

# Time-Dependent Perturbation Theory for Nonequilibrium Lattice Models

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Received February 28, 1992; final September 29, 1992

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We develop a time-dependent perturbation theory for nonequilibrium interacting particle systems. We focus on models such as the contact process which evolve via destruction and autocatalytic creation of particles. At a critical value of the destruction rate there is a continuous phase transition between an active steady state and the vacuum state, which is absorbing. We present several methods for deriving series for the evolution starting from a single seed particle, including expansions for the ultimate survival probability in the super- and subcritical regions, expansions for the average number of particles in the subcritical region, and short-time expansions. Algorithms for computer generation of the various expansions are presented. Rather long series (24 terms or more) and precise estimates of critical parameters are presented.

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**KEY WORDS:** Interacting particle systems; nonequilibrium critical points; series expansions; Padé analysis.

## 1. INTRODUCTION

The study of many-particle systems is an important problem in many branches of physics, chemistry, biology, and even sociology.<sup>(1,2)</sup> While equilibrium statistical mechanics has developed in great depth and a canonical description is at hand, no such unifying approach exists for nonequilibrium systems. Since the steady-state probability distribution is not known *a priori*, analysis of nonequilibrium systems must start from the *dynamics*. Of particular interest are systems exhibiting nonequilibrium phase transitions. Nonequilibrium critical points have many features in common with equilibrium critical phenomena: long-range correlations, a

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well-defined order parameter, and singularities characterized by critical exponents.

Present knowledge about nonequilibrium phase transitions is mainly based upon Monte Carlo simulations,<sup>(3–10)</sup> mean-field theory (MFT),<sup>(11,12)</sup> field-theoretic renormalization group (RG) methods,<sup>(13–17)</sup> and series expansions.<sup>(18–21)</sup> While MFT often yields qualitatively correct phase diagrams,<sup>(11,12)</sup> it does not provide accurate results for critical parameters. More progress has been achieved via RG methods,<sup>(13–17)</sup> but while these methods are successful in predicting the universality classes for nonequilibrium second-order phase transitions in simple models, they are not very effective in determining critical parameters, and they cannot be used to predict nonuniversal properties. The utility of field theories in distinguishing nonequilibrium universality classes for more complex models has been cast into doubt.<sup>(16)</sup> Series expansions<sup>(18–21)</sup> have proven very efficient tools for calculating the critical parameters, and also provide information about off-critical behavior. The method developed in this paper yields high-order series expansions for the asymptotic behavior of nonequilibrium systems exhibiting a continuous transition into an absorbing state.

In this paper we consider stochastic lattice models which evolve via annihilation and autocatalytic creation of particles. As there is no spontaneous creation of particles, the vacuum state is absorbing. Evidently, any finite system will eventually become trapped in this state. In addition to this trivial state, the system may possess (in the infinite-size limit) a nontrivial (“active”) steady state, with a nonzero average concentration  $\rho$  of particles, when the annihilation rate  $\lambda$  is sufficiently small. The models studied in this paper exhibit a continuous phase transition from the active to the absorbing state at some critical value  $\lambda_c$ . The steady-state concentration of particles (which is the appropriate order parameter) decays asymptotically as  $\rho \propto (\lambda_c - \lambda)^\beta$  when  $\lambda \rightarrow \lambda_c^-$ . One of the major achievements in the study of nonequilibrium phase transitions is the discovery that a wide variety of models exhibiting this kind of transition belong to the same universality class. Among these models one could mention the contact process (CP),<sup>(22,23)</sup> Schlögl’s first and second models,<sup>(3,13,16,24)</sup> directed percolation (DP),<sup>(4,14,25,26)</sup> Reggeon field theory (RFT),<sup>(3,18)</sup> and the ZGB model.<sup>(5,6)</sup> Studies of related models via computer simulations<sup>(7–10)</sup> and steady-state series expansions<sup>(19,20)</sup> demonstrate the robustness of this universality class against a wide range of changes in the local kinetic rules, such as multiparticle processes, diffusion, and changes in the number of components. So there is substantial evidence in favor of the hypothesis<sup>(13,16,17)</sup> that RFT is the generic critical behavior for systems with a scalar order parameter and a single absorbing state. This

universality class is characterized by the order-parameter exponent  $\beta \approx 0.277$  for  $d = 1 + 1$ <sup>(18,20)</sup> (one space and one time dimension).

In this paper we employ an operator formalism as a convenient means for describing the evolution of interacting particle systems. Starting from the master equation, we derive a perturbative expansion for the long- and short-time behavior of quantities such as the survival probability and the mean particle number, when evolving from an initial state with a single seed particle. For a class of one-dimensional models we have devised a computer algorithm which enables us to obtain rather long series for time-dependent properties leading to very precise estimates of critical parameters.

Preliminary results on the time-dependent perturbation theory for the one-dimensional A model were presented recently in summary form.<sup>(27)</sup> In this paper we explain the details of the method and extend it to incorporate several new features. We apply the method to several one-dimensional systems with different evolution rules. The results very strongly support the notion of universality, i.e., the critical behavior does not depend on details of the evolution rules. The remainder of this paper is organized as follows. In Section 2 we introduce the models to be studied. The scaling behavior of the models is described in Section 3. An operator formalism for the master equation is presented in Section 4. In Section 5 we derive the time-dependent perturbation theory, and it is applied to the one-dimensional A model in Section 6. An example of the algorithms used to derive the actual series is described in Section 7 and the corresponding Fortran program is listed in the Appendix. The various series are listed in Section 8, which also contains the results of our Padé approximant analysis. Section 9 contains a brief summary and discussion.

## 2. THE CONTACT PROCESS AND RELATED MODELS

The systems considered in this work are stochastic lattice models or *interacting particle systems*<sup>(22)</sup> evolving according to a Markov process with local, intrinsically irreversible transition rules. We restrict our attention to one-component models in which each site can be either vacant or occupied by a single particle. The configuration of the system is characterized by a set of occupation variables  $\{\sigma_i\}$  ( $i \in Z^d$ , with  $\sigma_i = 0, 1$  corresponding to site  $i$  vacant or occupied, respectively). The model evolves via the following elementary processes: annihilation of particles at rate  $\lambda$  independent of the states of other sites, and autocatalytic creation of particles at vacant sites, with a rate depending on the number of occupied neighbors.

Perhaps the simplest such model is the *contact process* (CP).<sup>(23)</sup> It is

closely related to Schlögl's (first) model<sup>(24)</sup> of an autocatalytic chemical reaction, to directed percolation in  $(d+1)$  dimensions,<sup>(25)</sup> and to Reggeon field theory.<sup>(3,18)</sup> In the CP, particles are annihilated at rate  $\lambda$ . The creation rate at a vacant site is  $n_o/n_c$ , where  $n_o$  is the number of occupied nearest neighbors and  $n_c$  is the total number of nearest neighbors. The CP has an active steady state for all  $d \geq 1$ , when  $\lambda \leq \lambda_c(d)$ .<sup>(22,23)</sup> A number of rigorous results have been proven for the CP<sup>(22)</sup>; in particular, the phase transition is known to be continuous.<sup>(28)</sup> In addition, there are rigorous bounds on  $\lambda_c$ . Series expansions<sup>(20)</sup> for the steady-state density of particles in one-dimensional systems yield  $\lambda_c \simeq 0.3032$  and  $\beta \simeq 0.277$ , placing the CP in the RFT universality class.<sup>(18)</sup>

We have studied several variants of the contact process. The A model, introduced<sup>(19)</sup> as a simplified model for catalytic surface reactions<sup>(5)</sup> (for this interpretation to be valid one has to interchange the role played by vacancies and particles). The A model differs from the CP only in that vacancies are filled at unit rate provided at least one nearest neighbor is occupied. (There is no creation if all neighbors are empty.) Monte Carlo simulations<sup>(19)</sup> and steady-state series expansions<sup>(19,20)</sup> for  $d=1$  revealed that the A model has a critical point at  $\lambda_c \simeq 0.5741$  with critical exponent  $\beta \simeq 0.277$ , again reflecting RFT critical behavior. Another closely related model is the N3 model, which is identical to the CP except that vacancies with one occupied and one vacant nearest-neighbor become occupied at rate  $1/4$ . The N3 model was originally studied in ref. 20 because MFT predicted that it belonged to a new universality class. Steady-state series expansions showed, however, that  $\lambda_c \simeq 0.1621$  and  $\beta \simeq 0.279$ . Thus, we expect the N3 model to belong to the RFT universality class.

### 3. SCALING BEHAVIOR

In this section we review the scaling behavior of the contact process and similar models in order to motivate the perturbation expansions we have developed. We are primarily interested in describing the behavior close to critical points, and in particular the exponents characterizing this behavior. Both  $\lambda_c$  and various critical exponents, including  $\beta$ , can be obtained from the long-time behavior of certain quantities.

Following the work of Grassberger and de la Torre,<sup>(3)</sup> we consider the asymptotic behavior of the models when starting at  $t=0$  with a single seed particle at the origin, and  $\lambda \approx \lambda_c$ . According to the scaling hypothesis, one expects that any function of  $\mathbf{x}$ ,  $t$ , and  $\Delta$  (where  $\Delta = \lambda_c - \lambda$ ) depends on these variables only through  $\mathbf{x}^2/t^z$  and  $\Delta \cdot t^{1/\nu}$ , times some power of  $\mathbf{x}^2$ ,  $t$ , or  $\Delta$ . Here  $\nu$  and  $z$  are critical exponents. Notice that  $\nu$  is the  $\nu_{\parallel}$  of directed

percolation and that  $z$  is *not* the usual critical exponent from dynamic critical phenomena.

For the particle density one expects

$$\rho(\mathbf{x}, t) \propto t^{\eta - dz/2} F(\mathbf{x}^2/t^z, \Delta t^{1/\nu}) \quad (1)$$

and for the survival probability, i.e., the probability that the system has not entered the vacuum state at time  $t$ , one expects

$$P(t) \propto t^{-\delta} \phi(\Delta t^{1/\nu}) \quad (2)$$

where  $\eta$  and  $\delta$  are further critical exponents, while  $F$  and  $\phi$  are universal scaling functions.

From Eq. (1) we find for the mean number of particles  $\bar{n}(t)$  and the mean-square distance of spreading  $\bar{R}^2(t)$

$$\bar{n}(t) = \int d^d x \rho(\mathbf{x}, t) \propto t^\eta f(\Delta t^{1/\nu}) \quad (3)$$

and

$$\bar{R}^2(t) = \frac{1}{\bar{n}(t)} \int d^d x \mathbf{x}^2 \rho(\mathbf{x}, t) \propto t^z g(\Delta t^{1/\nu}) \quad (4)$$

From Eqs. (2)–(4) we immediately see that if  $\phi(y)$ ,  $f(y)$ , and  $g(y)$  are nonsingular at  $y=0$ , the asymptotic behavior of  $P(t)$ ,  $\bar{n}(t)$ , and  $\bar{R}^2(t)$  as  $t \rightarrow \infty$  at  $\lambda_c$  determines the critical exponents  $\delta$ ,  $\eta$ , and  $z$ . Numerous simulations<sup>(3,4,6–8,10,29)</sup> support the scaling hypothesis outlined above.

Let us now turn our attention to off-critical behavior. In the supercritical regime ( $\lambda < \lambda_c$ ) we see that by setting  $\psi(y) = y^{-\delta\nu} \phi(y)$  we may rewrite Eq. (2) as

$$P(t) \propto \Delta^{v\delta} \psi(\Delta t^{1/\nu}) \quad (5)$$

In the supercritical region there is a finite chance of survival. Thus, since  $P_\infty \equiv \lim_{t \rightarrow \infty} P(t)$  is finite,  $\lim_{y \rightarrow \infty} \psi(y)$  is finite, too, and we get

$$P_\infty \propto \Delta^{v\delta} \quad (6)$$

It can, however, be shown<sup>(3)</sup> that  $P_\infty$  and  $\rho$  are governed by the same critical exponent, leading to the important relation

$$\beta = v\delta \quad (7)$$

Turning to the subcritical regime ( $\lambda > \lambda_c$ ), we note that far from the critical point the correlations are short-ranged; one therefore expects an exponentially vanishing chance of survival. This can only be the case if

$$\phi(y) \propto (-y)^{\delta\nu} e^{-b(-y)^y} \quad \text{for } y \rightarrow -\infty \quad (8)$$

where  $b$  is a constant. When this is inserted in Eq. (2) we find

$$P(t) \propto (-\Delta)^{\nu\delta} e^{-b(-\Delta)^{\nu t}} \quad (9)$$

Taking the Laplace transform of this relation gives

$$\tilde{P}(s) = \int_0^\infty P(t) e^{-st} dt \propto \frac{(-\Delta)^{\nu\delta}}{s + b(-\Delta)^\nu} \quad (10)$$

and letting  $s \rightarrow 0$ , we find that

$$\tilde{P}(0) \propto (-\Delta)^{\beta-\nu} \quad (11)$$

where we have used Eq. (7).

