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Nonequilibrium Lattice Models: Series Analysis of Steady States

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A perturbation theory for steady states of interacting particle systems is developed and applied to several lattice models with nonequilibrium critical points near an absorbing state. The expansion is expressed directly in terms of the kinetic parameter (creation rate), rather than in powers of the interaction. An algorithm for generating series expansions for local properties is described. Order parameter series (16 terms) and precise estimates of critical properties are presented for the one-dimensional contact process and several related models.

KEY WORDS: Nonequilibrium phase transitions; Schlögl model; contact process; interacting particle systems.

1. INTRODUCTION

Despite the growing interest in nonequilibrium systems,[1-3] the statistical mechanics of nonequilibrium steady states lags far behind the equilibrium theory. One obvious source of difficulty is that unlike in equilibrium, the steady-state probability distribution on phase space is not known *a priori*, so that analysis of nonequilibrium systems must be based upon *dynamics*. Progress in understanding of steady-state behavior would be particularly valuable in the theory of nonequilibrium phase transitions, a topic of considerable interest in physics, chemistry, and biology.

At present, knowledge about nonequilibrium phase transitions is based upon (1) mean-field theory (MFT), which cannot, of course, be relied on for a quantitative description of critical behavior; (2) Monte Carlo simulations; and (3) field-theoretic renormalization group (RG) methods. While computer simulations will continue to play an essential

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role in this field, they must be complemented by analytic methods to provide a full understanding of phase transitions. RG methods[4-8] have yielded important insights into critical behavior, but their efficacy may be limited when the upper critical dimension d_c is significantly greater than the dimensionality of the system of interest. For example, the Schlögl model[9] exhibits interesting critical behavior for $d \geqslant 1$, while $d_c = 4$ for this model.[4] Another limitation of the RG approach is that it cannot be used to predict "nonuniversal" properties, which arise in comparisons between theory and experiment or simulation. The method described in this paper offers an alternative approach to nonequilibrium phase transitions in lattice models, analogous to series expansions in equilibrium theory.

In this paper I consider stochastic lattice models in which rates of creation, annihilation, and diffusion of particles are governed by local rules. The transition probabilities do not, in general, satisfy detailed balance with respect to any reasonable (finite-range) Hamiltonian, and so the models are inherently nonequilibrium. (In some instances the transition probabilities may be derived as a singular limit of a Hamiltonian model with detailed balance.[10]) One is interested in the nature of the steady state(s) as a function of kinetic parameters such as the creation or hopping rates. Various nonequilibrium lattice models have been found to exhibit phase transitions and critical points—nonanalytic dependence of steady-state properties on kinetic parameters. The nature of nonequilibrium "universality classes" is not well understood, although there has been some discussion of this issue for one-component reaction-diffusion systems recently.[6,7,11]

In the present situation, a method analogous to the high- and low-temperature expansions of equilibrium theory, but applicable to nonequilibrium models, would be most useful. In this paper, starting from the master equation, I derive a perturbation expansion for steady states of interacting particle systems and describe its application to several models. As in time-independent perturbation theory in quantum mechanics, one expands about a model whose time dependence may be solved exactly. This provides a formalism which may then be implemented for a particular model, as represented by its evolution operator. For a class of one-dimensional models, an algorithm has been devised which yields rather long series for steady-state properties, leading to precise estimates of critical properties.

The series-expansion method is applied to single-component models which exhibit a transition to an absorbing state. Some time ago. Brower *et al.*[12] derived an expansion for the Reggeon quantum spin model which belongs to the same universality class as the models considered here. Their field-theoretic high-temperature expansion yielded precise estimates

of the exponents η, ν, and z (for $d=1$ and 2) from an analysis of generalized susceptibilities. In contrast with the high-T expansion method, the present work deals with an expansion in powers of a kinetic parameter v (related to the particle creation rate), rather than in powers of the interaction. Thus far, v expansions have been derived only for the order parameter and short-range correlations, yielding the first *direct* estimate of the exponent β for these models. Long-range correlations and susceptibilities will be the subject of future work.

Preliminary results on the v expansion for one system (the "A-model") were presented recently in summary form.[13] In this paper the details of the method are explained, and several models with different evolution rules are considered. The results provide strong evidence of universality, i.e., the critical behavior is insensitive to variations in details of the evolution rules. The remainder of this paper is organized as follows. Section 2 introduces the models of interest. An operator formalism permitting compact expression of probability distributions and the master equation is set out in Section 3. Section 4 presents a formal perturbation theory for the steady-state probability distribution. Detailed applications are described in Sections 5–7. In Section 8, I describe a computer algorithm which generates extended series for the order parameter and short-range correlation functions. The results of such computations, and determination of critical properties, are given in Section 9. Section 10 contains a brief summary and discussion.

2. MODELS

One expects that, as in equilibrium theory, it will be profitable to focus on the simplest models which exhibit the phenomena of interest. The models considered here are Markov processes with a discrete state space $\{0,..., n\}^{\Lambda}$ ($\Lambda \subseteq \mathbf{Z}^d$). One physical interpretation is a lattice whose sites may be vacant or occupied by a particle of type i ($i \in \{1,..., n\}$; in the examples considered, $n=1$). A configuration $\{\sigma_j\}$ ($j \in \Lambda$) specifies the occupation status of each site. Transitions between configurations occur via certain "elementary processes"—creation, annihilation, and (in some instances), hopping of particles—with probabilities depending on the local environment and on certain kinetic parameters. Examples of such Markov processes are dynamic Ising models or lattice gases (equilibrium and nonequilibrium), surface reaction models, reaction-diffusion models, and epidemic models. They are known collectively as *interacting particle systems* (IPS).[14]

When realized in Monte Carlo simulations, the models follow a discrete-time evolution. In a unit interval, at most one elementary process

occurs, at a randomly chosen site, and the configuration is immediately updated. This sort of evolution may be termed *sequential*, in contrast with a stochastic cellular automaton (SCA).[15] In the latter, each site is updated simultaneously. While the dynamic *and* static properties of a sequential IPS and the corresponding SCA (i.e., one having the same elementary processes and kinetic parameters) can be quite different, the two models may nevertheless belong to the same universality class. An example is the contact process (an IPS), which belongs to the same universality class as the corresponding SCA, directed percolation.[15-18]

The present work is mainly concerned with sequential models. In the analysis, it is convenient to use a continuous-time description in which the probability for some elementary process to occur in a short time dt is $R\,dt$, where R is a rate. The state of the system is described by the probability distribution on configuration space, which evolves via the master equation. This equation is expressed in an operator formalism in the following section. The remainder of this section is devoted to introducing the models studied in Sections 3–9. Much of the discussion of Sections 3 and 4 is applicable to IPS in general.

The *contact process* (CP) was introduced by Harris[19] as a model of an epidemic. It is closely related to Schlögl's (first) model[9] of an autocatalytic chemical reaction, to directed percolation,[17] and to Reggeon field theory.[12,20] The elementary processes may be thought of as adsorption and desorption of particles at the lattice sites. Particles appear randomly at vacant sites, at rate λ, independent of the states of other sites (each site is either vacant or singly occupied). Occupied sites are vacated at rate n_v/z, where n_v is the number of vacant nearest neighbors and z the total number of nearest neighbors. Evidently, a fully occupied lattice (called "poisoned") is an absorbing state of the Markov process. However, the contact process is known to possess in addition (in the infinite-size limit), a nontrivial ("active") steady state for sufficiently small values of λ.[14,19] The precise value of λ_c (above which there is only the poisoned steady state), is not known, nor is it rigorously established whether the transition is continuous or discontinuous. Monte Carlo simulations[20] and field-theoretic series analysis[12] in one dimension provide strong evidence of a *continuous* transition at $\lambda_c \cong 0.303$.

Denoting the fraction of occupied sites by x, we have, for the 1d CP in the rate approximation (site mean-field theory)

$$\frac{dx}{dt} = (1-x)[\lambda - x] \tag{2.1}$$

For $\lambda < \lambda_c = 1$, the stable steady state is active ($\bar{x} = \lambda$), while for $\lambda \geqslant 1$ there is only the poisoned steady state, $\bar{x} = 1$. (The overbar denotes a steady-

state, average property.) The order parameter for the contact process (and for the other models considered below) is the fraction of vacant sites, $\rho = 1 - x$. We shall also consider the contact process with diffusion, in which particles attempt to hop to nearest neighbor sites at rate D.

