Time-Dependent Perturbation Theory for Nonequilibrium Lattice Models

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We develop a perturbation theory for the asymptotic survival probability of an interacting particle system which can become trapped in an absorbing state. The method is applied to a simple model describing the poisoning of a catalytic surface. Analysis of the resulting series (in powers of the annihilation rate) leads to very precise estimates for the location of the critical point and the order-parameter exponent β . Results for similar models and other expansions are presented briefly.

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Nonequilibrium systems are presently under intensive study in physics, chemistry, and biology [1,2]. Special attention has been given to systems exhibiting nonequilibrium phase transitions. Models of these processes cannot generally be studied via the traditional methods of statistical mechanics; appropriate theoretical tools are currently under active development. Some progress has been achieved via field-theoretic renormalization-group methods [3-6], but while these methods are successful in predicting the possible universality classes for second-order phase transitions, they are not very effective in determining critical parameters or phase diagrams. It is thus very important to develop new analytic methods which can be relied upon as efficient calculational tools. Here we present a time-dependent perturbation theory which allows us to derive high-order series expansions for the asymptotic behavior of systems exhibiting a second-order phase transition into an absorbing state. Analysis of the series yields very precise estimates for the critical parameters.

The systems considered in this work are nonequilibrium stochastic lattice models or interacting particle systems [7] evolving according to a Markov process with local, intrinsically irreversible transition rules. One of the simplest such models is the A model [8], which was introduced recently as a simplified model for the poisoning of a catalytic surface. The A model is closely related to the contact process [9] describing the spreading of an epidemic, to Schlögl's (first) model [10] of an autocatalytic chemical reaction, to directed percolation [11], and to Reggeon field theory (RFT) [12,13]. In the A model each site can be either vacant or occupied, so that the state of the system is characterized by occupation variables $\{\sigma_i\}$ $(i \in \mathbb{Z}^d$, with $\sigma_i = 0, 1$ corresponding to site i vacant or occupied, respectively). The evolution of the system is governed by simple local rules: Particles are annihilated at rate λ independent of the states of other sites, and vacancies become occupied at a unit rate, provided that at least one nearest neighbor is occupied. As there is no spontaneous creation of particles the vacuum is an absorbing state for the Markov process. In addition to this trivial state the A model has for sufficiently small λ (in the infinite-size limit) a nontrivial ("active") steady state with a nonzero average particle concentration ρ . Monte Carlo simulations [8] and steady-state series expansions [8,14] for the A model and related models provide very strong evidence of a continuous phase transition from the active state to the absorbing state at a critical value λ_c . This kind of phase transition is also found in more complicated models for catalytic surface reactions [15,16]. As in equilibrium the behavior of the system near λ_c is characterized by various critical exponents; e.g., the steady-state concentration of particles (which is the appropriate order parameter) decays asymptotically as $\rho \propto (\lambda_c - \lambda)^{\beta}$ as $\lambda \rightarrow \lambda_c^{-}$. Steady-state series expansions [8,14] in d=1 yield $\lambda_c \approx 0.5714$ and $\beta \approx 0.277$. This places the A model in the same universality class as RFT [12,13] and directed percolation.

Before venturing into a description of the time-dependent perturbation theory we review the scaling behavior of models exhibiting a continuous transition to an absorbing state. Following Grassberger and de la Torre [13] we consider the asymptotic behavior of the model, starting at t=0 with a single seed particle at the origin. According to the usual scaling hypothesis, one expects that any function of x, t, and $\Delta (\Delta = \lambda_c - \lambda)$ depends on these variables only through x^2/t^z and $\Delta t^{1/\nu}$, times some power of x^2 , t, or Δ , where v and z are new critical exponents. For the probability of survival, i.e., the probability that the system has not entered into the vacuum state at time t, one expects

$$P(t) \propto t^{-\delta} \phi(\Delta t^{1/\nu}), \qquad (1)$$

where δ is another critical exponent, while ϕ is a universal scaling function. In the supercritical region $(\lambda < \lambda_c)$ we see that by setting $\psi(y) = y^{-\delta v} \phi(y)$ we may rewrite (1) as

$$P(t) \propto \Delta^{\nu \delta} \psi(\Delta t^{1/\nu}) . \tag{2}$$

Since the system is in the supercritical region there must

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be a nonzero chance of survival; were this not the case any configuration would eventually die out, contrary to our knowledge that the system has an active steady state in this region. Thus since $P_{\infty} \equiv \lim_{t \to \infty} P(t)$ is finite, $\lim_{y \to \infty} \psi(y)$ is finite too, and we get

$$P_{\infty} \propto \Delta^{\nu \delta} \,. \tag{3}$$

It can, however, be shown [13] that P_{∞} and ρ have the same critical exponent, leading to the scaling relation $\beta = v\delta$.