Likewise we expect that the mean particle number decays exponentially:

$$f(y) \propto (-y)^{-\eta\nu} e^{-c(-y)^y} \quad \text{for } y \rightarrow -\infty \quad (12)$$

Inserting this result in Eq. (3) and taking the Laplace transform yields

$$\tilde{n}(0) \propto (-\Delta)^{-\nu(1+\eta)} \quad (13)$$

We expect that a surviving event will move in space according to a normal diffusion process, which leads to

$$g(y) \propto (-y)^{\nu(1-z)} \quad \text{for } y \rightarrow -\infty \quad (14)$$

$\bar{R}^2(t)$  grows linearly with  $t$  and it is therefore not easy to study its asymptotic behavior. Instead we study  $\bar{X}^2(t) = \bar{n}(t) \bar{R}^2(t)$ . From Eqs. (12) and (14) we find that

$$\bar{X}^2(t) \propto (-\Delta)^{\nu(1-z-\eta)} t e^{-c(-\Delta)^{\nu t}} \quad (15)$$

Which, after performing the Laplace transform, yields

$$\tilde{\bar{X}}^2(s) \propto \frac{(-\Delta)^{\nu(1-z-\eta)}}{[s + c(-\Delta)^\nu]^2} \quad (16)$$

and thus

$$\tilde{X}^2(0) \propto (-\Delta)^{-\nu(1+z+\eta)} \tag{17}$$

We have shown that by studying the asymptotic evolution of an ensemble of systems, each starting from a single “seed” particle, one may determine a set of critical exponents characterizing the model. As noted, this approach has been employed extensively in Monte Carlo simulations; in the remainder of this paper we develop series expansion methods for studying this evolution.

#### 4. OPERATOR FORMALISM

Markov processes in many-particle systems may be conveniently described via an operator formalism.<sup>(30-32)</sup> In this paper we use the formalism of ref. 20 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  $\{\sigma_i\}$  of the system can be written as a direct product

$$|\{\sigma_i\}\rangle = \prod_{i \in Z^d} |\sigma_i\rangle \tag{18}$$

The basic inner product is given by

$$\langle \{\sigma_i\} | \{\sigma'_i\} \rangle = \prod_{i \in Z^d} \delta_{\sigma_i, \sigma'_i} \tag{19}$$

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

$$\begin{aligned} A_i^\dagger |\sigma_i\rangle &= (1 - \sigma_i) |\sigma_i + 1\rangle \\ A_i |\sigma_i\rangle &= \sigma_i |\sigma_i - 1\rangle \end{aligned} \tag{20}$$

The state of the system at time  $t$  is

$$|\Psi(t)\rangle = \sum_{\{\sigma_i\}} p(\{\sigma_i\}, t) |\{\sigma_i\}\rangle \tag{21}$$

where the sum is over all configurations and  $p(\{\sigma_i\}, t)$  is the probability distribution on the configuration space. Only states  $|\Psi\rangle$  that satisfy positivity and normalization are physically relevant. These conditions are readily expressed as

$$\langle \{\sigma_i\} | \Psi \rangle \geq 0, \quad \forall \{\sigma_i\} \tag{22}$$

and

$$\sum_{\{\sigma_i\}} \langle \{\sigma_i\} | \Psi \rangle = 1 \quad (23)$$

The evolution of the probability distribution is governed by the master equation

$$\frac{d|\Psi(t)\rangle}{dt} = S|\Psi(t)\rangle \quad (24)$$

which has the formal solution (given that  $S$  is time independent)

$$|\Psi(t)\rangle = e^{St} |\Psi(0)\rangle \quad (25)$$

where  $|\Psi(0)\rangle$  is the initial probability distribution.

For the contact process and related models, the evolution operator  $S$  can be broken up in various ways that suggest a perturbative approach. Specifically for the A model we may write

$$S = \lambda W + V \quad (26)$$

where

$$W = \sum_{i \in \mathbb{Z}^d} (1 - A_i^\dagger) A_i \quad (27)$$

and

$$V = \sum_{i \in \mathbb{Z}^d} (1 - A_i) A_i^\dagger \left( 1 - \prod_j A_j A_j^\dagger \right) \quad (28)$$

where the product is over all nearest neighbors  $j$  of site  $i$ .

In this decomposition  $W$  only annihilates particles and  $V$  only creates particles. Next we consider the effects of the operators  $V$  and  $W$  on various configurations.  $W$  is simplest: operating on a configuration ( $\mathcal{C}$ ) containing  $r$  occupied sites, it gives a sum of  $r$  configurations ( $\mathcal{C}'$ ) (each having one of the  $r$  sites vacated), minus  $r$  times ( $\mathcal{C}$ ) itself:

$$W(\mathcal{C}) = \sum_{i=1}^r (\mathcal{C}'_i) - r(\mathcal{C}) \quad (29)$$

Consider a configuration ( $\mathcal{C}$ ) in which there are  $q$  vacant sites which are nearest neighbors of a particle. Operating on such a configuration,  $V$  yields



a sum of  $q$  configurations ( $\mathcal{C}''$ ) (each having one of the  $q$  vacancies now occupied), minus  $q$  times the original configuration:

$$V(\mathcal{C}) = \sum_{i=1}^q (\mathcal{C}_i'') - q(\mathcal{C}) \quad (30)$$

Note that both  $W$  and  $V$  annihilate the vacuum state  $|0\rangle$ .

## 5. PERTURBATION THEORY

There are several ways of expanding Eq. (25), e.g., in terms of  $t$  (short-time expansion), in terms of  $\lambda$ , or in  $\mu = \lambda^{-1}$ . The expansion in powers of  $t$  is obtained simply by choosing a value for  $\lambda$  (the obvious choice being  $\lambda_c$  as found from one of the other expansions) and then truncating the series obtained from Eq. (25) at some order  $n$ :

$$|\Psi(t)\rangle \approx \sum_{j=0}^n \frac{t^j}{j!} |\Psi_j\rangle \quad (31)$$

We will focus on the initial distribution  $|X_0\rangle$ , which assigns probability 1 to the configuration with a single particle at the origin, and all other sites vacant. Then we find the following recursive relation for  $|\Psi_j\rangle$ :

$$|\Psi_0\rangle = |X_0\rangle \quad (32)$$

and

$$|\Psi_j\rangle = (\lambda W + V) |\Psi_{j-1}\rangle; \quad j \geq 1 \quad (33)$$

As we operate with  $V$  once in each step, the "state"  $|\Psi_j\rangle$  is a sum over configurations containing up to  $j+1$  particles. The coefficient of  $t^j$  in the series for  $\bar{n}(t)$  is simply obtained by summing the products of the coefficient and the number of particles in each configuration. The coefficients in the expansion for  $P(t)$  could be obtained simply by summing all the coefficients to the configurations in  $|\Psi_j\rangle$ . It is, however, much simpler to calculate the *extinction* probability  $p(t)$ , the probability of having entered the absorbing state; obviously,  $P(t) = 1 - p(t)$ . The coefficient of  $t^j$  in the expansion of  $p(t)$  is simply the coefficient of the vacuum state  $|0\rangle$  in  $|\Psi_j\rangle$ , or, as  $W$  annihilates only one particle in each application, it is  $\lambda$  times the coefficient to the single-particle state in  $|\Psi_{j-1}\rangle$ . Note that as  $V$  ( $W$ ) only creates (destroys) single particles, we do not need to keep all configurations in  $|\Psi_j\rangle$ . In a calculation of  $p(t)$  to order  $n$ , we can discard all configurations with more than  $n-j$  particles, as these only contribute at orders higher than  $n$ .

Next we consider the long-time behavior in the supercritical region and derive a series expansion in powers of  $\lambda$  for the ultimate survival probability  $P_\infty$ . In this expansion we treat the annihilation operator  $W$  as a perturbation. The unperturbed evolution never reaches the vacuum state, so for small  $\lambda$  we are clearly in the supercritical region. We expect the critical point to be associated with the first singularity on the positive  $\lambda$  axis. Consider the Laplace transform of  $|\Psi(t)\rangle$ :

$$|\tilde{\Psi}(s)\rangle = \int_0^\infty e^{-st} |\Psi(t)\rangle = (s - S)^{-1} |\Psi(0)\rangle \quad (34)$$

Assuming that  $|\tilde{\Psi}(s)\rangle$  can be expanded in powers of  $\lambda$ ,

$$|\tilde{\Psi}(s)\rangle = |\tilde{\Psi}_0\rangle + \lambda |\tilde{\Psi}_1\rangle + \lambda^2 |\tilde{\Psi}_2\rangle + \dots \quad (35)$$

we find upon inserting Eqs. (35) and (26) in Eq. (34) that

$$|\tilde{\Psi}_0\rangle = (s - V)^{-1} |X_0\rangle \quad (36)$$

and

$$|\tilde{\Psi}_n\rangle = (s - V)^{-1} W |\tilde{\Psi}_{n-1}\rangle; \quad n \geq 1 \quad (37)$$

As can be seen from Eqs. (36) and (37), the operator  $(s - V)^{-1}$  plays an important role in this expansion. The effect of this operator on a configuration ( $\mathcal{C}$ ) can be found using the identity (valid for any configuration)

$$(s - V)^{-1} (\mathcal{C}) = s^{-1} (\mathcal{C}) + s^{-1} (s - V)^{-1} V (\mathcal{C}) \quad (38)$$

Inserting Eq. (30) and rearranging yields (for the A model)

$$(s - V)^{-1} (\mathcal{C}) = s_q \left[ (\mathcal{C}) + (s - V)^{-1} \sum_{i=1}^q (\mathcal{C}_i'') \right] \quad (39)$$

where  $s_q \equiv (s + q)^{-1}$ . The perturbation expansion derived above is generally valid. Only Eq. (39) differs slightly from model to model.

As  $V$  creates configurations having an additional particle, it is clear from Eq. (39) that  $(s - V)^{-1}$  operating on any configuration (apart from the vacuum) generates an infinite sequence of configurations. Thus it is impossible to calculate  $|\tilde{\Psi}(s)\rangle$  completely. What we can calculate rather easily, however, is the *extinction* probability  $\tilde{p}(s)$ . The extinction probability is readily obtained from Eq. (35), as the  $\lambda^j$  term in the expansion for  $\tilde{p}(s)$  is the coefficient of the vacuum state  $|0\rangle$  in  $|\tilde{\Psi}_j\rangle$ . Noting again that  $W$  only annihilates a single particle, we observe that configurations with more than  $j$  particles only contribute to the extinction probability at orders

higher than  $j$ . Thus, if we want to carry out the expansion to some order  $n$ , we only have to consider configurations containing up to  $n$  particles, and as  $|\tilde{\Psi}_0\rangle$  is generated from a single particle at the origin, the number of such configurations in  $|\tilde{\Psi}_0\rangle$  is finite (actually it is a sum over all lattice animals consisting of  $n$  or fewer sites). Furthermore, when we have carried the expansion to order  $j$  we can discard all configurations with more than  $n-j$  particles, as these can never reach the vacuum state during the remaining  $n-j$  applications of  $W$ . Another major simplification arises if we only focus on the ultimate survival probability  $P_\infty = 1 - \lim_{s \rightarrow 0} s\tilde{p}(s)$ ; then the algebraic factor  $s_q$  in Eq. (39) reduces to the purely numerical factor  $1/q$ .

