lambda_c = 3.297\,98(1)$ and for the time correlation critical exponent $\nu_\parallel = 1.734\,65(8)$.

II. OCCUPATION REPRESENTATION

In the contact process particles are created catalytically in the sites of a regular lattice with rate λ and annihilated spontaneously with rate 1. In the usual occupation representation, one defines an occupation variable η_i that takes the value 0 or 1 according to whether the site i is empty or occupied by a particle. A configuration is then denoted by $\eta = (\eta_1, \eta_2, \ldots, \eta_N)$ where N is the number of sites of the lattice. The transition rate $w_i(\eta)$ at which the site i changes its state is given by

$$w_i(\eta) = w_i^{\mathrm{a}}(\eta) + w_i^{\mathrm{c}}(\eta), \tag{1}$$

where

$$w_i^{\mathrm{a}}(\eta) = \eta_i \tag{2}$$

is the annihilation transition rate, and

$$w_i^c(\eta) = \frac{\lambda}{2}(1-\eta_i)(\eta_{i-1}+\eta_{i+1}) \tag{3}$$

is the creation transition rate. We are considering a one-dimensional lattice.

The time evolution of the probability $P(\eta,t)$ of a configuration η at time t is governed by the master equation

$$\frac{d}{dt}P(\eta,t) = \sum_i \{w_i(\eta^i)P(\eta^i,t) - w_i(\eta)P(\eta,t)\}, \tag{4}$$

where η^i is that configuration obtained from η by changing η_i to $1-\eta_i$.

It is convenient to use the vector representation

$$|\psi(t)\rangle = \sum_\eta P(\eta,t)|\eta\rangle, \tag{5}$$

in which the vector

$$|\eta\rangle = |\eta_1,\eta_2,\ldots,\eta_N\rangle \tag{6}$$

represents a state of the system. Is is straightforward to show that the state vector $|\psi(t)\rangle$ evolves in time according to

$$\frac{d}{dt}|\psi(t)\rangle = W|\psi(t)\rangle, \tag{7}$$

where $W=W_0+\lambda V$ is the evolution operator and W_0 and V are the operators associated with the annihilation and creation processes, respectively. They are given by

$$W_0 = \sum_i B_i \tag{8}$$

and

$$V = \sum_i Q_i(n_{i-1}+n_{i+1}). \tag{9}$$

The local operators B_i, Q_i, and the number operator n_i are defined by

$$B_i|\bigcirc\rangle = 0, \quad B_i|\bullet\rangle = |\bigcirc\rangle - |\bullet\rangle, \tag{10}$$

$$Q_i|\bigcirc\rangle = \frac{1}{2}(|\bullet\rangle - |\bigcirc\rangle), \quad Q_i|\bullet\rangle = 0, \tag{11}$$

and

$$n_i|\bigcirc\rangle = 0, \quad n_i|\bullet\rangle = |\bullet\rangle. \tag{12}$$

The symbols "○" and "●" represent an empty site ($\eta_i=0$) and an occupied site ($\eta_i=1$), respectively.

III. σ REPRESENTATION

Since W_0 is a sum of independent operators B_i, its eigenvectors will be a direct product of the eigenvectors of B_i. The right eigenvectors of B_i are $|\bigcirc\rangle$ and $|\bullet\rangle-|\bigcirc\rangle$, with eigenvalues 0 and -1, respectively. The corresponding left eigenvectors are $\langle\bullet|+\langle\bigcirc|$ and $\langle\bullet|$, respectively.

It is convenient to change from the occupation representation spanned by the vectors $|\bigcirc\rangle$ and $|\bullet\rangle$ to a representation spanned by the vectors $|0\rangle$ and $|1\rangle$, which we call the σ representation, defined by

$$|0\rangle = |\bigcirc\rangle, \quad |1\rangle = |\bullet\rangle - |\bigcirc\rangle. \tag{13}$$

The transformations of the left vectors are

$$\langle 0| = \langle\bigcirc| + \langle\bullet|, \quad \langle 1| = \langle\bullet|. \tag{14}$$