Markov processes in many-particle systems can be conveniently described via an operator formalism [17–19], as demonstrated by the successful application of the formalism to nonequilibrium steady states of interacting particle systems [14] and the dynamics of random sequential adsorbtion [20]. In this paper we use the formalism of Ref. [14] in which only single occupancy of sites is allowed. The basis states of a given site $i \in Z^d$ are $|\sigma_i\rangle$ with $\sigma_i = 0, 1$ when site *i* is vacant or occupied, respectively. Any configuration $\{\sigma_i\} \to \Pi_i \in Z^d |\sigma_i\rangle$.

Creation and annihilation operators for site i are defined in the obvious manner:

$$A_{i}^{\dagger}|\sigma_{i}\rangle = (1 - \sigma_{i})|\sigma_{i} + 1\rangle,$$

$$A_{i}|\sigma_{i}\rangle = \sigma_{i}|\sigma_{i} - 1\rangle.$$
(4)

The state of the system at time t is

$$|\Psi(t)\rangle = \sum_{\{\sigma_i\}} p(\{\sigma_i\}, t) |\{\sigma_i\}\rangle, \qquad (5)$$

where the sum is over all configurations and $p(\{\sigma_i\}, t)$ is the probability distribution on configuration space. The evolution of the probability distribution is governed by the master equation

$$\frac{d|\Psi(t)\rangle}{dt} = S|\Psi(t)\rangle, \qquad (6)$$

which has the formal solution

$$|\Psi(t)\rangle = e^{St} |\Psi(0)\rangle, \qquad (7)$$

where $|\Psi(0)\rangle$ is the initial probability distribution. The evolution operator S for the one-dimensional A model can be written as

$$S = \lambda W + V, \qquad (8)$$

where

$$W = \sum_{i} (1 - A_i^{\dagger}) A_i , \qquad (9)$$

and

$$V = \sum_{i} (1 - A_i) A_i^{\dagger} [1 - A_{i-1} A_{i-1}^{\dagger} A_{i+1} A_{i+1}^{\dagger}].$$
(10)

In this decomposition W only annihilates, and V only creates particles. The evolution operator S fulfills the conditions required for a probability interpretation, i.e., it

preserves positivity and normalization. Next we consider the effect of the operators V and W on various configurations. W is simplest: Operating on a configuration (r)containing m particles, it gives a sum of m configurations (r') (each having one of the m sites vacated), minus mtimes (r) itself:

$$W(r) = \sum_{i=1}^{m} (r_i') - m(r) .$$
(11)

Consider a configuration (r) in which there are q vacancies having at least one occupied nearest neighbor (i.e., q sites where a new particle may appear). Operating on such a configuration, V yields

$$V(r) = \sum_{i=1}^{q} (r_i'') - q(r) , \qquad (12)$$

where (r'') is a configuration with one of the vacancies now occupied. Note that both W and V give 0 when operating on the vacuum state $|0\rangle$.

There are several ways of expanding (7), e.g., in terms of t (short-time expansion) [20] or in terms of λ or λ^{-1} . Here we consider the long-time behavior in the supercritical region. A more detailed account will be presented elsewhere [21]. The supercritical expansion is obtained by taking the Laplace transform of (7) and then treating λW perturbatively. In this way we can derive an expansion in powers of λ for the ultimate survival probability P_{∞} . Having derived such a series, we expect the critical point to be first singularity on the positive- λ axis. Consider the Laplace transform of $|\Psi(t)\rangle$:

$$\left|\tilde{\Psi}(z)\right\rangle = \int_0^\infty e^{-zt} \left|\Psi(t)\right\rangle dt = (z-S)^{-1} \left|\Psi(0)\right\rangle.$$
(13)