Finally, we consider the long-time behavior in the subcritical region. This expansion is very similar to the supercritical case, but now we treat  $V$  perturbatively instead of  $W$ . First we rewrite Eq. (26) as

$$S = W + \mu V \quad (40)$$

where  $\mu = \lambda^{-1}$ , and we have absorbed a factor  $\lambda$  into a rescaling of the time variable in Eq. (24). One immediately sees that the unperturbed evolution operator  $e^{Wt}$  simply corresponds to an exponentially decaying chance of survival. Thus in the infinite-time limit only the vacuum state remains, and we are studying the subcritical regime. Again we take the Laplace transform of Eq. (25), and assuming that  $|\tilde{\Psi}(s)\rangle$  can be expanded in powers of  $\mu$ ,

$$|\tilde{\Psi}(s)\rangle = |\tilde{\Psi}_0\rangle + \mu |\tilde{\Psi}_1\rangle + \mu^2 |\tilde{\Psi}_2\rangle + \dots \quad (41)$$

we find in analogy with Eqs. (36) and (37)

$$|\tilde{\Psi}_0\rangle = (s - W)^{-1} |X_0\rangle \quad (42)$$

and

$$|\tilde{\Psi}_n\rangle = (s - W)^{-1} V |\tilde{\Psi}_{n-1}\rangle; \quad n \geq 1 \quad (43)$$

An identity equivalent to Eq. (39) holds for  $(s - W)^{-1}$ :

$$(s - W)^{-1} (\mathcal{C}) = s_r \left[ (\mathcal{C}) + (s - W)^{-1} \sum_{i=1}^r (\mathcal{C}'_i) \right] \quad (44)$$

where  $s_r \equiv (s + r)^{-1}$  and  $r$  is the number of particles in the configuration  $\mathcal{C}$ . As  $W$  destroys particles,  $(s - W)^{-1}$  operating on any configuration produces only a finite number of new configurations.

In this case we can derive an expansion for  $\tilde{P}(0)$  directly. The coefficient of  $\mu^j$  in the expansion for  $\tilde{P}(0)$  is the sum of the coefficients of all configurations, except the vacuum, in  $|\tilde{\Psi}_j\rangle$ . The corresponding coefficient in the expansion for  $\tilde{n}(0)$  is just the sum of the product of the coefficient and the number of particles for each configuration. Again the calculation is greatly simplified by the fact that  $s_r$  is replaced simply by  $1/r$ .

## 6. APPLICATION TO THE ONE-DIMENSIONAL A MODEL

As an illustration of the methods derived in Section 5, we compute the poisoning probability  $\tilde{p}(z)$  for the one-dimensional A model to  $\mathcal{O}(\lambda^3)$ . First we need a convenient notation for configurations. Since we are focusing on situations where most of the sites are vacant, we will denote an occupied site by  $\bullet$ , and a vacant site by  $\circ$ . Typically the set of occupied sites will be embedded in an otherwise empty lattice—so we assume that all sites to the right (left) of the first (last)  $\bullet$  are vacant. We will furthermore use the translational invariance of the lattice. Thus  $(\bullet\bullet) = \sum_i A_i^\dagger A_{i+1}^\dagger |0\rangle$  denotes a translationally invariant configuration with two adjacent occupied sites and the rest vacant,  $(\bullet\circ\bullet) = \sum_i A_i^\dagger A_{i+2}^\dagger |0\rangle$  has two occupied sites separated by a vacancy, etc.

Iterating Eq. (39), we obtain

$$|\tilde{\Psi}_0\rangle = s_2(\bullet) + 2s_2^2(\bullet\bullet) + 4s_2^3(\bullet\bullet\bullet) + \dots$$

where we have discarded all configurations with more than 3 particles, as they do not contribute to the extinction probability at this order. Using Eq. (29), we get

$$W|\tilde{\Psi}_0\rangle = s_2[(0) - (1 - 4s_2)(\bullet) - 4s_2(1 - 2s_2)(\bullet\bullet) + 4s_2^2(\bullet\circ\bullet) + \dots]$$

where the omitted terms have three or more particles. Then Eqs. (37) and (39) imply

$$|\tilde{\Psi}_1\rangle = s_2[s^{-1}(0) - (1 - 4s_2)s_2(\bullet) - 2s_2^2(3 - 8s_2)(\bullet\bullet) + 4s_2^2s_3(\bullet\circ\bullet) + \dots]$$

Similarly,

$$W|\tilde{\Psi}_1\rangle = -s_2^2[(1 - 4s_2)(0) - (1 - 16s_2 + 32s_2^2 + 8s_2s_3)(\bullet) + \dots]$$

$$|\tilde{\Psi}_2\rangle = -s_2^2[s^{-1}(1 - 4s_2)(0) - s_2(1 - 16s_2 + 32s_2^2 + 8s_2s_3)(\bullet) + \dots]$$

$$W|\tilde{\Psi}_2\rangle = s_2^3(1 - 16s_2 + 32s_2^2 + 8s_2s_3)(0) + \dots$$

$$|\tilde{\Psi}_3\rangle = s^{-1}s_2^3(1 - 16s_2 + 32s_2^2 + 8s_2s_3)(0) + \dots$$

Collecting coefficients of (0) yields

$$\tilde{p}(s) = s^{-1} [s_2 \lambda - (1 - 4s_2) s_2^2 \lambda^2 + (1 - 16s_2 + 32s_2^2 + 8s_2 s_3) s_2^3 \lambda^3 + \dots]$$

Note that in the expansion of  $|\tilde{\Psi}(s)\rangle$  it is only (0) which carries the factor  $s^{-1}$ . All other configurations carry one or more  $s_q$  factors, corresponding to an eventual exponential decay in the probability. The ultimate survival probability is

$$P_\infty = 1 - \lim_{s \rightarrow 0} s \tilde{p}(s) = 1 - \frac{1}{2} \lambda - \frac{1}{4} \lambda^2 - \frac{7}{24} \lambda^3 + \dots \quad (45)$$

The coefficients of  $\lambda^j$  in the expansion for  $\tilde{p}(s)$  are already quite complicated at this low level and will evidently become more so at higher orders. For this reason we calculate only the ultimate survival probability. [The coefficient of  $\lambda^j$  in  $P_\infty$  is  $-1$  times the coefficient of  $(\bullet)$  in  $|\tilde{\Psi}_{j-1}\rangle$ .] Restricting attention to  $P_\infty$  allows us to anticipate the limit  $s \rightarrow 0$ , so that we can replace  $s_q$  by  $1/q$ , resulting in a major simplification of algebra. This enables us to obtain a much longer series for  $P_\infty$  at the expense of information about the behavior at intermediate times.

Next we take a look at the subcritical expansions for  $\tilde{P}(0)$  and  $\tilde{n}(0)$ . Using Eq. (44), we find

$$|\tilde{\Psi}_0\rangle = s_1(\bullet) + s^{-1}(0)$$

Notice that this  $|\tilde{\Psi}_0\rangle$  is very different from the corresponding quantity in the supercritical expansion. From Eq. (30) we get

$$V |\tilde{\Psi}_0\rangle = 2s_1[(\bullet\bullet) - (\bullet)]$$

Using Eq. (44), we find

$$|\tilde{\Psi}_1\rangle = 2s_1 s_2(\bullet\bullet) + 2s_1^2(2s_2 - 1)[(\bullet) + s^{-1}(0)]$$

As can be seen, the coefficients are already becoming quite complicated. But we are interested in the series only at  $s=0$  and we can therefore replace  $s_r$  by  $1/r$ . We will also discard the vacuum state, as the survival probability and average number of particles are obtained from the other configurations. We then find

$$|\tilde{\Psi}_1\rangle = (\bullet\bullet)$$

Continuing in the same manner, we obtain, for  $s=0$ ,

$$V |\tilde{\Psi}_1\rangle = 2(\bullet\bullet\bullet) - 2(\bullet\bullet)$$

$$|\tilde{\Psi}_2\rangle = \frac{2}{3}(\bullet\bullet\bullet) + \frac{1}{3}(\bullet\circ\bullet) - \frac{1}{3}(\bullet\bullet)$$

$$\begin{aligned}
V|\tilde{\Psi}_2\rangle &= \frac{4}{3}(\bullet\bullet\bullet\bullet) + \frac{1}{3}[(\bullet\bullet\bullet\bullet) + (\bullet\bullet\bullet\bullet)] \\
&\quad - \frac{5}{3}(\bullet\bullet\bullet) - (\bullet\bullet\bullet) + \frac{2}{3}(\bullet\bullet) \\
|\tilde{\Psi}_3\rangle &= \frac{1}{3}(\bullet\bullet\bullet\bullet) + \frac{2}{9}[(\bullet\bullet\bullet\bullet) + (\bullet\bullet\bullet\bullet)] + \frac{2}{9}(\bullet\bullet\bullet\bullet) \\
&\quad - \frac{1}{3}(\bullet\bullet\bullet) - \frac{4}{9}(\bullet\bullet\bullet) + \frac{2}{9}(\bullet\bullet)
\end{aligned}$$

Summing the coefficients in  $|\tilde{\Psi}_j\rangle$ , we find

$$\tilde{P}(0) = 1 + \mu + \frac{2}{3}\mu^2 + \frac{4}{9}\mu^3 + \dots \quad (46)$$

and forming the sum of the product of coefficients and number of particles, we find

$$\tilde{n}(0) = 1 + 2\mu + 2\mu^2 + \frac{5}{3}\mu^3 + \dots \quad (47)$$

Next we consider the expansion for  $\tilde{X}^2(0)$ . This expansion is more complicated, as we must keep track of the origin in each configuration. We now mark the origin by an overbar, e.g.,  $(\bullet\bar{\bullet})$  denotes a configuration in which the origin is vacant while its neighbors are occupied. As before, all sites to the left and right of the particles are vacant. We use reflection symmetry so that  $(\bar{\bullet}\bullet) \equiv \frac{1}{2}[(\bar{\bullet}\bullet) + (\bullet\bar{\bullet})]$ , etc. Using the rules for the subcritical expansion, we obtain, for  $s=0$ , and neglecting the vacuum state,

$$\begin{aligned}
|\tilde{\Psi}_0\rangle &= (\bar{\bullet}) \\
V|\tilde{\Psi}_0\rangle &= 2(\bar{\bullet}\bullet) - 2(\bar{\bullet}) \\
|\tilde{\Psi}_1\rangle &= (\bar{\bullet}\bullet) + (\bar{\bullet}\bullet) - (\bar{\bullet}) \\
V|\tilde{\Psi}_1\rangle &= (\bar{\bullet}\bullet\bullet) + (\bullet\bar{\bullet}\bullet) + (\bar{\bullet}\bullet\bullet) - 3(\bar{\bullet}\bullet) - 2(\bar{\bullet}\bullet) + 2(\bar{\bullet}) \\
|\tilde{\Psi}_2\rangle &= \frac{1}{3}(\bar{\bullet}\bullet\bullet) + \frac{1}{3}(\bullet\bar{\bullet}\bullet) + \frac{2}{3}(\bar{\bullet}\bullet\bullet) + \frac{1}{6}(\bar{\bullet}\bullet\bullet) \\
&\quad + \frac{1}{6}(\bullet\bar{\bullet}\bullet) + \frac{5}{6}(\bar{\bullet}\bullet\bullet) - (\bar{\bullet}\bullet) - 2(\bar{\bullet}\bullet) + \frac{7}{6}(\bar{\bullet}) \\
V|\tilde{\Psi}_2\rangle &= \frac{1}{3}(\bar{\bullet}\bullet\bullet\bullet) + (\bullet\bar{\bullet}\bullet\bullet) + \frac{2}{3}(\bar{\bullet}\bullet\bullet\bullet) + \frac{1}{6}(\bar{\bullet}\bullet\bullet\bullet) + \frac{1}{6}(\bullet\bar{\bullet}\bullet\bullet) \\
&\quad + \frac{1}{3}(\bullet\bar{\bullet}\bullet\bullet) - \frac{5}{6}(\bar{\bullet}\bullet\bullet\bullet) - \frac{3}{2}(\bullet\bar{\bullet}\bullet\bullet) + \frac{5}{6}(\bar{\bullet}\bullet\bullet\bullet) - \frac{5}{2}(\bar{\bullet}\bullet\bullet\bullet) \\
&\quad - \frac{1}{2}(\bar{\bullet}\bullet\bullet) - \frac{1}{2}(\bullet\bar{\bullet}\bullet) + \frac{7}{3}(\bar{\bullet}\bullet) - \frac{5}{3}(\bar{\bullet}\bullet\bullet) + 4(\bar{\bullet}\bullet) - \frac{7}{3}(\bar{\bullet}) \\
|\tilde{\Psi}_3\rangle &= \frac{1}{12}(\bar{\bullet}\bullet\bullet\bullet) + \frac{1}{4}(\bullet\bar{\bullet}\bullet\bullet) + \frac{1}{4}(\bar{\bullet}\bullet\bullet\bullet) + \frac{1}{12}(\bar{\bullet}\bullet\bullet\bullet) + \frac{1}{36}(\bar{\bullet}\bullet\bullet\bullet) \\
&\quad + \frac{7}{36}(\bullet\bar{\bullet}\bullet\bullet) + \frac{5}{36}(\bullet\bar{\bullet}\bullet\bullet) - \frac{1}{6}(\bar{\bullet}\bullet\bullet\bullet) - \frac{5}{12}(\bullet\bar{\bullet}\bullet\bullet) + \frac{7}{12}(\bar{\bullet}\bullet\bullet\bullet) \\
&\quad + \frac{5}{36}(\bar{\bullet}\bullet\bullet\bullet) + \frac{1}{18}(\bar{\bullet}\bullet\bullet\bullet) + \frac{1}{6}(\bullet\bar{\bullet}\bullet\bullet) - \frac{10}{9}(\bar{\bullet}\bullet\bullet) - \frac{2}{9}(\bar{\bullet}\bullet\bullet) \\
&\quad - \frac{13}{36}(\bullet\bar{\bullet}\bullet) + \frac{3}{4}(\bar{\bullet}\bullet) + \frac{7}{9}(\bar{\bullet}\bullet\bullet\bullet) - \frac{9}{4}(\bar{\bullet}\bullet\bullet) + \frac{29}{9}(\bar{\bullet}\bullet) - \frac{7}{4}(\bar{\bullet})
\end{aligned}$$