In this new representation B_i is diagonal, that is,

$$B_i|0\rangle = 0, \quad B_i|1\rangle = -|1\rangle. \tag{15}$$

The eigenvectors of W_0 are then

$$|\sigma\rangle = |\sigma_1,\sigma_2,\ldots,\sigma_N\rangle, \tag{16}$$

where $\sigma_i=0$ or 1, with eigenvalues

$$\Lambda(\sigma) = -\sum_i \sigma_i. \tag{17}$$

Next we need to known how the operator V acts on a vector $|\sigma\rangle$ of the σ representation. We begin by rearranging the terms in V in the form

$$V = \sum_i (Q_i n_{i+1} + n_i Q_{i+1}). \tag{18}$$

From the definition of Q_i and n_i and using the transformation (13) it follows that

$$Q_i|0\rangle = \frac{1}{2}|1\rangle, \quad Q_i|1\rangle = -\frac{1}{2}|1\rangle, \tag{19}$$

and that

$$n_i|0\rangle = 0, \quad n_i|1\rangle = |0\rangle + |1\rangle. \tag{20}$$

From these relations one gets the following important rules:

$$(Q_i n_{i+1} + n_i Q_{i+1})|00\rangle = 0, \tag{21}$$

$$(Q_i n_{i+1} + n_i Q_{i+1})|01\rangle = \frac{1}{2}|10\rangle + \frac{1}{2}|11\rangle, \tag{22}$$

$$(Q_i n_{i+1} + n_i Q_{i+1})|10\rangle = \frac{1}{2}|01\rangle + \frac{1}{2}|11\rangle, \tag{23}$$

$$(Q_i n_{i+1} + n_i Q_{i+1})|11\rangle = -\frac{1}{2}|10\rangle - \frac{1}{2}|01\rangle - |11\rangle. \tag{24}$$

IV. PERTURBATION SERIES EXPANSION

The state devoid of particles $|O\rangle$ is the eigenvector of W with zero eigenvalue, that is,

$$W|O\rangle = 0. \tag{25}$$

It is also the eigenvector or W_0 with zero eigenvalue

$$W_0|O\rangle = 0. \tag{26}$$

The subdominant eigenvector of W_0, which we denote by $|\psi_0\rangle$, has eigenvalue -1, that is,

$$W_0|\psi_0\rangle = -|\psi_0\rangle. \tag{27}$$

We are interested in determining the subdominant eigenvector of W, that is, the eigenvector $|\psi\rangle$ whose eigenvalue is the closest to zero. Denoting by A this eigenvalue then

$$W|\psi\rangle = A|\psi\rangle. \tag{28}$$

We define the gap Γ as the difference between the dominant eigenvalue and the subdominant eigenvalue, that is, $\Gamma=-A$ since the dominant eigenvalue is 0. Next we assume that $|\psi\rangle$ and A can be expanded in powers of λ, that is,

$$|\psi\rangle = |\psi_0\rangle + \lambda|\psi_1\rangle + \lambda^2|\psi_2\rangle + \cdots \tag{29}$$

and

$$A = A_0 + A_1\lambda + A_2\lambda^2 + \cdots, \tag{30}$$

where $A_0=-1$. The coefficients of the expansion of the gap

$$\Gamma = c_0 + c_1\lambda + c_2\lambda^2 + \cdots \tag{31}$$

are simply $c_n=-A_n$. In addition, we choose the vectors $|\psi_n\rangle$ to be orthogonal to $|\psi_0\rangle$, that is,

$$\langle\psi_0|\psi_n\rangle = 0, \quad n \neq 0. \tag{32}$$

It is straightforward to show that this is always possible to do.

Substituting (29) and (30) into (28) and collecting terms of the same power in λ we get the following relations:

$$W_0|\psi_0\rangle = A_0|\psi_0\rangle \tag{33}$$

and

$$W_0|\psi_n\rangle + V|\psi_{n-1}\rangle = \sum_{m=0}^{n} A_m|\psi_{n-m}\rangle, \tag{34}$$

valid for $n\geq 1$. Taking into account that $\langle\psi_0|W_0=A_0\langle\psi_0|$, the orthogonality relation (32), and the normalization $\langle\psi_0|\psi_0\rangle=1$, it follows from Eq. (34) that

$$A_n = \langle\psi_0|V|\psi_{n-1}\rangle, \tag{35}$$

valid for $n\geq 1$.