The *A-model*, introduced recently[13] as a simplified description of the poisoning of a catalytic surface,[21-24] is identical to the CP, except that particles desorb at unit rate provided they have *at least one* vacant nearest neighbor. Particles surrounded by occupied sites are trapped, as in the CP. For a given configuration, the desorption rate in the A-model is greater than or equal to that in the contact process, which implies $\lambda_{c,\mathrm{A}} > \lambda_{c,\mathrm{CP}}$.[2] Simulations and series analysis[13] indicate a continuous poisoning transition at $\lambda_c \cong 0.574$ in one dimension.

In the mean-field treatments of the contact process and the A-model, the order parameter vanishes linearly with $\lambda_c - \lambda$. Thus, the critical exponent β, defined through the relation $\bar{\rho}(\lambda) \sim (\lambda_c - \lambda)^{\beta}$, is 1. The mean-field value is very different from series and simulation results, which yield $\beta \cong 0.277$ and 0.585 in one[12,13] and two[12] dimensions, respectively.

A third, closely related model is identical to the contact process, except that (in one dimension) particles with one vacant and one occupied nearest neighbor leave the lattice at rate 1/4. This model is more prone to poisoning than the CP, but it is reasonable to expect that it, too, exhibits an active steady state for sufficiently small λ. The motivation for this choice of desorption rates is that in the rate equation approximation, the active steady-state solution is $\bar{\rho} = (1 - 2\lambda)^{1/2}$ for $\lambda < 1/2$, i.e., simple mean-field theory predicts $\beta = 1/2$. It is interesting to see if this model—called "N3" because of the cubic loss term in the rate equation—really has a β value which differs from that of the CP.

The last model ("A2") to be studied in detail has desorption rates identical to the CP, but the particles now adsorb in *pairs* at vacant nearest-neighbor sites, at rate λ. Pairwise adsorption is a feature of certain surface reaction models,[21] and it is of interest to determine its relevance to critical behavior.

3. OPERATOR FORMALISM

An operator formalism is a convenient way to describe Markov processes in many-body systems.[25-27] Here we employ the formalism of ref. 13, in which multiple occupancy of sites is forbidden. The basis states

[2] This inequality follows from Corollary III.1.7 of Ref. 14.

for a given site are $|\phi_{0,i}\rangle$ and $|\phi_{1,i}\rangle$, corresponding to site i vacant and occupied, respectively. The basic inner product is

$$\langle \phi_{j,i} | \phi_{k,i} \rangle = \delta_{j,k} \tag{3.1}$$

A configuration $\{\sigma_i\}$ is written as a direct product

$$|\{\sigma_i\}\rangle = \prod_i |\phi_{\sigma_i,i}\rangle \tag{3.2}$$

so that

$$\langle \{\sigma_i\} | \{\sigma_i'\} \rangle = \prod_i \delta_{\sigma_i,\sigma_i'} \tag{3.3}$$

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

$$\begin{aligned} A_i^\dagger |\phi_{0,i}\rangle &= |\phi_{1,i}\rangle \\ A_i^\dagger |\phi_{1,i}\rangle &= 0 \\ A_i |\phi_{1,i}\rangle &= |\phi_{0,i}\rangle \\ A_i |\phi_{0,i}\rangle &= 0 \end{aligned} \tag{3.4}$$

Note that $A_i A_i^\dagger + A_i^\dagger A_i = 1$.

The state of the system at time t is

$$|\Psi(t)\rangle = \sum_{\{\sigma_i\}} p(\{\sigma_i\}, t) |\{\sigma_i\}\rangle \tag{3.5}$$

where the sum is over all configurations and p is the probability distribution. Physical states $|\Psi\rangle$ must satisfy the positivity and normalization conditions

$$\langle \{\sigma_i\} | \Psi \rangle \geqslant 0, \qquad \forall \{\sigma_i\} \tag{3.6}$$

and

$$\langle \cdot | \Psi \rangle = 1 \tag{3.7}$$

where

$$\langle \cdot | \equiv \prod_j (\langle \phi_{0,j}| + \langle \phi_{1,j}|) = \sum_{\{\sigma_i\}} \langle \{\sigma_i\}| \tag{3.8}$$

is the projection onto all possible configurations.

Observables are represented by operators which are diagonal in the occupation representation. The expectation of obsrvable $\mathcal{O}$ is given by

$$\langle \mathcal{O} \rangle_{\Psi} = \langle \cdot | \mathcal{O} | \Psi \rangle \tag{3.9}$$

For example, the number operator at site j is $N_j = A_j^\dagger A_j$, and $N_j | \{\sigma_i\} \rangle = \sigma_j | \{\sigma_i\} \rangle$. The average density is

$$\langle N_j \rangle_{\Psi} = \sum_{\{\sigma_i\}} \sigma_j \langle \{\sigma_i\} | \Psi \rangle = \langle \cdot | N_j | \Psi \rangle \tag{3.10}$$

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

$$\frac{d | \Psi \rangle}{dt} = S | \Psi \rangle \tag{3.11}$$

The time evolution e^{tS} must preserve positivity and normalization; the latter condition is succinctly expressed as $\langle \cdot | S = 0$.

We may now write down the evolution operators for the 1d models to be considered in detail. The simplest, in terms of operator content, is the CP, which involves only 1- and 2-site terms:

$$S_{\mathrm{CP}} = \sum_i \{\lambda(1 - A_i) A_i^\dagger + (1 - A_i^\dagger) A_i [1 - \tfrac{1}{2}(A_{i-1}^\dagger A_{i-1} + A_{i+1}^\dagger A_{i+1})]\} \tag{3.12}$$

Since the CP involves only 2-site interactions, it is helpful to regroup this into a sum of 1- and 2-site operators,

$$\begin{aligned} S_{\mathrm{CP}} &= \sum_i \{\lambda(1 - A_i) A_i^\dagger + (1 - A_i^\dagger) A_i \\ &\quad - \tfrac{1}{2}[(1 - A_i^\dagger) A_i A_{i-1}^\dagger A_{i-1} + (1 - A_{i-1}^\dagger) A_{i-1} A_i^\dagger A_i]\} \\ &\equiv \sum_i S_{\mathrm{CP},i} \end{aligned} \tag{3.13}$$

The evolution operator for the CP with diffusion may then be written in the form

$$S_{\mathrm{CP},D} = \sum_i \{(1 - D) S_{\mathrm{CP},i} + D \mathscr{D}_i\} \tag{3.14}$$

where

$$\mathscr{D}_i = \tfrac{1}{2}[(1 - A_{i-1} A_i^\dagger) A_{i-1}^\dagger A_i + (1 - A_i A_{i-1}^\dagger) A_i^\dagger A_{i-1}] \tag{3.15}$$

describes nearest-neighbor hopping.

If we define

$$S_\eta = S_{\mathrm{CP}} + \eta \sum_i (1 - A_i^\dagger) A_i [A_{i-1}^\dagger A_{i-1} A_{i+1} A_{i+1}^\dagger + A_{i+1}^\dagger A_{i+1} A_{i-1} A_{i-1}^\dagger] \tag{3.16}$$

then $\eta = 1/2$ yields the evolution operator for the A-model, while the N3-model corresponds to $\eta = -1/4$. This shows that the latter models are obtained by adding a three-site interaction to the CP. The results presented in Section 9 indicate that this perturbation of the CP is irrelevant to critical behavior.