from which we find

$$\tilde{X}^2(0) = 2\mu + 7\mu^2 + 12\frac{5}{6}\mu^3 + \dots \quad (48)$$

Finally we turn our attention to the expansion in powers of  $t$  as given in Eqs. (31)–(33). For the A model in one dimension, the first few terms are as follows:

$$\begin{aligned} S |\Psi(0)\rangle &= 2[(\bullet\bullet) - (\bullet)] + \lambda[(0) - (\bullet)] \\ S^2 |\Psi(0)\rangle &= 4(\bullet\bullet\bullet) - 2(4 + 3\lambda)(\bullet\bullet) + (4 + 8\lambda + \lambda^2)(\bullet) - \lambda(2 + \lambda)(0) \\ S^3 |\Psi(0)\rangle &= 8(\bullet\bullet\bullet\bullet) - 24(1 + \lambda)(\bullet\bullet\bullet) + 2(12 + 26\lambda + 7\lambda^2)(\bullet\bullet) \\ &\quad + 4\lambda(\bullet\bullet\bullet) - (8 + 36\lambda + 22\lambda^2 + \lambda^3)(\bullet) + \lambda(4 + 8\lambda + \lambda^2)(0) \end{aligned}$$

which implies for the survival probability

$$P(t) = 1 - \lambda t + \frac{\lambda(2 + \lambda)}{2!} t^2 - \frac{\lambda(4 + 8\lambda + \lambda^2)}{3!} t^3 + \mathcal{O}(t^4) \quad (49)$$

and for the mean particle number

$$\bar{n}(t) = 1 + (2 - \lambda)t - \frac{\lambda(4 - \lambda)}{2!} t^2 - \frac{4\lambda + 6\lambda^2 - \lambda^3}{3!} t^3 + \mathcal{O}(t^4) \quad (50)$$

In all cases, calculating successive terms rapidly becomes very complicated. The rules are, however, simple enough that they can be codified as a computer algorithm.

## 7. COMPUTER ALGORITHM

The series expansions derived in Section 5 are based on the recursive determination of  $|\Psi_j\rangle$  as expressed in Eqs. (31)–(33), (35)–(37), and (41)–(43). The process consists of many similar elementary steps, creation and annihilation of particles, which are readily represented in a computer algorithm.

Each component  $|\Psi_j\rangle$  in the expansion is a sum over many configurations. In one dimension, any configuration is conveniently expressed as a binary number, with 0's representing vacancies and 1's representing particles. Due to translational invariance we can assume that the first site is occupied by a particle, so that a configuration corresponds to an odd integer. We will refer to a configuration by its integer analog  $[(\bullet\bullet\bullet) = (5)$ , etc.]. The operators  $V$  and  $W$  are readily expressed via logical bitwise operations on configuration ( $i$ ).

In the following we will use the supercritical expansion to exemplify the algorithm. The full program is listed in the Appendix. Let  $\text{COEF}(i)$  be the coefficient of configuration  $(i)$ ,  $\text{IND}(i)$  the number of particles in the configuration once it has been created [i.e.,  $\text{IND}(i)=0$  if the configuration has not yet appeared in the expansion],  $\text{IS}(k)$  a mask whose bytes are all 0 except for the  $k$ th [i.e.,  $\text{IS}(k)=2^k$ ], and finally let  $\text{NS}(k)$  be the bitwise compliment of  $\text{IS}(k)$  [i.e.,  $\text{NS}(k)=\text{NOT}(\text{IS}(k))$ ]. As can be seen from Eq. (37), the evaluation of  $|\Psi_j\rangle$  consists of two steps: first, the operation of the annihilation operator  $W$  on (the previously determined) component  $|\Psi_{j-1}\rangle$ , then operation with  $(s-V)^{-1}$ . The configurations  $(i')$  generated by  $W$  as it operates on  $(i)$  are evaluated [e.g., via the operation  $i'=\text{IAND}(\text{NS}(k), i)$ , where  $\text{IAND}$  is the bitwise logical AND]. Now,  $i' < i$  if site  $k$  was occupied and thus a new configuration generated. The various new configurations are simply produced by letting  $k$  run from 0 through the maximal possible number of particles in a configuration.  $\text{COEF}(i'+1)$  [which temporarily stores the coefficient of  $(i')$ ] is augmented by  $\text{COEF}(i)$ , and  $\text{COEF}(i+1)$  is decreased by  $\text{COEF}(i)*\text{IND}(i)$ . After having gone through all the configurations one resets the coefficients, i.e., one sets  $\text{COEF}(i)=\text{COEF}(i+1)$  and  $\text{COEF}(i+1)=0$  for all odd integers  $i$ .

The operation of  $(s-V)^{-1}$  is a little more involved, as can be seen from Eq. (39). It is, however, easily expressed as an algorithm. The three models studied in this paper differ only in the rules for creating particles. In the one-dimensional case studied here this difference can be represented through a parameter  $\alpha$  which controls the rate of creation at a site with just one occupied neighbor (the rate of creation is 1 when both neighbors are occupied); in this way  $\alpha=1$  corresponds to the A model,  $\alpha=1/2$  to the CP, and  $\alpha=1/4$  to the N3 model. Notice that the configurations in  $|\tilde{\Psi}_0\rangle$  are the same, but the coefficients are generalized to  $1/(2\alpha)$ . The recursive nature of  $(z-V)^{-1}$  is realized by treating the configurations in ascending order. This ensures that  $(z-V)^{-1}$  is applied to the configurations created by  $V$  because the new configuration  $i' > i$ . A new configuration  $i'$  is produced from  $i$  by adding a particle at an empty site [i.e., if  $\text{IAND}(i, \text{IS}(k))=0$ ] with at least one occupied neighbor [i.e., if  $\text{IAND}(i, \text{IS}(k-1)) > 0$  or  $\text{IAND}(i, \text{IS}(k+1)) > 0$ ]. If both neighbors are occupied, the new configuration  $(i')$ , where  $i'=\text{IOR}(i, \text{IS}(k))$ , is given weight 1, and if only one neighbor is occupied  $(i')$  it is given weight  $\alpha$ . The newly created configurations and their weights are stored temporarily. After having gone through all the positions in configuration  $(i)$ , the weights are added up in  $\text{SUM}$  and the coefficient of  $(i)$  is changed to  $\text{COEF}(i)/\text{SUM}$ . Finally, the coefficients of the new configurations  $(i')$  are incremented by  $\text{COEF}(i)*\text{WEIGHT}(i')$  [with  $\text{COEF}(i)$  being the newly changed value].

As noted in Section 5, there are restrictions on the number of particles



in configurations which need to be retained at each step of the calculation. These restrictions enable us to derive the various series with little expenditure of computer time (typically 15–20 min on an IBM 3090).

## 8. RESULTS AND ANALYSIS

### 8.1. Supercritical Expansion

We have derived series for the ultimate survival probability for the A model, the contact process, and the N3 model to  $\mathcal{O}(\lambda^{24})$ . The coefficients are given in Table I. We then formed various Padé approximants to the series for  $(d/d\lambda) \ln P_\infty$ , thus obtaining unbiased estimates for  $\lambda_c$ , the first

Table I. Coefficients of  $\lambda^n$  in the Supercritical Expansion for the Ultimate Survival Probability  $P_\infty$

$n$	A model	Contact process	N3 model
0	1	1	1
1	$-\frac{1}{2}$	-1	-2
2	$-\frac{1}{4}$	-1	-4
3	$-\frac{7}{24}$	-2	$-13\frac{1}{3}$
4	$-\frac{163}{432}$	$-4\frac{1}{2}$	$-50\frac{481}{300}$
5	$-\frac{3841}{7776}$	-11	$-233\frac{953}{1215}$
6	-0.6546460619570188	$-28\frac{1249}{2000}$	$-1.136548638317330 \times 10^3$
7	-0.9160621981452912	$-77\frac{11}{128}$	$-5.695698596607674 \times 10^3$
8	-1.356981446217977	$-2.137216796874996 \times 10^2$	$-2.977016730062130 \times 10^4$
9	-2.052404865011525	$-6.049109971788211 \times 10^2$	$-1.571425361355731 \times 10^5$
10	-3.088808063863888	$-1.739640020676603 \times 10^3$	$-8.498400295925013 \times 10^5$
11	-4.711980262430326	$-5.074116017903053 \times 10^3$	$-4.634960582084085 \times 10^6$
12	-7.373187827483772	$-1.494581753539295 \times 10^4$	$-2.560631593768748 \times 10^7$
13	-11.64098743777937	$-4.447736306471725 \times 10^4$	$-1.426950583017804 \times 10^8$
14	-18.31374655286935	$-1.332435717211703 \times 10^5$	$-8.004785860447677 \times 10^8$
15	-29.09696095266492	$-4.022276206150533 \times 10^5$	$-4.528272714746211 \times 10^9$
16	-46.84094923091073	$-1.220343327302971 \times 10^6$	$-2.570217654083986 \times 10^{10}$
17	-75.46270213626647	$-3.723196360389418 \times 10^6$	$-1.469947275905127 \times 10^{11}$
18	$-1.216314724443718 \times 10^2$	$-1.140871210580868 \times 10^7$	$-8.422148793647517 \times 10^{11}$
19	$-1.978953411341986 \times 10^2$	$-3.509071017053852 \times 10^7$	$-4.856567304563910 \times 10^{12}$
20	$-3.230966492170077 \times 10^2$	$-1.083954944690878 \times 10^8$	$-2.804254339803976 \times 10^{13}$
21	$-5.277431752339135 \times 10^2$	$-3.355197890181546 \times 10^8$	$-1.627400816255525 \times 10^{14}$
22	$-8.644497240830738 \times 10^2$	$-1.043396858362474 \times 10^9$	$-9.458146911335279 \times 10^{14}$
23	$-1.427559659906972 \times 10^3$	$-3.246061423205646 \times 10^9$	$-5.516901623641276 \times 10^{15}$
24	$-2.342271155757435 \times 10^3$	$-1.015175910777746 \times 10^{10}$	$-3.224002599773613 \times 10^{16}$

pole on the positive  $\lambda$  axis, and  $\beta$ , the residue of the Padé approximant at this pole. Figure 1 shows the flow of  $(\lambda_c - \lambda)$  times the value of the Padé approximants to the series for  $(d/d\lambda) \ln P_\infty$  evaluated at  $\lambda$ , in the vicinity of  $\lambda_c$  for various Padé approximants. This analysis yields the residue and thus the exponent  $\beta$ . The results of the analysis are summarized in Table II. The estimates of  $\lambda_c$  are very stable, as they only differ in the sixth digit. The estimates for  $\beta$  were obtained as the "central" value of the flows shown in Fig. 1. As can be seen, the estimates for  $\beta$  are in good internal agreement, with the discrepancy between the models being somewhat more pronounced. The error in the values for  $\beta$  can be estimated from the spread of various

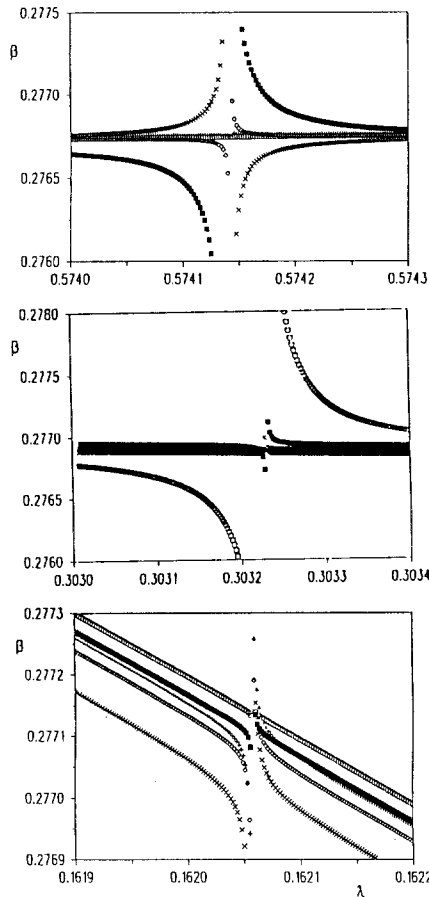


Fig. 1. Flow of the residue  $\beta$  from various Padé approximants to the series  $(d/d\lambda) \ln P_\infty$  for the A model (top), the contact process (middle), and the N3 model (bottom).