Now we write the operator W_0 as

$$W_0 = \sum_{\sigma}{}' |\sigma\rangle\Lambda(\sigma)\langle\sigma|, \tag{36}$$

where the summation is over the subspace orthogonal to the vector $|O\rangle$, and define the operator R by

$$R = \sum_{\sigma}{}'' |\sigma\rangle\frac{1}{\Lambda(\sigma)-A_0}\langle\sigma|, \tag{37}$$

where the summation is over the eigenvectors σ except those corresponding to eigenvalues 0 and -1. Therefore,

$$R(W_0 - A_0) = \sum_{\sigma}{}'' |\sigma\rangle\langle\sigma| = 1 - |O\rangle\langle O| - |\psi_0\rangle\langle\psi_0|. \tag{38}$$

Writing (34) as

$$(W_0 - A_0)|\psi_n\rangle = -V|\psi_{n-1}\rangle + \sum_{m=1}^{n} A_m|\psi_{n-m}\rangle \tag{39}$$

and multiplying from the left by R, we get, for $n=1$,

$$|\psi_1\rangle = -RV|\psi_0\rangle \tag{40}$$

and, for $n\geq 2$,

$$|\psi_n\rangle = -RV|\psi_{n-1}\rangle + \sum_{m=1}^{n-1} A_m R|\psi_{n-m}\rangle, \tag{41}$$

where we used the fact that $|\psi_m\rangle$, for $m\neq 0$, is orthogonal to $|O\rangle$ and to $|\psi_0\rangle$. We have used also that $R|\psi_0\rangle=0$. We remark that multiplying both the right- and left-hand sides by $\langle\psi_0|$ and taking into account that $\langle\psi_0|R=0$ it follows that $\langle\psi_0|\psi_n\rangle=0$, as expected.

Equations (35), (40), and (41) allow us to determine A_n and $|\psi_n\rangle$ recursively starting from $|\psi_0\rangle=|.1.\rangle$. The first vectors are

$$|\psi_1\rangle = |.11.\rangle, \tag{42}$$

$$|\psi_2\rangle = -2|.11.\rangle + |.101.\rangle + \frac{1}{2}|.111.\rangle, \tag{43}$$

$$|\psi_3\rangle = \frac{11}{2}|.11.\rangle - \frac{7}{2}|.101.\rangle - \frac{5}{4}|.111. + |.1001.\rangle + \frac{3}{8}|.1101.\rangle + \frac{3}{8}|.1011.\rangle + \frac{1}{6}|.1111.\rangle. \tag{44}$$

The two dots in the notation $|.x.\rangle$ mean that all sites at the right and at the left of x are in the state 0.

Up to terms of order λ^5 the gap Γ is given by

$$\Gamma = 1 - \lambda + \lambda^2 - 2\lambda^3 + \frac{11}{2}\lambda^4 - \frac{69}{4}\lambda^5. \tag{45}$$

Other coefficients of the gap expansion up to 49th order are listed in Table I. They were obtained by using quadruple precision (REAL*16 in FORTRAN coding). The calculations were performed on a computer machine with a 64-bit reduced instruction set computer (RISC) processor of 667 MHz. The determination of the 49 coefficients shown in Table I needed about 1 gigabyte of random access memory and consumed 8 min of CPU time.

V. CRITICAL BEHAVIOR AND PADÉ APPROXIMANTS

At the critical point the gap has a singular behavior given by

$$\Gamma \sim (\lambda_c - \lambda)^{\nu_\parallel}, \tag{46}$$

where $\nu_\parallel$ is the exponent related to the time correlation length τ, defined as the inverse of the gap, that is, $\tau=1/\Gamma$. To obtain the exponent $\nu_\parallel$ as well as the critical parameter λ_c from the coefficients of the series for Γ we have used an analysis by Padé approximants [12,13] for the logarithm derivative of the gap, which behaves as

TABLE I. Coefficients $c_n=-A_n$ of λ^n for the gap Γ between the dominant and subdominant eigenvalues.