Finally, the evolution operator for the A2-model is

$$\begin{aligned} S_{\mathrm{A2}} = \sum_i \{ & \lambda (1 - A_{i-1} A_i) A_{i-1}^\dagger A_i^\dagger \\ & + \tfrac{1}{2} [(1 - A_i^\dagger) A_i A_{i-1} A_{i-1}^\dagger + (1 - A_{i-1}^\dagger) A_{i-1} A_i A_i^\dagger] \} \end{aligned} \tag{3.17}$$

4. PERTURBATION THEORY

We wish to determine the stationary probability distribution, i.e., the solution(s) to $S|\bar{P}\rangle = 0$. Let us decompose the evolution operator

$$S = S^0 + V \tag{4.1}$$

such that the evolution under S^0 is solvable, and $\langle \cdot | S^0 = \langle \cdot | V = 0$. (Note that $\langle \bar{P}^0 | = \langle \cdot |$, i.e., the left eigenvector of S^0 with eigenvalue zero is the normalization bra.) In this section we derive a formal expression for $|\bar{P}\rangle$ in terms of a reference state $|\bar{P}^0\rangle$, the exact steady state for a model with evolution S^0. Let $[S^0]^{-1}$ be the inverse of S^0 in the nonzero subspace. If we multiply the equation $S|\bar{P}\rangle = 0$ by $[S^0]^{-1}$, and use $[S^0]^{-1} S^0 = 1 - |\bar{P}^0\rangle\langle\bar{P}^0|$ and the normalization condition on $|\bar{P}\rangle$, we find

$$(1 + [S^0]^{-1} V) |\bar{P}\rangle = |\bar{P}^0\rangle \tag{4.2}$$

This is the formal solution for the stationary state. We shall be interested in a systematic expansion of (4.2).

For a finite system with periodic boundary conditions, the unique steady state is the absorbing state $|\Phi\rangle$. We verify that $|\Phi\rangle$ satisfies (4.2), for the A-model on a ring of N sites, in the Appendix. In the infinite-size limit, and for sufficiently small λ, there is also an active steady state which we seek to represent by expanding (4.2). On the basis of simulations and mean-field theory, we expect the steady states of the models under consideration to exhibit a critical point at λ_c. Since there appears to be a

well-defined active steady state for small λ, we interpret, for any observable expressed as a series in λ, the first singularity on the positive-λ axis as marking the critical point. Thus, we require an expansion of (4.2) in powers of λ or a related quantity, in contrast with the usual "high-T" expansion in powers of the interaction V. In fact, the parameter λ appears in the part of evolution operator which describes a *noninteracting* system. After transforming to a basis of eigenstates of S^0, we shall find that V is a polynomial in $v = \lambda/(1+\lambda)$. The portion of V which is $O(v^0)$ is retained to all orders at each stage of the calculation. The particle density in the reference state $|\bar{P}^0\rangle$ vanishes when $v \to 0$; in effect, we expand about the vacant lattice (i.e., the opposite of the absorbing state).

5. APPLICATION TO THE A-MODEL

Referring to the evolution operator (3.16), we see that the obvious choice for the reference system is

$$S^0 = \sum_i \{\lambda(1-A_i)\, A_i^\dagger + (1-A_i^\dagger)\, A_i\} = \sum_i S_i^0 \tag{5.1}$$

since this portion of S describes a noninteracting system. The interaction is

$$V = -\sum_i (1-A_i^\dagger)\, A_i A_{i-1}^\dagger A_{i-1} A_{i+1}^\dagger A_{i+1} \equiv \sum_i V_i \tag{5.2}$$

S_i^0 has eigenvalues 0 and $-(1+\lambda)$, with corresponding right eigenvectors

$$|\psi_{0,i}\rangle = (1-v)\,|\phi_{0,i}\rangle + v\,|\phi_{1,i}\rangle \tag{5.3}$$

$$|\psi_{1,i}\rangle = |\phi_{0,i}\rangle - |\phi_{1,i}\rangle \tag{5.4}$$

and left eigenvectors

$$\langle\psi_{0,i}| = \langle\phi_{0,i}| + \langle\phi_{1,i}| \tag{5.5}$$

$$\langle\psi_{1,i}| = v\langle\phi_{0,i}| - (1-v)\langle\phi_{1,i}| \tag{5.6}$$

where $v = \lambda/(1+\lambda)$. We shall refer to states $\langle\psi_{0,i}|$ and $\langle\psi_{1,i}|$ as "ground" and "excited" states, respectively, at site i. Note that $\langle\psi_{i,k}|\psi_{j,k}\rangle = \delta_{i,j}$ and that S^0 has the unique steady state $|\bar{P}^0\rangle = \prod_j |\psi_{0,j}\rangle$. S^0 has eigenstates $|i_1,\ldots,i_m\rangle$ (sites $i_1,\ldots,i_m$ excited, all others in ground state) with corresponding eigenvalues $-m(1+\lambda)$. Let P_m be the projection onto the subspace of states with exactly m excited sites. Then

$$[S^0]^{-1} = -(1-v)\sum_{m=1}^{\infty} m^{-1} P_m \equiv -(1-v)\, M^{-1} \tag{5.7}$$

M^{-1} is simply division by the number of excited sites. Define raising and lowering operators $B_i^\dagger$ and B_i such that

$$\begin{aligned} B_i^\dagger \,|\psi_{0,i}\rangle &= |\psi_{1,i}\rangle \\ B_i^\dagger \,|\psi_{1,i}\rangle &= 0 \\ B_i \,|\psi_{1,i}\rangle &= |\psi_{0,i}\rangle \\ B_i \,|\psi_{0,i}\rangle &= 0 \end{aligned} \tag{5.8}$$

B_i and $B_i^\dagger$ are related to the creation and annihilation operators by

$$A_i^\dagger = B_i[1 + (1-v)\,B_i^\dagger] - (1-v)\,B_i^\dagger[(1-v) + B_i] \tag{5.9}$$

$$A_i = B_i(vB_i^\dagger - 1) - vB_i^\dagger(B_i - v) \tag{5.10}$$

Note that $B_i\,|\bar{\Psi}^0\rangle = \langle\bar{\Psi}^0|\,B_i^\dagger = 0$. The number operator is

$$N_i = A_i^\dagger A_i = [(1-v)\,B_i^\dagger - 1]\,B_i + v[B_i - (1-v)]\,B_i^\dagger \tag{5.11}$$

and the steady-state occupation fraction is

$$\begin{aligned} \bar{x} &= \langle\bar{\Psi}^0|\,(vB_iB_i^\dagger - B_i)\,|\bar{\Psi}\rangle \\ &= v - \langle\bar{\Psi}^0|\,B_i\,|\bar{\Psi}\rangle \end{aligned} \tag{5.12}$$

We also note the expressions for the pair occupancy fraction

$$\langle N_iN_j\rangle = \bar{x}^2 - \langle\bar{\Psi}^0|\,B_i\,|\bar{\Psi}\rangle^2 + \langle\bar{\Psi}^0|\,B_iB_j\,|\bar{\Psi}\rangle \tag{5.13}$$

and the pair correlation

$$g_{|i-j|} = \langle N_iN_j\rangle - \langle N_i\rangle\langle N_j\rangle = \langle\bar{\Psi}^0|\,B_iB_j\,|\bar{\Psi}\rangle - \langle\bar{\Psi}^0|\,B_i\,|\bar{\Psi}\rangle^2 \tag{5.14}$$

The interaction now takes the form

$$\begin{aligned} V_i = B_i^\dagger(B_i - v)\{&[(1-v)\,B_{i-1}^\dagger - 1]\,B_{i-1} + v[B_{i-1} - (1-v)]\,B_{i-1}^\dagger\} \\ \times\ \{&[(1-v)\,B_{i+1}^\dagger - 1]\,B_{i+1} + v[B_{i+1} - (1-v)]\,B_{i+1}^\dagger\} \end{aligned} \tag{5.15}$$

Note that $[S^0]^{-1}\,V$ is a sixth-degree polynomial in v, while λ appears to all orders in this operator. We therefore adopt v as the expansion parameter. Let

$$1 + [S^0]^{-1}\,V = 1 - R + \sum_{j=1}^{6} v^jT_j \tag{5.16}$$

Expanding the stationary distribution as

$$|\bar{\Psi}\rangle = |\bar{\Psi}^0\rangle + v\,|\bar{\Psi}_1\rangle + v^2\,|\bar{\Psi}_2\rangle + \cdots \tag{5.17}$$

we have, from (4.2),

$$|\bar{\Psi}_n\rangle = -(1-R)^{-1} \sum_{j=1}^{\min[n,6]} T_j\,|\bar{\Psi}_{n-j}\rangle \tag{5.18}$$

which permits recursive determination of the $|\bar{\Psi}_n\rangle$.