**Table II. Unbiased Estimates for the Location of the Critical Point  $\lambda_c$  and the Value of the Critical Exponent  $\beta$  As Obtained from Various Padé Approximants to the Series  $d/d\lambda \ln P_\infty$ , with the Series for  $P_\infty$  Given in Table I**

Model	Approximant	$\lambda_c$	$\beta$
A	[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
CP	[10, 11]	0.303228	0.27688
	[11, 10]	0.303228	0.2769
	[11, 11]	0.303230	0.27693
	[10, 12]	0.303228	0.27686
	[12, 10]	0.303229	0.27690
N3	[10, 11]	0.162057	0.27710
	[11, 10]	0.162056	0.27702
	[11, 11]	0.162058	0.27715
	[11, 12]	0.162058	0.27712
	[12, 11]	0.162057	0.27707

Padé approximants. This leads to the following estimates for  $\lambda_c$  and  $\beta$ : For the A model we estimate that  $\lambda_c = 0.574141(3)$  and  $\beta = 0.27674(4)$ , for the CP we estimate that  $\lambda_c = 0.303228(2)$  and  $\beta = 0.27690(5)$ , and for the N3 model we estimate that  $\lambda_c = 0.162057(2)$  and  $\beta = 0.27710(5)$ . We strongly believe that the models belong to the same universality class and thus should have the same critical exponents. However, the values of  $\beta$  do not agree within the cited uncertainty. Rather than seeing this as a violation of universality, we believe it reflects systematic errors that cannot be estimated from any of the individual models. These errors could be caused by corrections to scaling or be inherent to the method. This suggests the need for better methods for analyzing the series, a problem we hope to address in the future.

As pointed out by Guttman,<sup>(33)</sup> it is difficult to quantify error bounds and when they are stated they are generally subjective confidence limits, frequently measuring the enthusiasm of the author rather than the quality of the data. Our work suggests that one way to obtain a more realistic estimate of the exponent uncertainties is to study several closely related models. In conclusion we adopt  $\beta = 0.2769(2)$  as our final estimate. This value is in good agreement with the earlier results  $\beta = 0.277(1)$ <sup>(20)</sup> obtained from time-independent expansions for the same models as studied in this work. Our estimate for  $\beta$  agrees only marginally with series expansion results for directed percolation,<sup>(26)</sup> which yielded  $\beta = 0.2764(1)$ . However,

our result does not agree with the conjecture<sup>(34)</sup> that  $\beta = 199/720 = 0.2763888\dots$ . This conjecture is also contradicted by recent results obtained by ben-Avraham *et al.*<sup>(35)</sup>

Better estimates for critical exponents can often be obtained if one has prior knowledge of the location of the critical point. In this case it is useful to study Padé approximants to the series for  $(\lambda_c - \lambda)(d/d\lambda) \ln P_\infty$  which, when evaluated at  $\lambda_c$ , yields the critical exponent  $\beta$ . Since we do not know  $\lambda_c$ , we use a generalization of this approach.<sup>(36)</sup> We form the series mentioned above using a trial value  $\tilde{\lambda}_c$  for  $\lambda_c$  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  $\tilde{\beta}$

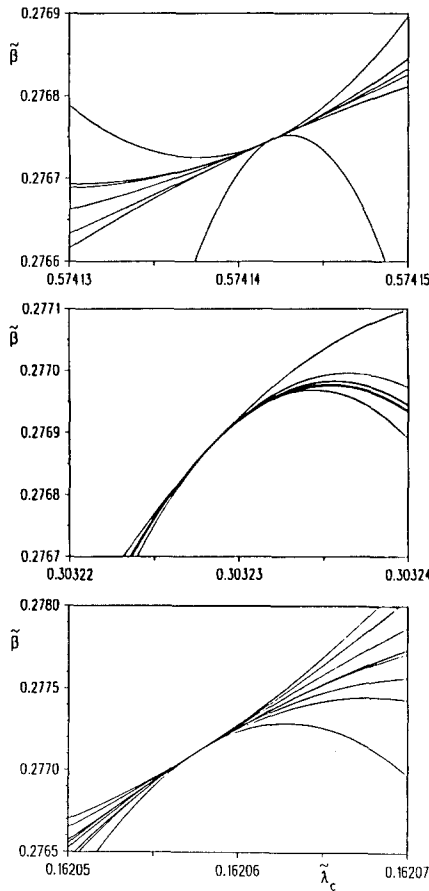


Fig. 2. Biased estimates  $\tilde{\beta}$  as a function of  $\tilde{\lambda}_c$  derived from Padé approximants to the series  $(\tilde{\lambda}_c - \lambda)(d/d\lambda) \ln P_\infty$  evaluated at  $\tilde{\lambda}_c$  for the A model (top), the contact process (middle), and the N3 model (bottom).

versus  $\tilde{\lambda}_c$  we expect the curves to intersect at the point  $(\lambda_c, \beta)$ . Figure 2 shows the result of this approach for the three models studied in this paper. Notice that with the unbiased flow shown in Fig. 1 we first form Padé approximants to  $(d/d\lambda) \ln P_\infty$ , evaluate them at  $\lambda$ , and then multiply by  $(\lambda_c - \lambda)$ , whereas with the biased flow shown in Fig. 2 we first form the series  $(\tilde{\lambda}_c - \lambda)(d/d\lambda) \ln P_\infty$ , then form Padé approximants and evaluate them at  $\tilde{\lambda}_c$ . In all cases we see a very narrow intersection of the Padé approximants, showing the utility of this approach. The estimates of  $\lambda_c$  and  $\beta$  from this analysis are consistent with those obtained from the unbiased estimates. The method therefore seems to be very efficient in determining  $\lambda_c$  and the central value of the critical exponent. As in the unbiased case, the estimates from the various models disagree in the fourth significant figure.

**Table III. Coefficients of  $\mu^n$  in the Subcritical Expansion for the Survival Probability  $\tilde{P}(0)$**

$n$	A model	Contact process	N3 model
0	1	1	1
1	1	$\frac{1}{2}$	$\frac{1}{4}$
2	$\frac{2}{3}$	$\frac{1}{6}$	$\frac{1}{24}$
3	$\frac{4}{9}$	$\frac{5}{72}$	$\frac{7}{576}$
4	$\frac{3}{10}$	$\frac{11}{720}$	$-\frac{1}{2880}$
5	0.1490123456790121	$1.1705246913580190 \times 10^{-2}$	$1.4754533179012440 \times 10^{-3}$
6	0.1646778365667236	$-1.9142416225749440 \times 10^{-3}$	$-6.7660136730232340 \times 10^{-4}$
7	$-2.8811662607430620 \times 10^{-2}$	$4.4907832577475000 \times 10^{-3}$	$4.4972546370998570 \times 10^{-4}$
8	0.2121663707056365	$-3.1941193130690740 \times 10^{-3}$	$-2.6418492028906710 \times 10^{-4}$
9	$-0.2820407842914748$	$3.2229252772281540 \times 10^{-3}$	$1.5854790789034080 \times 10^{-4}$
10	0.5687162235151362	$-2.8750665234452790 \times 10^{-3}$	$-9.3188779446962200 \times 10^{-5}$
11	$-0.9974391841175399$	$2.6788542008882720 \times 10^{-3}$	$5.4288026096361380 \times 10^{-5}$
12	1.841874510257309	$-2.4600519771159420 \times 10^{-3}$	$-3.1277155056983060 \times 10^{-5}$
13	$-3.360767324839372$	$2.2715585623241610 \times 10^{-3}$	$1.7876722473684250 \times 10^{-5}$
14	6.182306478228222	$-2.0962191122760940 \times 10^{-3}$	$-1.0162176389621450 \times 10^{-5}$
15	$-11.38763552142269$	$1.9392143142618080 \times 10^{-3}$	$5.7639334933744500 \times 10^{-6}$
16	21.04866017478824	$-1.7982824768918780 \times 10^{-3}$	$-3.2716828675659270 \times 10^{-6}$
17	$-39.01546762347390$	$1.6728497523677200 \times 10^{-3}$	$1.8629110322197100 \times 10^{-6}$
18	72.53879002343065	$-1.5612586716720530 \times 10^{-3}$	$-1.0657037197092720 \times 10^{-6}$
19	$-1.352619056531210 \times 10^2$	$1.4618649182260920 \times 10^{-3}$	$6.1280401160814620 \times 10^{-7}$
20	$2.529419096358465 \times 10^2$	$-1.3729522763817930 \times 10^{-3}$	$-3.5405660124621110 \times 10^{-7}$
21	$-4.742899292554566 \times 10^2$	$1.2929675172696700 \times 10^{-3}$	$2.0532367564803330 \times 10^{-7}$
22	$8.916112189172460 \times 10^2$	$-1.2205746184416090 \times 10^{-3}$	$-1.1935297072315820 \times 10^{-7}$
23	$-1.680121716999735 \times 10^3$	$1.1546841927474370 \times 10^{-3}$	$6.9447180040513229 \times 10^{-8}$
24	$3.172971217367947 \times 10^3$	$-1.0944295167454210 \times 10^{-3}$	$-4.0399392599242160 \times 10^{-8}$

## 8.2. Subcritical Expansions

In the subcritical regime we have derived series for the ultimate survival probability and the average number of particles to 24th order in  $\mu = \lambda^{-1}$ . For the quantity  $\bar{X}^2$  we have derived a series to 18th order. The coefficients in these series are listed in Tables III–V. One immediately notices that the series are not so well behaved. The alternating sign of consecutive terms is an indication that the dominant singularity is located on the negative  $\mu$  axis. We analyzed the series using the same methods as for the supercritical series. The results of the unbiased analysis for the survival probability are summarized in Table VI and for the number of particles in Table VII. The critical singularity is not as stable as in the supercritical case and the value of  $\mu_c$  differs quite a bit from  $\lambda_c^{-1}$ . The lack of stability of  $\mu_c$  of course leads to a less accurate determination of the critical

**Table IV. Coefficients of  $\mu^n$  in the Subcritical Expansion for the Average Number of Particles  $\bar{n}(0)$**

$n$	A model	Contact process	N3 model
0	1	1	1
1	2	1	$\frac{1}{2}$
2	2	$\frac{1}{2}$	$\frac{1}{4}$
3	$1\frac{2}{3}$	$\frac{1}{4}$	$\frac{1}{24}$
4	$1\frac{1}{3}$	$\frac{1}{12}$	$\frac{1}{384}$
5	$\frac{8}{9}$	$\frac{7}{144}$	$\frac{7}{1536}$
6	$\frac{7}{9}$	$\frac{1}{288}$	$\frac{85}{55296}$
7	0.2493827160493821	$1.4660493827160410 \times 10^{-2}$	$1.1886031539351770 \times 10^{-3}$
8	0.6884773662551446	$-7.2402263374484451 \times 10^{-3}$	$-6.7031671971449939 \times 10^{-4}$
9	-0.5108470507544979	$9.0599815672151569 \times 10^{-3}$	$4.0924264831960010 \times 10^{-4}$
10	1.449847050754300	$-7.6807060363794850 \times 10^{-3}$	$-2.3972546903848020 \times 10^{-4}$
11	-2.359832016297594	$7.4357531647106270 \times 10^{-3}$	$1.4002098834551620 \times 10^{-4}$
12	4.577409663674890	$-6.8295967100518310 \times 10^{-3}$	$-8.0701830317584079 \times 10^{-5}$
13	-8.342415514885291	$6.3779501429536061 \times 10^{-3}$	$4.6170685752736690 \times 10^{-5}$
14	15.54134106412082	$-5.9146293588482440 \times 10^{-3}$	$-2.6265373384772920 \times 10^{-5}$
15	-28.78362454239583	$5.5016525380336909 \times 10^{-3}$	$1.4908816489589680 \times 10^{-5}$
16	53.54002284758874	$-5.1218195645679460 \times 10^{-3}$	$-8.4677533119365099 \times 10^{-6}$
17	-99.73136975399839	$4.7809842965747750 \times 10^{-3}$	$4.8237629118719750 \times 10^{-6}$
18	$1.862806886599634 \times 10^2$	$-4.4747077329947890 \times 10^{-3}$	$-2.7600574945468440 \times 10^{-6}$
19	$-3.487878336242023 \times 10^2$	$4.2001643605226410 \times 10^{-3}$	$1.5869689698041270 \times 10^{-6}$
20	$6.547130632379355 \times 10^2$	$-3.9531987663530880 \times 10^{-3}$	$-9.1657233120783739 \times 10^{-7}$
21	$-1.23190408305394 \times 10^3$	$3.7300645132853410 \times 10^{-3}$	$5.3123407568589100 \times 10^{-7}$
22	$2.323193188630013 \times 10^3$	$-3.5273608481607640 \times 10^{-3}$	$-3.0858483756500820 \times 10^{-7}$
23	$-4.390456106249723 \times 10^3$	$3.3422832038918550 \times 10^{-3}$	$1.7942087455647910 \times 10^{-7}$
24	$8.313559411785390 \times 10^3$	$-3.1725654739756720 \times 10^{-3}$	$-1.0430187154798440 \times 10^{-7}$