We focus on the initial distribution $|X_0\rangle$ which assigns probability 1 to the configuration with the origin occupied, and all other sites vacant. Assuming that $|\tilde{\Psi}(z)\rangle$ can be expanded in powers of λ ,

$$|\tilde{\Psi}(z)\rangle = |\tilde{\Psi}_{0}\rangle + \lambda |\tilde{\Psi}_{1}\rangle + \lambda^{2} |\tilde{\Psi}_{2}\rangle + \cdots, \qquad (14)$$

we find upon inserting (14) and (8) in (13) that

$$|\tilde{\Psi}_0\rangle = (z - V)^{-1} |X_0\rangle \tag{15}$$

and

$$|\tilde{\Psi}_n\rangle = (z-V)^{-1}W|\tilde{\Psi}_{n-1}\rangle, \quad n \ge 1.$$
(16)

As can be seen from (15) and (16) the operator $(z-V)^{-1}$ plays an important role in this expansion. The effect of this operator on a configuration (r) can be found using the identity

$$(z-V)^{-1}(r) = z^{-1}(r) + z^{-1}(z-V)^{-1}V(r). \quad (17)$$

Inserting (12) and rearranging yields

$$(z-V)^{-1}(r) = z_q \left[(r) + (z-V)^{-1} \sum_{i=1}^q (r_i'') \right], \quad (18)$$

where $z_q \equiv (z+q)^{-1}$. If we let (n) denote a configuration

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with a string of n occupied sites surrounded by vacancies we find, in particular,

$$(z-V)^{-1}(n) = z_2(n) + 2z_2(z-V)^{-1}(n+1)$$
$$= \sum_{j=0}^{\infty} 2^j z_2^{j+1}(n+j).$$
(19)

With n = 1, the right-hand side is $|\tilde{\Psi}_0\rangle$.

From (19) it is clear that $|\tilde{\Psi}_0\rangle$ involves infinitely many configurations so it is impossible to calculate $\tilde{\Psi}(z)$. What we can calculate, however, is the *extinction* probability $\tilde{p}(z)$, i.e., the probability of having entered the absorbing state. The λ^j term in the expansion for $\tilde{p}(z)$ is simply the coefficient of $|0\rangle$ in $|\tilde{\Psi}_j\rangle$. As each application of W annihilates at most one particle it follows from (16) that in a calculation of $\tilde{p}(z)$ to $\mathcal{O}(\lambda^n)$ we can discard (j) for

 $P_{\infty} = 1 - \frac{1}{2}\lambda - \frac{1}{4}\lambda^{2} - \frac{7}{24}\lambda^{3} - \frac{163}{432}\lambda^{4}$ $- 0.4939557613168719\lambda^{5} - 0.6546460619570188\lambda^{6}$ $- 0.9160621981452912\lambda^{7} - 1.356981446217977\lambda^{8}$ $- 2.052404865011525\lambda^{9} - 3.088808063863888\lambda^{10}$ $- 4.711980262430326\lambda^{11} - 7.373187827483772\lambda^{12}$ $- 11.64098743777937\lambda^{13} - 18.31374655286935\lambda^{14}$ $- 29.09696095266492\lambda^{15} - 46.84094923091073\lambda^{16}$ $- 75.46270213626647\lambda^{17} - 121.6314724443718\lambda^{18}$ $- 197.8953411341986\lambda^{19} - 323.0966492170077\lambda^{20}$ $- 527.7431752339135\lambda^{21} - 864.4497240830738\lambda^{22}$ $- 1427.559659906972\lambda^{23} - 2342.271155757435\lambda^{24} + \mathcal{O}(\lambda^{25}).$

We have formed various Padé approximants to the series for $(d/d\lambda)\ln P_{\infty}$, thus obtaining unbiased estimates for λ_c , the first pole on the positive- λ axis, and β , the residue of the Padé approximant at this pole. The results of this analysis are summarized in Table I. The Padé approximants are in excellent agreement yielding the very precise estimates $\lambda_c = 0.574141(2)$ and $\beta = 0.27674(2)$, where the uncertainty on the last digit is given in parentheses.

Better estimates for the critical exponent can often be obtained if one has prior knowledge of the location of the critical point. In such a situation one often looks at Padé approximants to the series for $(\lambda_c - \lambda)(d/d\lambda) \ln P_{\infty}$ which,

TABLE I. Unbiased estimates for λ_c and β derived from Padé approximants to the series $(d/d\lambda)\ln P_{\infty}$ for the A model.