The operators R and T_j are as follows:

$$R = M^{-1} \sum_i B_i^\dagger B_i D_{i-1} D_{i+1} \tag{5.19}$$

$$T_1 = M^{-1} \sum_i B_i^\dagger \{(B_i+1)\, D_{i-1} D_{i+1} + B_i [D_{i-1} C_{i+1} + D_{i+1} C_{i-1}]\} \tag{5.20}$$

$$T_2 = -M^{-1} \sum_i B_i^\dagger \{(D_{i-1} D_{i+1} + (B_i+1)[D_{i-1} C_{i+1} + D_{i+1} C_{i-1}] + B_i [B_{i-1} D_{i+1} + B_{i+1} D_{i-1}]\} \tag{5.21}$$

$$T_3 = M^{-1} \sum_i B_i^\dagger \{D_{i-1} C_{i+1} + D_{i+1} C_{i-1} + (B_i+1)\, C_{i-1} C_{i+1} + B_i [B_{i-1}^\dagger C_{i+1} + B_{i+1}^\dagger C_{i-1}]\} \tag{5.22}$$

$$T_4 = -M^{-1} \sum_i B_i^\dagger \{C_{i-1} C_{i+1} + B_{i-1}^\dagger D_{i+1} + B_{i+1}^\dagger D_{i-1} + (B_i+1)[B_{i-1}^\dagger C_{i+1} + B_{i+1}^\dagger C_{i-1}] + B_i B_{i-1}^\dagger B_{i+1}^\dagger\} \tag{5.23}$$

$$T_5 = M^{-1} \sum_i B_i^\dagger \{B_{i-1}^\dagger C_{i+1} + B_{i+1}^\dagger C_{i-1} + (B_i+1)\, B_{i-1}^\dagger B_{i+1}^\dagger\} \tag{5.24}$$

$$T_6 = -M^{-1} \sum_i B_i^\dagger B_{i-1}^\dagger B_{i+1}^\dagger \tag{5.25}$$

where

$$C_i = B_i^\dagger B_i - (B_i - 1)\, B_i^\dagger \tag{5.26}$$

and

$$D_i = (B_i^\dagger - 1)\, B_i \tag{5.27}$$

The algebra is greatly simplified by introducing a graphical notation. Note that R and T_j consist of products of operators associated with three consecutive sites. If the rightmost operator associated with site j is B_j ($B_j^\dagger$),

then site j must be excited (unexcited) in the "incoming" state. Similarly, if the leftmost operator is $B_j^\dagger$ (B_j), then site j is excited (unexcited) in the outgoing state. We represent the operators associated with site j by a $\times$ and an excited site in the incoming (outgoing) state by a line above (below) the $\times$. Thus we have the following "nodes":

$$\begin{aligned} B_i &\leftrightarrow \overset{|}{\times} \\ B_i^\dagger &\leftrightarrow \underset{|}{\times} \\ B_i B_i^\dagger &\leftrightarrow \times \\ B_i^\dagger B_i &\leftrightarrow \overset{|}{\underset{|}{\times}} \end{aligned} \tag{5.28}$$

Each term in R and T_j may then be represented as a "vertex" containing three nodes. Note that there is always a line emerging below the central node. The operator R is

$$R = M^{-1}[\overset{|}{\times}\times\times - \times\overset{|}{\times}\times - \times\times\overset{|}{\times} + \overset{|}{\times}\overset{|}{\times}\overset{|}{\times}] \tag{5.29}$$

where the sum over sites (prior to operation of M^{-1}) is now understood. Further simplification is possible if we note that the vertices in a given operator always occur in symmetrical combinations. We therefore use a blob with n_i incoming and n_0 outgoing lines to represent the sum of all allowed vertices of that kind. For example,

$$\overset{|}{\bigcirc}\!\!\!\!\underset{|}{} = \overset{|}{\times}\times\overset{|}{\times} + \times\overset{|}{\times}\times \tag{5.30}$$

$$\overset{|}{\bigcirc}\!\!\!\!\underset{|}{} = \overset{|}{\times}\times\times + \times\overset{|}{\times}\times + \times\times\overset{|}{\times} + \underset{|}{\times}\overset{|}{\times}\times + \underset{|}{\times}\times\overset{|}{\times} + \times\underset{|}{\times}\overset{|}{\times} \tag{5.31}$$

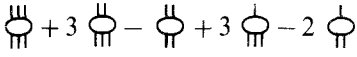
$$\bigcirc\!\!\!\!\underset{|}{} = \overset{|}{\times}\times\times + \times\overset{|}{\times}\times + \times\times\overset{|}{\times} \tag{5.32}$$

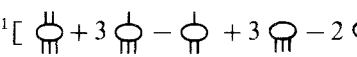
etc. In terms of this notation we have

$$R = M^{-1}[\ \overset{|}{\bigcirc}\!\!\!\!\underset{|}{} - \bigcirc + \bigcirc\ ] \tag{5.33}$$

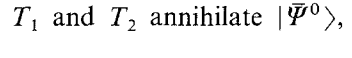
$$T_1 = M^{-1}[3\,\overset{|}{\bigcirc}\!\!\!\!\underset{|}{} - 2\,\bigcirc + \bigcirc + \overset{|}{\bigcirc}\!\!\!\!\underset{|}{} - \bigcirc + \bigcirc\ ] \tag{5.34}$$

$$\begin{aligned} T_2 = -M^{-1}[3\,\overset{|}{\bigcirc}\!\!\!\!\underset{|}{} - \bigcirc + 3\,\underset{|}{\bigcirc} - 2\,\bigcirc \\ + \bigcirc + \underset{|}{\bigcirc} - \bigcirc + \bigcirc\ ] \end{aligned} \tag{5.35}$$

$T_3 = M^{-1}[$  $]$ (5.36)

$T_4 = -M^{-1}[$  $]$ (5.37)

$T_5 = M^{-1}[$  $]$ (5.38)

$T_6 = -M^{-1}$  (5.39)

It is immediately apparent from this representation that R creates no new excited sites, and that T_1 and T_2 annihilate $|\bar{\Psi}^0\rangle$, so that (5.18) yields $|\bar{\Psi}_1\rangle = |\bar{\Psi}_2\rangle = 0$.

The lowest-order correction to $|\bar{\Psi}\rangle$ is

$$|\bar{\Psi}_3\rangle = (1-R)^{-1}\, T_3\, |\bar{\Psi}^0\rangle \tag{5.40}$$

Referring to (5.36), we see that

$$T_3\, |\bar{\Psi}^0\rangle = \tfrac{1}{3}(|\,|\,|) - (|\,|) + (|) \tag{5.41}$$

where we have introduced the notation

$$(|\,|\,|) \equiv \sum_i |i-1, i\rangle = \sum_i B^\dagger_{i-1} B^\dagger_i\, |\bar{\Psi}^0\rangle \tag{5.42}$$

etc., for translation-invariant states in which excited sites are arranged in a specified sequence. Referring now to (5.33), we see that $R(|) = R(|\,|) = 0$. To evaluate $(1-R)^{-1}\,(|\,|\,|)$, we note the identity

$$(1-R)^{-1} = 1 + (1-R)^{-1} R \tag{5.43}$$

Now,

$$R(|\,|\,|) = \tfrac{1}{3}(|\,|\,|) - (|\,|) + (|) \tag{5.44}$$

so that

$$(1-R)^{-1}\,(|\,|\,|) = \tfrac{3}{2}\{(|\,|\,|) - (|\,|) + (|)\} \tag{5.45}$$

and

$$|\bar{\Psi}_3\rangle = -\tfrac{1}{2}\{(|\,|\,|) - 3(|\,|) + 3(|)\} \tag{5.46}$$

Notice that evaluation of $(1-R)^{-1}$ is straightforward because R does not produce any new excited sites.

Following the same procedure, one finds the next correction to be

$$\begin{aligned} |\bar{\Psi}_4\rangle &= -(1-R)^{-1}\,[T_1\,|\bar{\Psi}_3\rangle + T_4\,|\bar{\Psi}^0\rangle] \\ &= \tfrac{1}{2}(|\,|\,|\,|) - \tfrac{1}{3}[(|\,|0|\,|) + (|0|\,|\,|)] + (|0|\,|) \\ &\quad - \tfrac{1}{4}(|\,|\,|) + \tfrac{1}{4}(|\,|\,|) - \tfrac{7}{4}(|) \end{aligned} \tag{5.47}$$

where

$$(|0|) = \sum_i B_{i-2}^{\dagger} B_i^{\dagger}\,|\bar{\Psi}^0\rangle \tag{5.48}$$

and the obvious generalizations to $(|\,|0|)$, etc., are used to denote translation-invariant states with a specified sequence of excited $(|)$ and ground (0) sites.