n	c_n
0	$0.10000000000000000000000000000000\times 10^{1}$
1	$-0.10000000000000000000000000000000\times 10^{1}$
2	$0.10000000000000000000000000000000\times 10^{1}$
3	$-0.20000000000000000000000000000000\times 10^{1}$
4	$0.55000000000000000000000000000000\times 10^{1}$
5	$-0.17250000000000000000000000000000\times 10^{2}$
6	$0.58145833333333333333333333333333\times 10^{2}$
7	$-0.20510590277777777777777777777778\times 10^{3}$
8	$0.74666145833333333333333333333333\times 10^{3}$
9	$-0.27824315562307098765432098765432\times 10^{4}$
10	$0.10559185065224729938271604938272\times 10^{5}$
11	$-0.40663499522422089334705075445816\times 10^{5}$
12	$0.15850374353381124390932213077275\times 10^{6}$
13	$-0.62416873644121251663698726375553\times 10^{6}$
14	$0.24793994576864424804924054920036\times 10^{7}$
15	$-0.99233930054414026478039202932240\times 10^{7}$
16	$0.39978654898019013324234457383972\times 10^{8}$
17	$-0.16199801451968107022751997742955\times 10^{9}$
18	$0.65981369639291419050601201601903\times 10^{9}$
19	$-0.26997580096879531020601305076810\times 10^{10}$
20	$0.11092209297248709929693796251047\times 10^{11}$
21	$-0.45743350460118092150449102676524\times 10^{11}$
22	$0.18928029884376209635971554568753\times 10^{12}$
23	$-0.78563509376340460662879241091594\times 10^{12}$
24	$0.32701013907692385731672303696029\times 10^{13}$
25	$-0.13646680852412971308162844694013\times 10^{14}$
26	$0.57086118938854129284225101308734\times 10^{14}$
27	$-0.23932811976660851165137006830232\times 10^{15}$
28	$0.10054192030943096670903950606937\times 10^{16}$
29	$-0.42318341439092303787922371853344\times 10^{16}$
30	$0.17843588063020210045178951401720\times 10^{17}$
31	$-0.75362860155990246095601666265477\times 10^{17}$
32	$0.31879281024944268725247836567465\times 10^{18}$
33	$-0.13504986432216258095509813738375\times 10^{19}$
34	$0.57289693646299782489328815094175\times 10^{19}$
35	$-0.24334423341123914346226741790539\times 10^{20}$
36	$0.10348948680444338916147654741416\times 10^{21}$
37	$-0.44062893667556268780621415759995\times 10^{21}$
38	$0.18781259265016825428034037111797\times 10^{22}$
39	$-0.80135821495218346358410935162745\times 10^{22}$
40	$0.34226005448402586074770570757498\times 10^{23}$
41	$-0.14631612772304272471387311414664\times 10^{24}$
42	$0.62605875064111692466722579274380\times 10^{24}$
43	$-0.26810611002829694690537544522708\times 10^{25}$
44	$0.11490796574366077070676746286450\times 10^{26}$
45	$-0.49286681369242956973843558582605\times 10^{26}$
46	$0.21155840492692774297831181794147\times 10^{27}$
47	$-0.90873751841185413631021365534459\times 10^{27}$
48	$0.39060803456546541299848897891520\times 10^{28}$
49	$-0.16800658077463921600253273431846\times 10^{29}$

$$\frac{d}{d\lambda}\ln\Gamma \sim \frac{\nu_{\|}}{\lambda-\lambda_c}. \tag{47}$$

The critical exponent $\nu_{\|}$ and the critical parameter λ_c are identified as the residue and pole, respectively, of a given Padé approximant of the logarithm derivative.

Table II shows the estimates of λ_c and the exponent $\nu_{\|}$ obtained from the coefficients of Table I by the use of Padé approximants for the logarithmic derivative of the gap. The determination of the deviations of the results given by the Padé approximants from the true values represents a difficult problem. We may look at the convergence of the results as one increases the order of the Padé approximants. However, the convergence may not be clear. Alternatively, we used a biased analysis in which we form the series for the quantity in the left-hand side of

$$(\lambda-\lambda_c^*)\frac{d}{d\lambda}\ln\Gamma \sim \nu_{\|} \tag{48}$$

for a trial value of λ_c^* and then determine the Padé approximants which are evaluated at $\lambda=\lambda_c^*$.