**Table V. Coefficients of  $\mu^n$  in the Subcritical Expansion for the Spreading of Particles  $\bar{X}^2(0)$**

$n$	A model	Contact process	N3 model
0	1	1	1
1	2	1	$\frac{1}{2}$
2	7	$1\frac{3}{4}$	$\frac{7}{16}$
3	$12\frac{5}{8}$	$1\frac{5}{8}$	0.1901041666666664
4	$17\frac{1}{3}$	$1\frac{21}{144}$	$6.3856336805555660 \times 10^{-2}$
5	$19\frac{2}{3}$	$\frac{197}{288}$	$1.8213568793402790 \times 10^{-2}$
6	$19\frac{17}{18}$	$\frac{23}{64}$	$3.2796026159218070 \times 10^{-3}$
7	18.48827160493976	0.1847029320987510	$1.8780726080147860 \times 10^{-3}$
8	16.59480452675448	$7.5126189557623050 \times 10^{-2}$	$-5.7276977523249870 \times 10^{-4}$
9	13.02176611795439	$4.6265994727462590 \times 10^{-2}$	$6.2998195943861600 \times 10^{-4}$
10	12.63513940315905	$4.3215107092355370 \times 10^{-3}$	$-4.2079635990711300 \times 10^{-4}$
11	5.016808260411231	$1.9412633075471370 \times 10^{-2}$	$3.0050740557312060 \times 10^{-4}$
12	14.7131239188803	$-1.1829981046481720 \times 10^{-2}$	$-2.0231631304122020 \times 10^{-4}$
13	-12.78410961292725	$1.6803662542129920 \times 10^{-2}$	$1.3399796119614990 \times 10^{-4}$
14	41.64442947988799	$-1.6553333878337960 \times 10^{-2}$	$-8.6835578895642670 \times 10^{-5}$
15	-77.92125019899402	$1.8117922209656310 \times 10^{-2}$	$5.5388981758386310 \times 10^{-5}$
16	170.4662114678585	$-1.8769963628250040 \times 10^{-2}$	$-3.4837951093368030 \times 10^{-5}$
17	-348.5483087264899	$1.9567813401686720 \times 10^{-2}$	$2.1651650208454030 \times 10^{-5}$
18	721.4541831732130	$-2.0133059273039680 \times 10^{-2}$	$-1.3314308116140040 \times 10^{-5}$

**Table VI. Unbiased Estimates for the Location of the Critical Point  $\mu_c$  and the Value of the Critical Exponent  $\nu - \beta$  As Obtained from Various Padé Approximants to the Series  $d/d\mu \ln \bar{P}(0)$ , with the Series for  $\bar{P}(0)$  Given in Table III**

Model	Approximant	$\mu_c$	$\nu - \beta$
A	[10, 11]	1.74141	1.4520
	[11, 10]	1.74182	1.4565
	[11, 11]	1.74131	1.4510
	[11, 12]	1.74140	1.4520
	[12, 11]	1.74161	1.4545
CP	[10, 10]	3.29785	1.4575
	[11, 10]	3.29790	1.4578
	[10, 11]	3.29804	1.4589
	[11, 11]	3.29791	1.4579
	[11, 12]	3.29793	1.4580
N3	[10, 11]	6.17328	1.4682
	[11, 10]	6.17304	1.4678
	[11, 11]	6.17263	1.4666
	[11, 12]	6.17224	1.4650
	[12, 11]	6.17205	1.4646

exponents. The discrepancy between the three models is also more pronounced. We tried to transform the series in order to remove any singularity closer to the origin than  $\mu_c$ , but none of these transformations led to improved estimates for the critical exponents. The series for the spreading is so ill-behaved that this kind of analysis does not yield any useful results.

An analysis of the biased exponents, similar to the one presented in Fig. 2 for the supercritical series, was done for the subcritical series. The analysis of the series for the survival probability yielded  $\mu_c = 1.74135$  and  $\nu - \beta = 1.4515$  for the A model,  $\mu_c = 3.29791$  and  $\nu - \beta = 1.4579$  for the CP, and  $\mu_c = 6.1727$  and  $\nu - \beta = 1.467$  for the N3 model. From the series for the average number of particles we find  $\mu_c = 1.74195$  and  $\nu(1 + \eta) = 2.2821$  for the A model,  $\mu_c = 3.29782$  and  $\nu(1 + \eta) = 2.2772$  for the CP, and  $\mu_c = 6.17155$  and  $\nu(1 + \eta) = 2.2824$  for the N3 model. Again this kind of analysis does not yield any useful results from the series for the spreading.

Because the supercritical series are so well-behaved and the estimates for  $\lambda_c$  so stable, we are inclined to believe strongly in these estimates. Using these values for  $\lambda_c$  we can obtain biased estimates for the critical exponents from the subcritical series. The results of this analysis are given in Table VIII. The internal agreement of various approximants within each model is quite good, and furthermore the agreement between the models is improved significantly. In conclusion, we estimate that  $\nu - \beta = 1.457(2)$ ,

**Table VII. Unbiased Estimates for the Location of the Critical Point  $\mu_c$  and the Value of the Critical Exponent  $\nu(1 + \eta)$  As Obtained from Various Padé Approximants to the Series  $d/d\mu \ln \tilde{n}(0)$  Given in Table IV**

Model	Approximant	$\mu_c$	$\nu(1 + \eta)$
A	[10, 10]	1.74186	2.2805
	[10, 11]	1.74196	2.2820
	[11, 10]	1.74190	2.2815
	[11, 11]	1.74195	2.2825
	[12, 11]	1.74192	2.2820
CP	[10, 10]	3.29782	2.2775
	[11, 10]	3.29793	2.2786
	[10, 11]	3.29801	2.2800
	[11, 11]	3.29780	2.2775
	[12, 11]	3.29804	2.2800
N3	[10, 11]	6.17223	2.2850
	[11, 11]	6.17135	2.2818
	[12, 10]	6.17161	2.2829
	[11, 12]	6.17165	2.2830
	[12, 11]	6.17188	2.2839



**Table VIII. Biased Estimates of the Critical Exponents  $\nu - \beta$ ,  $\nu(1 + \eta)$ , and  $\nu(1 + \eta + z)$  As Obtained from Various Padé Approximants, with the Original Series Given in Tables III–V**

Exponent	Approximant	A model	CP	N3 model
$\nu - \beta$	[10, 11]	1.4558	1.4576	1.4627
	[11, 10]	1.4558	1.4576	1.4619
	[11, 11]	1.4547	1.4575	1.4600
	[11, 12]	1.4560	1.4576	1.4586
	[12, 11]	1.4560	1.4576	1.4581
$\nu(1 + \eta)$	[10, 11]	2.2784	2.2777	2.2799
	[11, 10]	2.2778	2.2777	2.2796
	[11, 11]	2.2723	2.2777	2.2792
	[11, 12]	2.2778	2.2777	2.2818
	[12, 11]	2.2773	2.2777	2.2800
$\nu(1 + \eta + z)$	[7, 8]	4.4723	4.4678	
	[8, 7]	4.4782	4.8555	
	[8, 8]	4.4699	4.4723	
	[8, 9]	4.4723	4.4704	
	[9, 8]	4.4802	4.4690	

$\nu(1 + \eta) = 2.278(2)$ , and  $\nu(1 + \eta + z) = 4.47(1)$ . This in turn leads to the estimates  $\nu = 1.734(2)$ ,  $\eta = 0.314(3)$ , and  $z = 1.264(10)$ . If we use the scaling relation<sup>(3)</sup>  $\delta = \beta/\nu$ , we find that  $\delta = 0.1597(3)$ . We can use the hyperscaling relation  $dz = 4\delta + 2\eta$ ,<sup>(3)</sup> where  $d$  is the spatial dimension of the system, to check the consistency of our estimates. In this manner we find  $z = 1.266(7)$ , in excellent agreement with the other estimate. Our estimates are in good agreement with earlier results, which yielded  $\nu = 1.736(1)$ ,  $\eta = 0.317(2)$ ,  $\delta = 0.160(3)$ , and  $z = 1.272(7)$  from high-temperature series expansions for Reggeon field theory,<sup>(18)</sup> and  $\nu = 1.691(18)$ ,  $\eta = 0.308(9)$ ,  $\delta = 0.162(4)$ , and  $z = 1.263(8)$ , from computer simulations of the contact process and related models.<sup>(3)</sup>

### 8.3. Critical Time Series

As noted in Section 6, one may derive quite long series for the survival probability and the mean particle number in powers of  $t$  for any given value of  $\lambda$ . We focus on the case  $\lambda = \lambda_c$ , and consider how the exponents  $\delta$  and  $\eta$  may be determined from the series. The method of analysis parallels the approach applied in ref. 37 to another, albeit simpler, non-equilibrium process, random sequential adsorption (RSA).

From Eqs. (2) and (3) it follows that the asymptotic evolution of the survival probability and the mean particle number in the critical process

are governed by power laws:  $P(t; \lambda_c) \propto t^{-\delta}$ ,  $\bar{n}(t; \lambda_c) \propto t^n$ . We also expect that the approach to the power law involves corrections to scaling, for example,

$$P(t; \lambda_c) \approx At^{-\delta}(1 + at^{-d} + \dots) \quad (51)$$

Similar corrections are expected for  $\bar{n}(t)$ .

Relating the long-time behavior to the expansion  $P(t; \lambda) = 1 - \lambda t + O(t^2) + \dots$  about  $t = 0$  evidently hinges upon our ability to find an analytic continuation connecting the two representations. It is not obvious that such a connection can always be found. Nevertheless, our experience with RSA—in which the analysis of short-time series produced high-precision results for the asymptotic coverage—suggests that useful estimates may be derived via suitable transformation and analysis of the  $t$  series. In fact, since  $P(t)$  and  $\bar{n}(t)$  and all of their derivatives are well-defined for  $0 \leq t < \infty$ , we expect that the analytic continuation exists in principle. We seek to construct an approximate continuation using Padé approximants.<sup>(38,39)</sup>

Using the  $\lambda_c$  values found in our analysis of the supercritical series, we have determined the series coefficients for  $P(t)$  in the critical A model and contact process to 36th order, as listed in Table IX. A simple ratio analysis suggests that each series has a singularity on the negative  $t$  axis, not far from the origin, so that the direct expansion for  $P(t)$  is useful only for rather short times. There is, of course, no point in extrapolating the limiting value of the survival probability: we already know it is zero! Similarly, the mean particle number diverges as  $t \rightarrow \infty$ . We want to analyze series for quantities which remain finite as  $t \rightarrow \infty$ , and which provide information on the exponents. We have found two transformations to be particularly useful. If  $f(t)$  is the Taylor series expansion of some quantity about  $t = 0$ , we define

$$F[f(t)] = t \frac{d \ln f}{dt} \quad (52)$$

and

$$G[f(t)] = \frac{1}{tf(t)} \int^t dt' f(t') \quad (53)$$

If  $f \sim At^\alpha$  as  $t \rightarrow \infty$ , then  $F(t) \rightarrow \alpha$ , while  $G(t) \rightarrow 1/(1 + \alpha)$ . Given  $f(t)$ , it is straightforward to construct the series for  $F$  and  $G$ . Other transformations—involving repeated integrations and/or differentiations—may also be considered, but we have not found these to have such consistent and regular behaviors as  $F$  and  $G$ .