From (5.12) we see that $\bar{x}_n$, the nth-order contribution to $\bar{x}$, is just the coefficient of $-(|)$ in $|\bar{\Psi}_n\rangle$. Thus we have

$$\bar{x} = v + \tfrac{3}{2}v^3 + \tfrac{7}{4}v^4 + O(v^5) \tag{5.49}$$

Similarly, the nearest-neighbor pair occupancy fraction is, from (5.13),

$$\begin{aligned} \langle N_{i-1} N_i\rangle &= v^2 - 2vc_{(|)} + c_{(|\,|)} \\ &= v^2 + \tfrac{3}{2}v^3 + \tfrac{13}{4}v^4 + O(v^5) \end{aligned} \tag{5.50}$$

where $c_{(|)}$ is the coefficient of $(|)$ in $|\bar{\Psi}\rangle$, etc. The nearest-neighbor pair correlation is

$$g_1 = c_{(|\,|)} - c_{(|)}^2 = \tfrac{3}{2}v^3 + \tfrac{1}{4}v^4 + O(v^5) \tag{5.51}$$

which shows the expected positive correlation, due to inhibited desorption.

Since the direct evaluation of further terms in the expansion becomes quite tedious, the derivation of long series requires an efficient computer algorithm. In principle, one would like to determine the steady-state probability distribution (i.e., the $|\bar{\Psi}_n\rangle$), but in practice the calculation of a local property such as $\bar{x}$ or g_1 is much simpler. This is because only a small subset of the states in $|\bar{\Psi}_n\rangle$ are relevant to local properties. In Section 8 an algorithm is described which generates the states required to evaluate $\bar{x}$ and g_1.

The expansions for the CP and the N3-model parallel the derivation outlined above, as we may again take S^0 as in (5.1). For the evolution operator (3.16), one finds that the lowest-order correction to $|\bar{\Psi}\rangle$ is

$$|\bar{\Psi}_2\rangle = \frac{2\eta - 1}{2\eta + 1}\,[2(|) - (|\,|)] \tag{5.52}$$

where the CP corresponds to $\eta = 0$ and N3 to $\eta = -1/4$. Extended series for these models are given in Section 9.

6. THE CONTACT PROCESS WITH DIFFUSION

In this section we consider steady-state perturbation theory for a model which incorporates hopping in the unperturbed evolution. Absorbing a factor of $(1-D)$ into a rescaled time variable, we write the evolution operator for the 1d CP with nearest-neighbor hopping (at rate D) as

$$S=\sum_i \{S_{\mathrm{CP},i}+\bar{D}\mathscr{D}_i\} \tag{6.1}$$

where $\bar{D}=D/(1-D)$, and $S_{\mathrm{CP},i}$ and $\mathscr{D}_i$ are given by (3.13) and (3.15), respectively. Several perturbative approaches are possible: (1) Take the noninteracting creation and annihilation terms [i.e., the rhs of (5.1)] together with $D\mathscr{D}$ as S^0, and work in a basis of eigenstates (characterized by a set of wavevectors) of this new reference system; (2) take S^0 as in the A-model, and derive an expansion in v *and* $\bar{D}$; (3) take S^0 as in the A-model, but treat diffusion nonperturbatively. In the present, preliminary application, we pursue the last-mentioned approach to second order in v.

We may write S^0 in the form

$$S^0=-(1+\lambda)\sum_{m=0}^{\infty} mP_m=-\frac{M}{1-v} \tag{6.2}$$

In terms of raising and lowering operators, we have

$$\mathscr{D}_i=\tfrac{1}{2}[(1-B_{i-1}^{\dagger}B_i)\,B_{i-1}B_i^{\dagger}+(1-B_i^{\dagger}B_{i-1})\,B_iB_{i-1}^{\dagger}] \tag{6.3}$$

or, in the notation of (5.28),

$$\mathscr{D}=\tfrac{1}{2}\{\nwarrow\!\!\times+\times\!\!\nwarrow-\nwarrow\!\!\times-\times\!\!\nwarrow\} \tag{6.4}$$

so that the hopping operator transfers excitations between neighboring sites, but does not create or destroy them.

From (3.13), one has for the interaction

$$V_i=-\tfrac{1}{2}[(1-A_i^{\dagger})\,A_iA_{i-1}^{\dagger}A_{i-1}+(1-A_{i-1}^{\dagger})\,A_{i-1}A_i^{\dagger}A_i]\} \tag{6.5}$$

It proves convenient to introduce the v expansion of $|\bar{\Psi}\rangle$ directly into $(S^0+\bar{D}\mathscr{D}+V)\,|\bar{\Psi}\rangle=0$. Hence, we expand V (rather than $[S^0]^{-1}V$) in powers of v, obtaining

$$V=\sum_{j=0}^{3} v^j t_j \tag{6.6}$$

where

$$t_0 = \tfrac{1}{2} \tag{6.7}$$

$$t_1 = -\tfrac{1}{2} \tag{6.8}$$

$$t_2 = \tfrac{1}{2} \tag{6.9}$$

$$t_3 = -\tfrac{1}{2} \tag{6.10}$$

and where

$$\equiv \times\times + \times\times + \times\times + \times\times \tag{6.11}$$

etc.

We may now derive the lowest-order (in v) correction to $|\bar{\Psi}\rangle$. Upon inserting the expansion (5.19) into

$$\left(-\frac{M}{1-v} + \bar{D}\mathscr{D} + V\right)|\bar{\Psi}\rangle = 0 \tag{6.12}$$

we obtain, at order v, an equation which implies that $|\bar{\Psi}_1\rangle = 0$, and at order v^2

$$(t_0 - M + \bar{D}\mathscr{D})\,|\bar{\Psi}_2\rangle = -t_2\,|\bar{\Psi}^0\rangle = (|) - (||) \tag{6.13}$$

The solution must be a translation-invariant sum of states with one or two excited sites; hence, we take

$$|\bar{\Psi}_2\rangle = c^{(2)}_{(|)}(|) + \sum_j b_j(/j/) \tag{6.14}$$

where

$$(/j/) \equiv \sum_i B^\dagger_{i-j} B^\dagger_i\,|\bar{\Psi}^0\rangle \tag{6.15}$$

so that $(/1/) = (||)$, $(/2/) = (|0|)$, etc. One readily verifies that

$$\mathscr{D}(|) = 0 \tag{6.16}$$

$$\mathscr{D}(/1/) = (/2/) - (/1/) \tag{6.17}$$

and

$$\mathscr{D}(/j/) = (/j-1/) + (/j+1/) - 2(/j/) \tag{6.18}$$

for $j \geqslant 2$. Also note that $t_0 |\bar{\Psi}_2\rangle = b_1[(||) - (|)]$. Upon inserting (6.14) in (6.13), we obtain, from the coefficient of $(||)$

$$0 = 1 - b_1 + \bar{D}[b_2 - b_1] \tag{6.19}$$

while the coefficient of $(/j/)$ (for $j \geqslant 2$) yields

$$0 = -2b_j + \bar{D}[b_{j-1} + b_{j+1} - 2b_j] \tag{6.20}$$

Notice that b_j in (6.19) and (6.20) may be interpreted as the average number of random walkers at site j in the steady state of the following 1d process. Independent random walkers appear at $j=1$, at rate $1+b_1$, disappear (from any site) at rate 2, and hop to neighboring sites at rate D, subject to a reflecting barrier at $j=0$. We may solve for the steady-state density by placing an image source of strength $1+b_0$ at $j=0$ and removing the barrier. One now has (for $j \in \mathbf{Z}$)

$$0 = (1+b_j)(\delta_{j,0} + \delta_{j,1}) - 2b_j + \bar{D}(b_{j-1} + b_{j+1} - 2b_j) \tag{6.21}$$

Introducing the generating function $g(k) = \sum_j e^{ijk} b_j$, one finds

$$g(k) = \frac{(1+e^{ik})(1+b)}{2(1+\bar{D})(1-\bar{D}\cos k)} \tag{6.22}$$

Using

$$b_1 = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-ik} g(k)$$

one then obtains

$$b_1 = \left(\frac{1-D}{1+D}\right)^{1/2} \tag{6.23}$$

When $D \to 0$, $|\bar{\Psi}_2\rangle = -2(|) + (||)$, in agreement with (5.51) for $\eta = 0$. The occupation fraction is

$$\bar{x} = v + (1+b_1)\, v^2 + O(v^3) \tag{6.24}$$

The v^2 term is largest when $D=0$, reflecting the breakup of clusters (hence easier desorption) as the diffusion rate grows.