For each trial value of λ_c^*, the biased Padé approximants give estimates of the exponent $\nu_{\|}$. A plot of $\nu_{\|}$ versus λ_c^* then gives the actual values of these two quantities at the intersection of the curves coming from several Padé approximants. From Fig. 1 the following results are obtained: $\lambda_c=3.297\,98(1)$ and $\nu_{\|}=1.734\,65(8)$. These results should be compared with the results $\lambda_c=3.297\,85(2)$, obtained for the

TABLE II. Estimates for the critical point λ_c and the value of the critical exponent $\nu_{\|}$ obtained from the Padé approximants to the logarithm derivative of the gap A.

Approximant	λ_c	$\nu_{\|}$
[10/10]	3.297880	1.735339
[11/11]	3.298395	1.736703
[12/12]	3.298410	1.736745
[13/13]	3.298413	1.736754
[14/14]	3.298412	1.736752
[15/15]	3.298428	1.736795
[16/16]	3.297941	1.734371
[17/17]	3.297942	1.734380
[18/18]	3.297921	1.734220
[19/19]	3.297976	1.734635
[20/20]	3.297985	1.734705
[21/21]	3.297986	1.734711
[22/22]	3.298006	1.734810
[23/23]	3.297988	1.734726

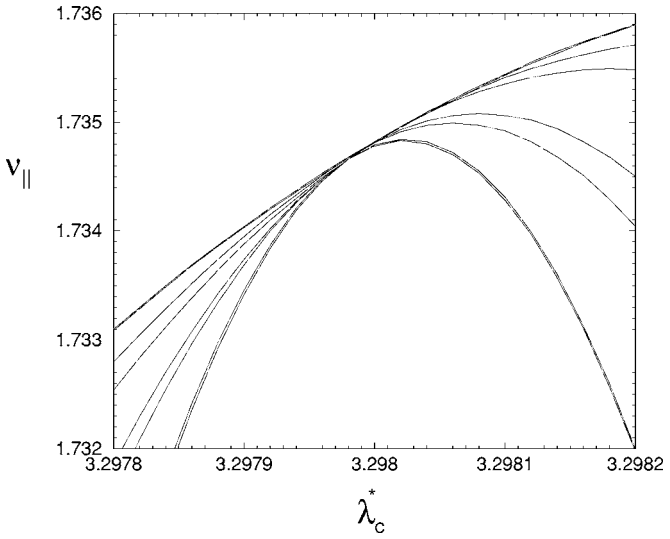

FIG. 1. The critical exponent $\nu_{\|}$ as a function of the creation rate λ obtained from the biased Padé aproximants.

one-dimensional contact process [7], and $\nu_{\|}=1.733\,83(3)$, obtained for directed percolation in two dimensions [16]. Although the values for λ_c and $\nu_{\|}$ differ by less than 0.004% and 0.04%, respectively, they are distinct if the statistical errors are taken into account. We remark that, even if we take into consideration the values obtained from the unbiased Padé approximants shown in Table II, namely, $\lambda_c=3.297\,96(4)$ and $\nu_{\|}=1.7345(3)$, the statistical errors will be greater but not sufficient to make an agreement with the results quoted.

The estimate of errors coming from a Padé analysis is a difficult task. One of the problems is that the convergence is not smooth. The figures seem to be displayed like stages of a staircase as can be seen in Table II. One observes clearly a stage from [11/11] to [15/15] and another from [16/16] to [23/23]. Conventionally, the error is defined as the statistical error contained in the figures of the last stage. Since the figures within a stage have a small dispersion, the statistical error will be small. However, there is no guarantee that another stage will not follow the last stage if we had more terms in the series expansion. Therefore, the error of a quantity determined by a Padé analysis may not coincide with the true error, defined as the deviation between the estimate of a quantity and its exact value. If the estimated error is not the true error, the Padé results coming from distinct series might not be comparable. As a result, a more realistic numerical estimate of a given quantity would be the average of estimates coming from distinct series.

VI. CONCLUSION

We have developed a perturbative series expansion for the contact process in which the operators associated with the spontaneous annihilation and the catalytic creation were treated as the unperturbed operator and the perturbation, respectively. A representation defined by the eigenvectors of the unperturbed operator was used in place of the usual occupation representation. We have computed 49 coefficients of the powers of the creation rate for the gap of the evolution operator associated with the contact process in one dimension. An analysis by Padé approximants allowed the determination of the critical creation rate and the time correlation exponent.

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