The series for the  $F$  and  $G$  transforms of  $P(t)$  and  $\bar{n}(t)$  again appear to have small radii of convergence, but they presumably represent short-time expansions of functions which are well-behaved for large  $t$ . To get at the long-time behavior, we study a set of Padé approximants to these series. The direct  $t$  series may be studied via the diagonal approximants

**Table IX. Series Coefficients for the Survival Probability  $P(t)$  in the Critical Contact Process and A Model**

$n$	Contact process	A model
0	1.0000000000000000	1.0000000000000000
1	-0.3032300000000000	-0.5741400000000000
2	0.1975892164500000	0.7389583698000000
3	-0.1164842091513778	-0.8538185924123239
4	$6.024654861682094 \times 10^{-2}$	0.8638487931050367
5	$-2.779249233086488 \times 10^{-2}$	-0.7785827928143218
6	$1.168865994190696 \times 10^{-2}$	0.6370211549405265
7	$-4.574374709742027 \times 10^{-3}$	-0.4809066254768587
8	$1.694874218920966 \times 10^{-3}$	0.3396289268635887
9	$-6.025873287567562 \times 10^{-4}$	-0.2270143835398018
10	$2.075363632335699 \times 10^{-4}$	0.1450385613988649
11	$-6.965423416871635 \times 10^{-5}$	$-8.929646194425331 \times 10^{-2}$
12	$2.285760830438168 \times 10^{-5}$	$5.332554361962063 \times 10^{-2}$
13	$-7.346976184814000 \times 10^{-6}$	$-3.104181153778206 \times 10^{-2}$
14	$2.315450103127075 \times 10^{-6}$	$1.767810218091046 \times 10^{-2}$
15	$-7.161310037527354 \times 10^{-7}$	$-9.873736609925353 \times 10^{-3}$
16	$2.175675321691604 \times 10^{-7}$	$5.417585323454907 \times 10^{-3}$
17	$-6.499886371038794 \times 10^{-8}$	$-2.923421768006476 \times 10^{-3}$
18	$1.911701592344971 \times 10^{-8}$	$1.552688940178137 \times 10^{-3}$
19	$-5.541437872176813 \times 10^{-9}$	$-8.122035956199857 \times 10^{-4}$
20	$1.584760002804068 \times 10^{-9}$	$4.186890414227672 \times 10^{-4}$
21	$-4.475525491599831 \times 10^{-10}$	$-2.128256818481803 \times 10^{-4}$
22	$1.249141390379286 \times 10^{-10}$	$1.067406150794438 \times 10^{-4}$
23	$-3.447980725341066 \times 10^{-11}$	$-5.285457067901271 \times 10^{-5}$
24	$9.418066427427577 \times 10^{-12}$	$2.585577039924513 \times 10^{-5}$
25	$-2.546998834664866 \times 10^{-12}$	$-1.250327599748272 \times 10^{-5}$
26	$6.822889473992474 \times 10^{-13}$	$5.980527257014955 \times 10^{-6}$
27	$-1.811193874824606 \times 10^{-13}$	$-2.831044450280031 \times 10^{-6}$
28	$4.766380424997410 \times 10^{-14}$	$1.326995581307090 \times 10^{-6}$
29	$-1.243935212649037 \times 10^{-14}$	$-6.161872316136795 \times 10^{-7}$
30	$3.220620472366028 \times 10^{-15}$	$2.835713668488498 \times 10^{-7}$
31	$-8.274686654070306 \times 10^{-16}$	$-1.293859062901805 \times 10^{-7}$
32	$2.110386135986964 \times 10^{-16}$	$5.855164708526439 \times 10^{-8}$
33	$-5.344290054620019 \times 10^{-17}$	$-2.628800439707885 \times 10^{-8}$
34	$1.344147938547451 \times 10^{-17}$	$1.171303502200469 \times 10^{-8}$
35	$-3.358434167661840 \times 10^{-18}$	$-5.180736640124616 \times 10^{-9}$
36	$8.337893152824442 \times 10^{-19}$	$2.275266648642259 \times 10^{-9}$

(the off-diagonal approximants have trivial  $t \rightarrow \infty$  limits.) Alternatively, we may perform a transformation of variable which maps  $t = \infty$  to a point in the finite plane; then the off-diagonal approximants also yield useful results. A transformation of variable can also yield a radical simplification of the series, when a large set of terms in the original series is subsumed into one power of the new variable. Such a simplification appears to facilitate the estimation of asymptotic properties. (This is precisely the situation in RSA: the exact solutions in one dimension<sup>(40)</sup> and on Bethe lattices<sup>(41)</sup> are well-behaved functions whose complicated structure leads to rather unpleasant power series in  $t$ . The series can be tamed by a change of variable.<sup>(37,42)</sup>)

There are of course many transformations that one might consider. The choice may to some extent be guided by our expectations regarding the asymptotic approach of the function to its limiting value. Given the correction to scaling behavior described by Eq. (51), one would expect the asymptotic correction term to decay as some negative power of  $t$ , perhaps proportional to  $t^{-1}$ , which would suggest that we perform an Euler transformation:

$$y = \frac{t}{a+t} \quad (54)$$

We shall also consider the exponential transformation

$$z = \frac{1 - e^{-bt}}{b} \quad (55)$$

which proved very useful in the analysis of lattice RSA series. In either case the transformation involves a parameter which cannot be fixed *a priori*. We shall adopt the strategy of Adler *et al.*<sup>(36)</sup> compute many Padé approximants for the quantity of interest, as a function of the transformation parameter. Then find the parameter values (if any) for which all or most of the approximants agree; if such a “crossing” exists, it is natural to adopt the associated exponent value as our estimate. The rationale is that for a suitable parameter value, the transformed series represents a function with a simple structure (having an isolated, simple pole, for example), which is well-represented by Padé approximants of various orders.

Consider first the survival probability series for the A model. The diagonal Padé approximants to the  $F$  transform give rather scattered estimates for the exponent  $\delta$ : 0.165, 0.168, 0.153, and 0.178 for the [18, 18], [17, 17], [16, 16], and [15, 15] approximants, respectively. However, when we make a change of variable using the Euler transformation, we obtain more useful results. In Fig. 3 we plot the  $\delta$  estimates which result from 25 Padé approximants (the diagonal series,  $[m, m]$ ,  $14 \leq m \leq 18$ , and

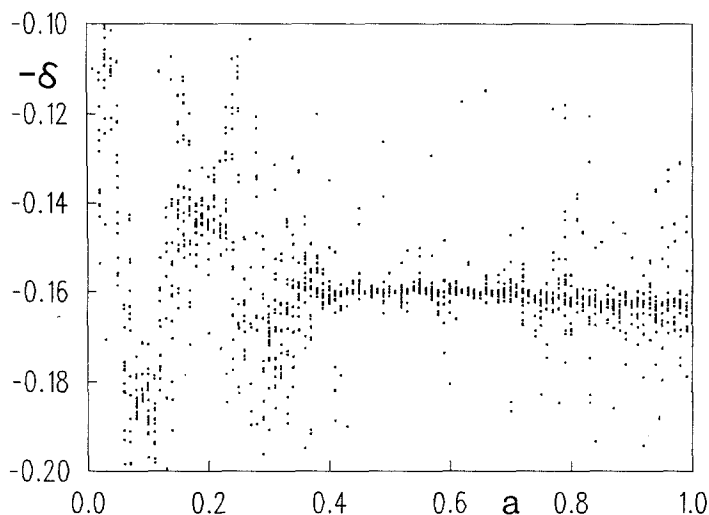


Fig. 3. Padé approximant estimates for the exponent  $\delta$  derived from the Euler-transformed series for  $F[P(t)]$  ( $F$ -transform of the survival probability series), for the A model. Twenty-five approximants are plotted as a function of  $a$ , the Euler transformation parameter.

the corresponding off-diagonals,  $[n, m]$ , with  $m - n = -2, -1, 1$ , or  $2$ ). There are very narrow crossings near  $a = 0.46$  and  $0.48$ , yielding the estimate  $\delta = 0.160(2)$ . (The uncertainty reflects the variation in  $\delta$  over the range  $0.4 \leq a \leq 0.7$ , where the estimates are generally well-behaved.) The  $G(t)$  series for the A-model survival probability yields slightly smaller, but consistent estimates. We note that diagonal approximants to the  $G$  series are quite stable, with the  $n = 12$ – $18$  approximants all giving  $\delta = 0.158$ , while the  $[11, 11]$  and  $[10, 10]$  approximants give  $0.159$  and  $0.157$ , respectively. The  $\delta$  estimates obtained via Euler transformation of the  $G$  series exhibit a narrow crossing near  $a = 1.1$ ,  $\delta = 0.158$  (with a width of about  $0.0002$ ). The estimates derived via the Euler transformation of the  $G$  series become constant (approximately  $0.158$ ) for  $a \geq 1.25$ . If we average over all estimates for  $0.01 \leq a \leq 1.25$ , restricting the sample to  $\delta$  values in the range  $[0.15, 0.17]$  (to exclude a few singularities of the approximants), we consistently obtain  $\delta = 0.157$ . From the entire set of estimates reported, we conclude that, for the A model,  $\delta$  lies in the range  $0.157$ – $0.162$ . We also note that the  $G$ -series estimates (direct and Euler-transformed) have a higher degree of internal consistency than the  $F$ -series estimates. Finally, we note that neither series yields well-behaved exponent estimates under the exponential transformation of Eq. (55).

The  $F$  and  $G$  series for the survival probability of the critical contact process have been analyzed similarly. When it is applied to the  $F(t)$  series,

the Euler transformation fails to yield useful results. The estimates for  $\delta$  fluctuate wildly for  $a \leq 2$ , while for somewhat larger  $a$  the approximants attain steady, but mutually inconsistent values. (We have not found any explanation for the irregular behavior of the Euler-transformed series.) In this case, the exponential transformation yields a much more consistent and well-behaved set of estimates, as may be seen from Fig. 4. In fact, there is a remarkably narrow crossing of the estimates (again obtained from a set of 25 Padé approximants) near  $b = 0.43$ , which gives  $\delta = 0.1620(5)$ . A second, somewhat less distinct crossing appears near  $b = 1.5$ , giving  $\delta \approx 0.1599$ . Furthermore, the approximants remain rather tightly clustered for  $b$  up to about 1.7,  $\delta \approx 0.159$ . We have confirmed that the behavior of the  $\delta$  estimates is stable under small,  $\mathcal{O}(10^{-5})$ , variations in the estimate for  $\lambda_c$ . Turning to the  $G$  series, we obtain the values 0.158, 0.159, 0.158, 0.158, and 0.156 from the diagonal approximants,  $n = 14-18$ , respectively. Applying the exponential transformation to this series yields irregular estimates (as for the A-model  $F$  and  $G$  series), but the Padé approximants to the Euler-transformed  $G$  series exhibit crossings at  $\delta = 0.156$ , 0.161, and 0.162,

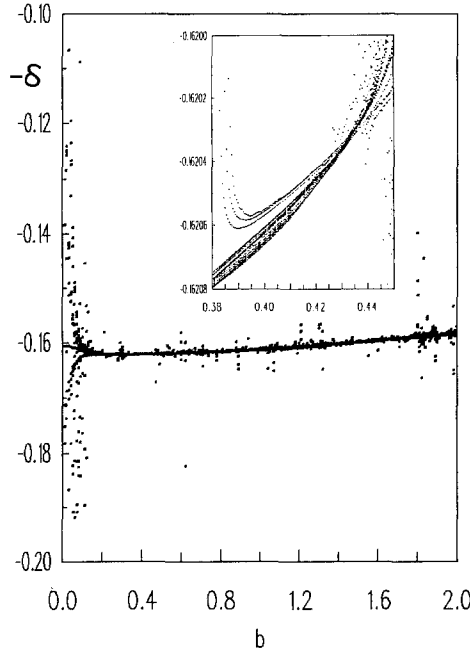


Fig. 4. Padé approximant estimates for the exponent  $\delta$  derived from the exponentially-transformed series for  $F[P(t)]$  for the contact process. Twenty-five approximants are plotted versus  $b$ , the transformation parameter. The inset is a detail of the crossing region.

while averages over all estimates for  $0.01 \leq a \leq 2$  yield values in the range 0.160–0.162. Thus for the contact process we may conclude that  $\delta = 0.159(3)$ .

Our results for the N3 model are relatively disappointing. The diagonal approximants yield  $\delta = 0.153$ – $0.156$  and  $0.166$ – $0.167$  for the  $F$  and  $G$  series, respectively. The Euler and exponential transformations yield generally irregular estimates, the former exhibiting somewhat diffuse crossing regions near  $\delta = 0.153(3)$  ( $F$  series) and  $0.153$  and  $0.175$  ( $G$  series). Thus we are unable to specify  $\delta$  for the N3 model with any precision, based upon the survival probability series.