7. THE A2-MODEL

As noted in Section 2, the distinctive feature of this model is pairwise adsorption of particles. This means that the single-site creation term in S^0,

as given by (5.1), is not part of the evolution operator for the A2-model, (3.17). Rather than adopting an S^0 which incorporates pairwise creation, we employ a noninteracting reference system. Since (3.17) does not suggest a specific choice for the coefficients of the creation and annihilation terms, we write

$$S^0 = \sum_i \{a(1-A_i)\,A_i^\dagger + b(1-A_i^\dagger)\,A_i\} \tag{7.1}$$

with $a = \alpha\lambda$, and α and b left unspecified for the moment. If we let $v = a/(a+b)$, then the eigenvectors of S_i^0 are as in (5.3)–(5.6), and the corresponding eigenvalues are 0 and $-(a+b)$. The inverse of S^0 (on the nonzero subspace) is $-(1-v)M^{-1}/b$, and (5.8)–(5.10), relating to the raising and lowering operators, are again valid. The interaction is now

$$\begin{aligned} V_i &= S_i - \frac{1}{2}[S_i^0 + S_{i-1}^0] \\ &= \lambda\{(1-A_{i-1}A_i)\,A_{i-1}^\dagger A_i^\dagger - \frac{\alpha}{2}[(1-A_i)\,A_i^\dagger + (1-A_{i-1})\,A_{i-1}^\dagger]\} \\ &\quad + \frac{1}{2}[(1-A_i^\dagger)\,A_i(A_{i-1}A_{i-1}^\dagger - b) + (1-A_{i-1}^\dagger)\,A_{i-1}(A_iA_i^\dagger - b)] \end{aligned} \tag{7.2}$$

If we express V_i in terms on raising and lowering operators and introduce graphical notation as above, we find that the resulting expression is simplest for a particular relation between a and b. In order that all of the vertices with one incoming and one outgoing line combine to give a multiple of  , we must choose $a+b=1$. Then $v=\alpha\lambda$ and $[S^0]^{-1} = -M^{-1}$, and

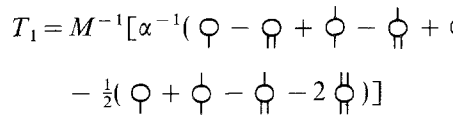
$$\begin{aligned} V_i = \frac{v}{\alpha}[&-(1-v)^2 \\ &+ (1-v)^2(1-2v) \\ &- (1-v) \\ &+ (1-v)(1-2v) \\ &- \\ &+ (1-2v) \\ &] \\ &+ \frac{1}{2}[v(1-v) \\ &+ 2v^2(1-v) \\ &+ v \\ &- v(1-2v) \\ &- \\ &+ 2(1-v) \\ &] \end{aligned} \tag{7.3}$$

We write $1 + [S^0]^{-1}\,V = 1 - R + \sum_{j=1}^4 v^j T_j$, where

$$R = M^{-1}[\ - \tfrac{1}{2}\ ] \tag{7.4}$$

and

$$T_1 = M^{-1}[\alpha^{-1}(\quad - \quad + \quad - \quad + \quad - \quad) - \tfrac{1}{2}(\quad + \quad - \quad - 2\quad)] \tag{7.5}$$



Notice that $T_1 |\bar{\Psi}^0\rangle \neq 0$, so that (unlike the models considered until now) there is a first-order correction to $|\bar{\Psi}\rangle$, given by

$$|\bar{\Psi}_1\rangle = -\frac{1}{1-R} T_1 |\bar{\Psi}^0\rangle = -\left[\frac{3}{\alpha} - 1\right](|) + \frac{1}{\alpha}(||) \tag{7.6}$$

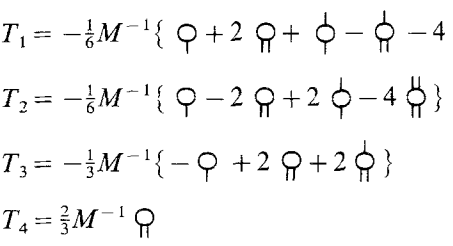
We now choose $\alpha = 3$, so that the first-order correction to $\bar{x}$ vanishes. [The result, $\bar{x} = 3\lambda + O(\lambda^2)$, is of course independent of our choice for α.] With this value for α, the T_j are given by

$$T_1 = -\tfrac{1}{6}M^{-1}\{\quad + 2\quad + \quad - \quad - 4\quad - 2\quad\} \tag{7.7}$$

$$T_2 = -\tfrac{1}{6}M^{-1}\{\quad - 2\quad + 2\quad - 4\quad\} \tag{7.8}$$

$$T_3 = -\tfrac{1}{3}M^{-1}\{-\quad + 2\quad + 2\quad\} \tag{7.9}$$

$$T_4 = \tfrac{2}{3}M^{-1}\quad \tag{7.10}$$



An expansion for the steady-state properties of the model may be derived using the algorithm described in the following section. We see that the absence of an identifiable noninteracting portion of S does not preclude the application of perturbation methods.

8. AN ALGORITHM FOR GENERATING SERIES EXPANSIONS

The expansions derived above involve recursive determination of the $|\bar{\Psi}_n\rangle$, as expressed in (5.16)–(5.18). The process consists of many similar elementary steps, which are readily coded into an algorithm. In calculations of local properties such as $\bar{x}$, the number of steps at each order in perturbation theory is finite.

The basic entities in the problem are the operators R and T_j and the components $|\bar{\Psi}_n\rangle$. The latter are represented [as in (5.48)] in terms of states of the form

$$(|s_{r-1}, \ldots, s_2|) = \sum_j B_{j-r}^\dagger B_j^\dagger \prod_{k|s_k=1} B_{j-k}^\dagger |\bar{\Psi}^0\rangle \tag{8.1}$$

where $s_i = 0$ or |. It is convenient to regard a string of 0's and |'s as a binary number, so that each corresponds to a different (odd) integer. We refer to a state by its label [(| |) = (3), etc.], and denote the coefficient of (r) in $|\bar{\Psi}_n\rangle$ by $C(n, r)$.

The operators R and T_j are represented by vertices with three nodes. (In this discussion we consider three-site operators; the generalization to n-site operators is obvious.) We may again code the incoming and outgoing patterns as binary numbers, so that, for example, the vertex  has input 7 and output 6. We use arrays $T(j, o, i)$ to represent the coefficient of output o, for input i, in T_j, and similarly for R. For example, the nonzero elements of R, (5.35), for the A-model are

$$\begin{aligned} R(2, 7) &= R(7, 7) = 1 \\ R(3, 7) &= R(6, 7) = -1 \end{aligned} \tag{8.2}$$

Note that these arrays cannot represent the nonlocal operator M^{-1} appearing in (5.33)–(5.39). The effect of M^{-1} is to introduce a factor m^{-1}, where m is the number of |'s in the string.

As is suggested by (5.18), evaluation of $|\bar{\Psi}_n\rangle$ proceeds in two stages: first, operation of the T_j on (previously determined) $|\bar{\Psi}_{n-j}\rangle$, then operation with $(1-R)^{-1}$. The first task, then, is to generate the strings representing the sum in (5.18). The states generated by T_j, as it operates upon the states in $|\bar{\Psi}_{n-j}\rangle$, are evaluated, and $C'(r)$ [which temporarily stores the coefficient of (r) in the sum] is updated. To begin, consider

$$T_j |\bar{\Psi}^0\rangle = \sum_r T(j, r, 0)(r) \tag{8.3}$$

where $r = 2$, 3, 6, or 7, corresponding to the strings (0|0), (0| |), (| |0), and (| | |), respectively. Clearly, any 0's lying to one side of all the 0's are superfluous (*all* of the sites outside the string are in the ground state). To eliminate this redundancy, each generated string (r) is divided by 2 until an odd-numbered string $(\underline{r})$ is obtained. Then $C'(\underline{r})$ is augmented by $T(j, r, 0)/m$, where m is the number of |'s in string (r). For example, when T_3, (5.36), operates on $|\bar{\Psi}^0\rangle$, the terms (2), $-(3)$, $-(6)$, and (7) are generated; (2) is converted to (1), (6) to (3). The number of |'s in each string is determined (to find m^{-1}), yielding $C'(1) = 1$, $C'(3) = -1$, and $C'(7) = 1/3$.