Padé approximants	λ_c	β
[10,11]	0.574143	0.27676
[11,10]	0.574141	0.27674
[11,11]	0.574142	0.27674
[11,12]	0.574139	0.27672
[12,11]	0.574142	0.27675

j > n in the expression for $|\tilde{\Psi}_0\rangle$. Similarly, we can ignore all configurations with more than n-k occupied sites in $|\tilde{\Psi}_k\rangle$, as none of these contribute to the extinction probability. Further simplifications arise if we just focus our attention on the ultimate survival probability P_{∞} . Taking the Laplace transform of (3) shows that $P_{\infty}=1$ $-\lim_{z\to 0} z\tilde{p}(z)$, which makes the application of Eq. (18) much simpler, as the algebraic factor z_q reduces to the numerical factor 1/q.

The algebra involved in the calculation of $\tilde{p}(z)$ rapidly becomes very complex. The steps used to generate the series are, however, simple enough to be codified as a computer algorithm. We have derived the series expansion for $\lim_{z \to 0} z\tilde{p}(z)$ to 24th order in λ (it takes a little more than 16 min on an IBM 3090). The resulting series for the ultimate survival probability is

when evaluated at λ_c , yields the critical exponent β . In principle we do not have any prior knowledge of λ_c , but we have used this approach in a modified form [22]. We form the series mentioned above using a trial value $\tilde{\lambda}_c$ for



FIG. 1. Biased estimates $\tilde{\beta}$ as a function of $\tilde{\lambda}_c$ derived from Padé approximants to the series $(\tilde{\lambda}_c - \lambda)(d/d\lambda) \ln P_{\infty}$ evaluated at $\tilde{\lambda}_c$.

TABLE II. Estimates for various critical exponents for the A model, the contact process, and the N3 model.

Exponent	A model	СР	N3 model
β	0.2767	0.2769	0.2771
v	1.731	1.735	1.737
η	0.318	0.313	0.312
Z	1.264	1.265	?

 λ_c and find the corresponding $\tilde{\beta}$. For each Padé approximant we obtain $\tilde{\beta}$ as a function of $\tilde{\lambda}_c$. In a plot of $\tilde{\beta}$ vs $\tilde{\lambda}_c$ we expect the curves to intercept at the point (λ_c, β) . Figure 1 shows the result of this approach. All the curves intercept very nicely for $\tilde{\lambda}_c = 0.5741420(5)$ and $\tilde{\beta} = 0.276750(5)$ in excellent agreement with the unbiased estimates.

Our results for λ_c and β are consistent with earlier studies of the A model which found (using steady-state series expansions [8,14]) $\lambda_c = 0.5414$ and $\beta = 0.277(1)$. Studies of Reggeon field theory yielded $\beta = 0.277(2)$ (from series analysis of generalized susceptibilities [12]), and $\beta = 0.273(6)$ (from Monte Carlo simulations [13]). For directed percolation the best (to our knowledge) result for β is 0.2765(5) [23].

We conclude with a brief summary of results from expansions for similar models and expansions in the subcritical regime which enable us to estimate the critical exponents v, η , and z. The subcritical expansion is very similar to the supercritical expansion, as one ends up with the expressions (14)-(18), but with the roles of V and W interchanged and λ replaced by $\mu = \lambda^{-1}$. As W annihilates particles $|\Psi_0\rangle$ becomes much simpler and it just consists of the one-particle state and the vacuum. Details of this expansion will be given elsewhere [21]. We have studied two models closely related to the A model, the contact process (CP) and the N3 model. In all the models particles spontaneously annihilated at rate λ and empty sites with two occupied neighbors are filled at unit rate, but sites with only one occupied neighbor are filled with rate 1 in the A model, with rate $\frac{1}{2}$ in the CP, and with rate $\frac{1}{4}$ in the N3 model. We expect these models to show the same critical behavior, a notion which is strongly supported by steady-state series expansions [14]. Our estimates for the critical exponents are summarized in Table II. The nearly identical exponent values for these different models strongly supports the hypothesis of universality; the small variation among exponent estimates presumably reflects the need to consider corrections to asymptotic scaling in the analysis of series. This issue, as well as applications to nonequilibrium models in two dimensions and models which include diffusion of particles, is currently under investigation.

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