A similar analysis has been applied to the  $\bar{n}(t)$  series, which, due to more extensive storage requirements, can only be obtained to 24th order. Our estimates for the exponent  $\eta$  are again based on analysis of the  $F$  and  $G$  transforms of the series. For the A model, diagonal approximants to the  $F$  series are quite useless (the [11, 11] and [12, 12] PAs yield 0.5 and  $-0.4!$ ). Studying a set of 25 approximants to the Euler-transformed series (diagonals with  $n = 8$ – $12$ , and the corresponding off-diagonals with  $n = m \pm 1, 2$ ), we find the estimates generally erratic. But the set does exhibit one rather narrow crossing, near  $a = 0.23$ ,  $\eta = 0.30$ – $0.31$ . Diagonal approximants to the  $G$  series are better behaved, yielding  $\eta = 0.30$ – $0.33$ . The 25 approximants to the Euler-transformed  $G$  series exhibit a more regular behavior, with a narrow crossing— $\eta = 0.310(1)$ —near  $a = 0.32$ . Averages over all  $\eta$  values in the range 0.2–0.4 obtained with  $0.01 \leq a \leq 1.2$  (the estimates attain constant values for larger  $a$ ) consistently yield estimates in the range 0.306–0.324. For the critical contact process, a set of 20 Padé approximants for the exponential transformation of the  $F$  series to  $\bar{n}(t)$  exhibit a crossing near  $b = 0.23$ , yielding  $\eta = 0.308(2)$ . The  $G$ -series estimates are fairly irregular, falling in the range 0.30–0.33. Based on these results, we conclude that for the contact process and the A model,  $\eta$  is almost surely in the range 0.30–0.33, and that very likely it lies between 0.305 and 0.320.

The results of this analysis demonstrate that it is possible to extract useful exponent estimates from the  $P(t)$  and  $\bar{n}(t)$  series. The exponent estimates derived from the  $P(t)$  series are of modest precision, and are in good agreement with the estimate<sup>(3)</sup>  $\delta = 0.162(4)$  and with the value obtained using the scaling relation,  $\delta = \beta/\nu = 0.1597(3)$ , using our own estimates for the latter exponents. Our  $t$ -series estimate for  $\eta$  is also in agreement with the value 0.314(3) derived above in our analyses of subcritical series. A disadvantage of the foregoing analysis is that one does not know in advance which transformations will yield consistent results. We have tried to compensate for the empirical character of the approach (present, to some extent, in all series analyses) by seeking a consensus of

estimates obtained through a variety of methods. The results, while not of the highest precision, are nonetheless of interest, as they suggest that analysis of time series may prove useful in studies of other models. In fact, we expect to be able to derive  $t$  expansions for a wide variety of diffusive, multicomponent, and higher-dimensional models which may resist more conventional perturbative analysis.

## 9. SUMMARY AND DISCUSSION

We have developed perturbation methods for the long- and short-time behavior of particle systems with a unique absorbing state. Using these methods, we studied three one-dimensional models. The methods are readily represented as computer algorithms, and should be applicable to a variety of lattice models exhibiting nonequilibrium phase transitions. We think that the subcritical expansions and in particular the time series will prove to be the methods of most general utility.

The numerical results presented in Section 8 yield precise estimates for the location of the critical points and the values of various critical exponents. Our results support the universality hypothesis for non-equilibrium particle systems, in that all of the models studied here belong to the universality class of Reggeon field theory or directed percolation.

Based on our results, we propose the following best estimates for the critical exponents of the DP/RFT class in one space dimension:  $\beta = 0.2769(2)$ , which is in excellent agreement with the estimate  $\beta = 0.2765(5)^{(26)}$  for directed percolation. From the biased exponents we estimate  $\nu = 1.734(2)$ ,  $\eta = 0.314(3)$ , and  $z = 1.264(10)$ . If we use the scaling relation<sup>(3)</sup>  $\delta = \beta/\nu$ , we find that  $\delta = 0.1597(3)$ . Using the hyperscaling relation<sup>(3)</sup>  $dz = 4\delta + 2\eta$ , we find  $z = 1.266(7)$ , in excellent agreement with the other estimate. Our estimates are in good agreement with earlier results, which yielded  $\nu = 1.736(1)$ ,  $\eta = 0.317(2)$ ,  $\delta = 0.160(3)$ , and  $z = 1.272(7)$  from high-temperature series expansions for Reggeon field theory.<sup>(18)</sup> Our estimate for  $\nu$  also agrees with the result for directed percolation  $\nu = 1.734(2)$ .<sup>(44,45)</sup>

## APPENDIX A. Program Listing

```
C*****
C Calculate super-critical expansion of the ultimate survival *
C probability for the generalized A-model in 1-dimension. *
C
C THE MODEL *
C Each particle occupies single sites on a 1-dimensional lattice*
```



```

C Particles are annihilated at rate LAMBDA.          *
C Particles created at UNIT rate if both neighbors are occupied,*
C and at rate ALPHA if only a single neighbor is occupied.    *
C Thus ALPHA = 1 corresponds to the A-model, ALPHA = 1/2 to the *
C Contact Process, and ALPHA = 1/4 to the N3-model.          *
C                                                         *
C Arrays:                                                         *
C COEF(i): Coefficient of configuration i.                    *
C IND(i) : Number of particles in configuration i. IND(i) = 0 if*
C          configuration i has not appeared in the expansion.  *
C IS(k)  : An indicator binary number which is ONE at site k and*
C          ZERO everywhere else (i.e. IS(k) = 2**k).          *
C          Thus IAND(IS(k),i) = 0 if i has a ZERO at position k *
C          else it equals IS(k).                               *
C NS(k)  : The bitwise compliment of IS(i). NS(i) = NOT(IS(i)). *
C RES(i) : Coefficient to LAMBDA**i in the expansion for P-inf. *
C Variables:                                                     *
C NORD   : Final order of calculation                          *
C IORD   : Present order of calculation                        *
C ICUT   : Maximal number of particles in configurations that *
C          contribute to the ultimate survival probability    *
C LSM    : Size of arrays COEF and IND                       *
C ALPHA  : Rate of creation at sites with one occupied neighbor *
C Subroutines:                                                 *
C ANNOP  : The annihilation operation. Does the job of W      *
C CREAOP : The creation operation. Does the job of 1/(z - V)  *
C*****

```

PROGRAM TDPAMOD

```

C Definition of common variables
PARAMETER(NORD = 24,LSM = 2**NORD)

```

```

      IMPLICIT REAL*8 (A-H,O-Z)
      INTEGER*2 IND(LSM)
      COMMON/CO/COEF(LSM),RES(NORD),ALPHA
      COMMON/IN/IND,IS(0:32),NS(0:32),IORD,ICUT
C      Initialization of variables
      ALPHA = 0.25
      DO 10 I = 1,LSM
          IND(I) = 0
10      COEF(I) = 0.
      DO 11 I = 0,31
          IS(I) = 2**I
11      NS(I) = NOT(IS(I))
          K = 0
      DO 12 I = 0,NORD-1
          K = K+2**I
          IND(K) = I+1
          RES(I+1) = 0.
12      COEF(K) = .5/ALPHA
C      Start of main loop
      DO 20 IORD = 1,NORD
          ICUT = NORD-IORD
          RES(IORD) = -COEF(1)
          CALL ANNOP
          CALL CREAOP
20      CONTINUE
          OPEN(1)
          WRITE(1,*) 0,1.0
          DO 30 I = 1,NORD
30      WRITE(1,*) I,RES(I)
      END

```

```

SUBROUTINE ANNOP
PARAMETER(NORD = 24,LSM = 2**NORD)
IMPLICIT REAL*8 (A-H,O-Z)
INTEGER*2 IND(LSM)
COMMON/CO/COEF(LSM),RES(NORD),ALPHA
COMMON/IN/IND,IS(0:32),NS(0:32),IORD,ICUT
INTEGER CONF
DO 100 CONF = 3,LSM,2
C      Go through all configurations
      IF (IND(CONF).GT.0.AND.IND(CONF).LE.(ICUT+1)) THEN
C          Operate on configurations that exist and contribute
C          Remove first particle and superfluous zeros
      NEWCONF = CONF/2
      DO 110 K = 1,NORD
          IF (IAND(NEWCONF,1).EQ.1) GO TO 115
110      NEWCONF = NEWCONF/2
115      IND(NEWCONF) = IND(CONF)-1
      COEF(NEWCONF+1) = COEF(NEWCONF+1)+COEF(CONF)
C          Coefficients are temporarily stored at NEWCONF+1
      DO 120 K = 1,NORD-1
C          Go through rest of positions, and remove particles
          NEWCONF = IAND(CONF,NS(K))
          IF (NEWCONF.LT.CONF) THEN
              IND(NEWCONF) = IND(CONF)-1
              COEF(NEWCONF+1) = COEF(NEWCONF+1)+COEF(CONF)
          END IF
120      CONTINUE
      COEF(CONF+1) = -IND(CONF)*COEF(CONF)+COEF(CONF+1)
      END IF
100  CONTINUE
      COEF(2) = -COEF(1)+COEF(2)

```

```

DO 130 J = 1,LSM,2
    COEF(J) = COEF(J+1)
130    COEF(J+1) = 0.DO
END

SUBROUTINE CREAOP
PARAMETER(NORD = 24,LSM = 2**NORD)
IMPLICIT REAL*8 (A-H,O-Z)
INTEGER*2 IND(LSM)
COMMON/CO/COEF(LSM),RES(NORD),ALPHA
COMMON/IN/IND,IS(0:32),NS(0:32),IORD,ICUT
INTEGER NEW(32), CONF
REAL*8 WEIGHT(32)
C    Temporary storage for created configurations (NEW)
C    and their weights (WEIGHT)
DO 200 CONF = 1,LSM,2
C    Go through all configurations.
C    No need to update IND as this routine does not create new
C    configurations not already created in ANNOP
    NCON = 0
    IF (IND(CONF).GT.0.AND.IND(CONF).LE.ICUT) THEN
C    Operate on existing configurations and configurations
C    whose 'offspring' contribute to survival probability

C    Create at position -1 with weight 1
        NEWCONF = CONF*2+1
        NCON = NCON+1
        NEW(NCON) = NEWCONF
        WEIGHT(NCON) = ALPHA
DO 210 K = 1,NORD
C    Go through rest of positions
        IF (IAND(CONF,IS(K)).EQ.0) THEN

```

```

C          Check if position K is vacant
          IF (IAND(CONF,IS(K-1)).GT.0.AND.
&          IAND(CONF,IS(K+1)).GT.0) THEN
C          Both neighbors occupied create with weight 1
          NEWCONF = IOR(CONF,IS(K))
          NCON = NCON+1
          NEW(NCON) = NEWCONF
          WEIGHT(NCON) = 1.
          ELSE IF (IAND(CONF,IS(K-1)).GT.0) THEN
C          Left neighbor occupied create with weight ALPHA
          NEWCONF = IOR(CONF,IS(K))
          NCON = NCON+1
          NEW(NCON) = NEWCONF
          WEIGHT(NCON) = ALPHA
          ELSE IF (IAND(CONF,IS(K+1)).GT.0) THEN
C          Right neighbor occupied create with weight ALPHA
          NEWCONF = IOR(CONF,IS(K))
          NCON = NCON+1
          NEW(NCON) = NEWCONF
          WEIGHT(NCON) = ALPHA
          END IF
          END IF
210      CONTINUE
          END IF
          IF (NCON.GT.0) THEN
C          Sum up the weights and update COEF(CONF)
          SUM = 0.DO
          DO 220 M = 1,NCON
220      SUM = SUM+WEIGHT(M)
          COEF(CONF) = COEF(CONF)/SUM
          IF (IND(CONF).LT.ICUT) THEN

```

```

C      If the offspring contribute update coefficients
      DO 230 K = 1,NCON
          NM = NEW(K)
230      COEF(NM) = COEF(NM)+COEF(CONF)*WEIGHT(K)
      END IF
      END IF
200  CONTINUE
      END

```

## ACKNOWLEDGMENTS

We wish to thank Vladimir Privman, George Baker, Jr., and Jose Duarte for helpful discussions, and Larry Schulman and Daniel ben-Avraham for helpful correspondence and comments on the subject of error estimation. One of us (I.J.) gratefully acknowledges the support of the Danish Research Academy. This research was supported in part by a grant from the City University of New York PSC-CUNY Research Award Program. Calculations were performed on the facilities of the University Computing Center of the City University of New York.

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