Now consider $T_j(r)$ $(r \neq 0)$. The state (r)—a string of 0's and |'s, embedded in an infinite sequence of 0's—is regarded as a static pattern, while T_j (which involves a sum over $\mathbf{Z}$), sweeps across the lattice. For example, if $r = 3$, T_j operates at each site in ...000| |000..., encountering the sequence of inputs: ...0, 0, 4, 6, 3, 1, 0, 0.... For each input i, T_j

may generate strings (r') by replacing i with a sequence o. For each (r'), the corresponding $(\underline{r}')$ (free of extraneous 0's) is formed, and $C'(\underline{r}')$ is augmented by $C(n-j, r)\, T(j, o, i)/m'$, where m' is the number of excited sites in (r').

Note that $T_j(r)$ comprises an infinite set of strings if $T(j, o, 0) \neq 0$ for some o. However, as will be shown below, only a restricted set of strings contributes in calculations of local properties. Suppose, then, that we need only consider strings up to $r_{\max}$, where $r_{\max} < 2^{n_{\max}}$, so that the strings extend over at most $n_{\max}$ sites. Let (r) extend over n sites. Then the range of operation of T_j need not extend beyond margins of $n_{\max} - n$ 0's to the right and left of the outermost |'s in (r), and a finite set of strings (r') is generated.

It remains to evaluate $-(1-R)^{-1}$ acting on $\sum_j T_j |\bar{\Psi}_{n-j}\rangle$. Let

$$R(r) = a_r(r) + \sum_{r'} a_{r'}(r') \tag{8.4}$$

Since R creates no new excited sites, $r' < r$. From (5.43) we have

$$(1-R)^{-1}(r) = (1-a_r)^{-1}\left[(r) + (1-R)^{-1}\sum_{r'} a_{r'}(r')\right] \tag{8.5}$$

Let the largest string in $\sum_j T_j |\bar{\Psi}_{n-j}\rangle$ be $(r_{\max})$. Applying (8.5) to $(r_{\max})$, one obtains

$$C(n, r_{\max}) = -C'(r_{\max})/(1-a_{r_{\max}}) \tag{8.6}$$

The r' terms in (8.4) are added in to the remaining terms in $C'(r')$, via

$$C'(r') \to C'(r') + C'(r_{\max})\, a_{r'}/(1-a_{r_{\max}})$$

This procedure is repeated for each string $r' < r_{\max}$, in descending order, to obtain the $C(n, r)$.

As noted above, only a finite set of strings need be retained at each order in the evaluation of a local property, even when $|\bar{\Psi}_n\rangle$ includes an infinite number of terms. Consider, for example, the calculation of $\bar{x}$ in the A-model, to $O(v^6)$. The only coefficient required for $\bar{x}$ is $C(n, 1)$, since $\bar{x} = v - \sum_n C(n, 1)\, v^n$. At nth order, then, we only require $C'(r)$ for those strings which yield a nonzero (1) component under repeated action of $(1-R)^{-1}$. Since R is nonzero only for input $i = 7$, $(|||)$, (r) contributes to $\bar{x}$ if and only if $(r) = (|||\ldots|)$, i.e., r must equal $2^m - 1$ for some m. If (r) includes any "gap" (one or more 0's between |'s), then all strings in $(1-R)^{-1}$ also contain a gap. Thus, in the sixth-order calculation, the entire series $(|||0|||)$, $(|||00|||)$,..., generated by $T_3 |\bar{\Psi}_3\rangle$ may be discarded; only $(||||||)$ contributes. Similarly, if the calculation were extended to seventh order, one would retain (in sixth order) $(|||0|||)$, but discard strings with

larger gaps, or with more than one gap, since T_1 (5.36), can only create a single new excited site. Considerations such as these lead to restrictions on the length, and the number of zeros, in strings which need be retained at each step of the calculation. Such restrictions are essential for deriving useful series with a reasonable expenditure of computer time. [For example, the calculations to $O(v^{16})$ presented in the following section require about 1.5 h on an IBM 3081. The CPU time increases by roughly a factor of 3 with each additional order.]

9. RESULTS AND ANALYSIS

Using the algorithm described in the preceding section, series for the occupation fraction x and for $c_{(|)}$ have been derived to $O(v^{16})$ for the CP, A, and N3-models. The coefficients are displayed in Tables I–III. To get a feeling for the behavior of the series and to derive preliminary estimates for critical properties, we examine the ratios $a_n = \bar{x}_n/\bar{x}_{n-1}$ of successive coefficients in the v expansion of $\bar{x}$ and the $n \to \infty$ intercept values extrapolated from successive ratio pairs. These are plotted versus n^{-1} in Figs. 1–3. While the ratios are most regular for the CP, there is in each case some transient superimposed on the linear asymptotic behavior

$$a_n = a\left(1 - \frac{b}{n}\right) \tag{9.1}$$

Table I. Coefficients in v Expansion for $\bar{x}$ and $c_{(|)}$ for the Contact Process

n	$\bar{x}_n$	$c_{(|)}^{(n)}$
1	1	0
2	2	1
3	5	3
4	$14\frac{1}{2}$	$11\frac{1}{2}$
5	46	$38\frac{1}{2}$
6	$154\frac{5}{8}$	$130\frac{1}{8}$
7	540.8359375	453.7109375
8	1946.94824218	1628.23730468
9	7163.09068467	5979.10337999
10	26805.78821403	22352.60670904
11	101690.65953520	84757.87118554
12	390112.71682587	325100.84536907
13	1510616.55538565	1258873.28617338
14	5895971.55468865	4913837.16374249
15	23168987.55131961	19312114.71645609
16	91584008.27053567	76350090.99372987

Table II. Coefficients in v Expansion for $\bar{x}$ and $c_{(||)}$ for the A-Model

n	$\bar{x}_n$	$c_{(||)}^{(n)}$
1	1	0
2	0	0
3	$\frac{3}{2}$	$\frac{3}{2}$
4	$\frac{7}{4}$	$\frac{1}{4}$
5	$4\frac{23}{24}$	$3\frac{5}{24}$
6	$9\frac{253}{432}$	$4\frac{271}{432}$
7	22.78375772	13.19810957
8	51.26263191	28.47887419
9	121.50081143[a]	70.23817952
10	288.96525435	167.46444292
11	699.61608118	410.65082683
12	1710.03808463	1010.42200345
13	4221.27861244	2511.24052781
14	10501.39300128	6280.11438884
15	26308.02818891	15806.63518763
16	66295.22638567	39987.19819676

[a] In ref. 12 this coefficient is incorrectly listed as 125.50... due to a typographical error.

Table III. Coefficients in v Expansion for $\bar{x}$ and $c_{(||)}$ for the N3-Model

n	$\bar{x}_n$	$c_{(||)}^{(n)}$
1	1	0
2	6	3
3	30	18
4	145	115
5	$727\frac{1}{6}$	$672\frac{1}{6}$
6	$3867\frac{23}{27}$	$3845\frac{37}{54}$
7	$21801\frac{1}{6}$	$22229\frac{22}{27}$
8	128549.55956218	131241.44845107
9	782443.14221051	792776.24931499
10	4868622.93831731	4888476.47479335
11	30776908.02315692	30662504.54753078
12	196913527.8192085	195005146.9990770
13	1272052154.464451	1254074932.323790
14	8283459402.101379	8138956748.130198
15	54309508850.35882	53224854413.13061
16	358180553658.0506	350317837908.6155

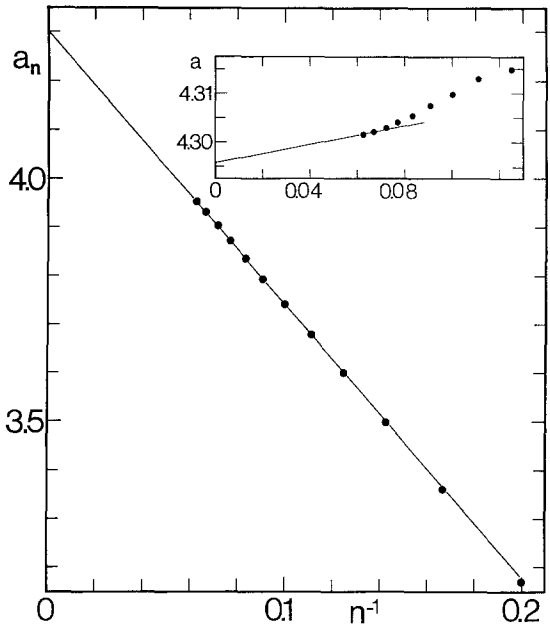


Fig. 1. Ratio plot for the 1d contact process. The inset shows the a values extrapolated from successive ratio pairs.

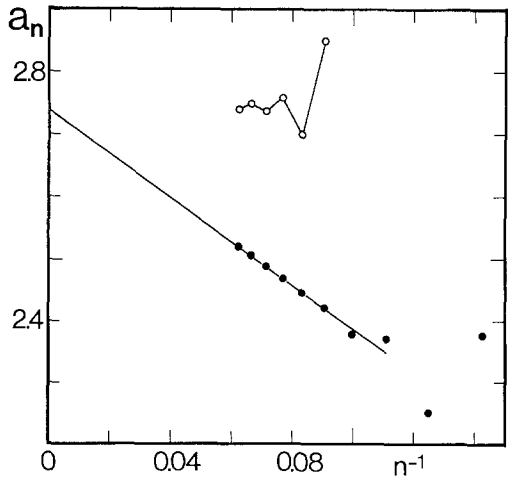


Fig. 2. Ratio plot for the A-model. (●) a_n, (9.1), (○) a values extrapolated from successive ratio pairs.

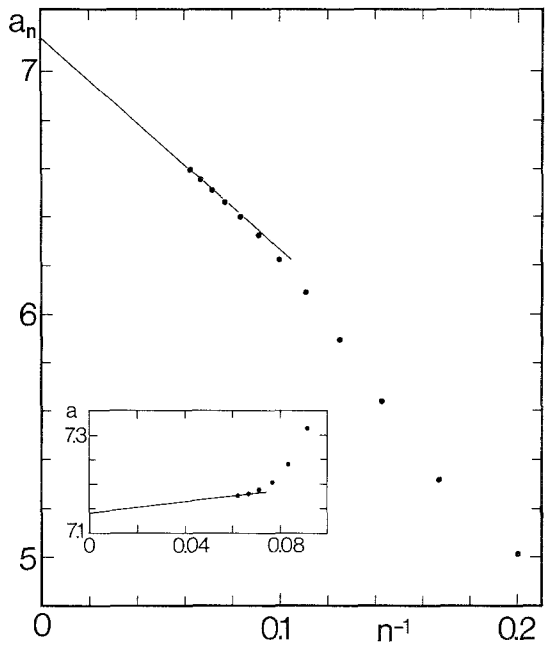


Fig. 3. Ratio plot for the N3-model. The inset shows the a values extrapolated from successive ratio pairs.

Table IV. Critical Parameters for the CP, A, and N3-Models Derived from Padé Approximants to Series for $d/dv \log(1-\hat{x})$

Model	Approximant	$\hat{\lambda}_c$	β
CP	[6, 7]	0.30323	0.2770
	[7, 6]	0.30327	0.2776
	[7, 8]	0.303243	0.2772
	[8, 7]	0.303237	0.2771
A	[6, 7]	0.57410	0.277
	[7, 6]	0.57410	0.276
	[7, 8]	0.57410	0.2765
	[8, 7]	0.57410	0.2765
N3	[6, 7]	0.1621	0.2795
	[7, 6]	0.1621	0.2794
	[7, 8]	0.16213	0.2797
	[8, 7]	0.16208	0.2780

Extrapolating $\lambda_c = (a-1)^{-1}$ and $\beta = b-1$ from the estimates derived from successive ratio pairs, one finds $\lambda_c \cong 0.575$, $\beta \cong 0.28$; $\lambda_c \cong 0.304$, $\beta \cong 0.27$; and $\lambda_c \cong 0.163$, $\beta \cong 0.27$, for the A, CP, and N3-models, respectively.

More precise estimates are obtained from Padé approximants to the series for $d/dv \log(1-\bar{x})$. The resulting values of λ_c and are given in Table IV. Included are two 14th-order series results, as well as the full 16th-order results, in order that the degree of convergence may be judged. The values for λ_c are seen to be quite stable. The β estimates for the three models are also quite close, although the N3 values are slightly higher than the others. It seems very reasonable to conclude that the CP, A, and N3-models belong to the same universality class, i.e., the three-site interaction introduced in (3.16) is irrelevant to critical behavior. Ratio and Padé approximant analyses of the coefficients $c_{(||)}^{(n)}$ and the pair occupancy fraction yield a similar behavior to the $\bar{x}$ series, and indicate that the critical singularity of these quantities is also governed by the exponent β.

Based on the results quoted in Table IV, I propose the value $\beta = 0.277 \pm 0.001$ for the CP/Schlögl model/Reggeon field theory class in one dimension (and, by extension, for directed percolation in $1+1$ dimensions). This result is in good agreement with previous estimates: $\beta = 0.277 \pm 0.002$ from series analysis of generalized susceptibilities in Reggeon field theory,[12] $\beta = 0.273 \pm 0.006$ from Monte Carlo simulations,[20] and, more recently, $\beta = 0.2765 \pm 0.0005$ from series analysis of directed percolation.[28] [These calculations furnish β indirectly, through the exponent relations $\beta = \delta\nu$ for Reggeon field theory, and $\beta = (\nu_{||} + \nu_{\perp} - \gamma)/2$ for directed percolation.[29]]

For the A2-model, only a relatively short series has been derived so far. Because *two* new excited sites may appear at each order in perturbation theory, the eight-order calculation for the A2-model makes CPU time and storage space demands comparable to the 16th-order calculations for the other models. The coefficients for $\bar{x}$ and $c_{(||)}$ in terms of $v = 3\lambda$ are given in Table IV. A glance reveals that the ratios do not follow a regular trend. In fact, analysis of the series for $d/dv \log(1-\bar{x})$ reveals an (unphysical) dominant singularity at $\lambda = -0.131$, whereas simulations[30] indicate $\lambda_c \cong 0.186$. This suggests that we transform to the variable $w = v/(1+v)$. The resulting series has a much more regular behavior; the ratios are plotted in Fig. 4. Extrapolation of the last ratio pair in the w series for $\bar{x}$ yields $\lambda_c = 0.187$, while the last pair in the series for $d/dw \log(1-\bar{x})$ yields $\lambda_c = 0.188$. The present series is too short to permit a precise estimate of λ_c, or any useful estimate of β for the A2-model.

In ref. 13 the Padé approximant for $d/dv \log(1-\bar{x})$ was used to derive predictions for the occupation fraction in very close agreement with Monte Carlo simulation results of the A-model. Figure 5 shows a similar com-

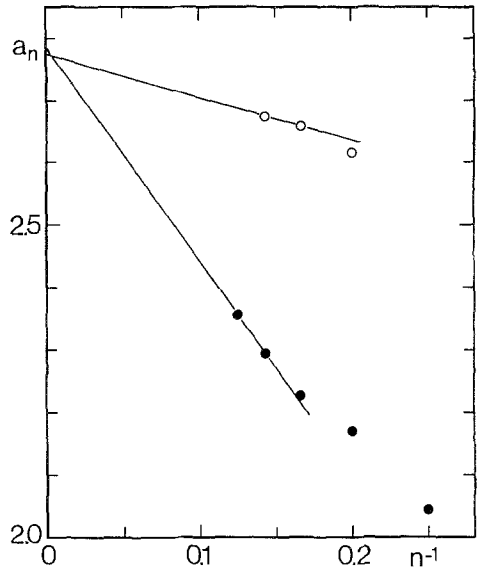


Fig. 4. Ratio plot for the A2-model. (●) a_n, (9.1). (○) Ratios of successive terms in the expansion of $d/dw \log(1-\bar{x})$.

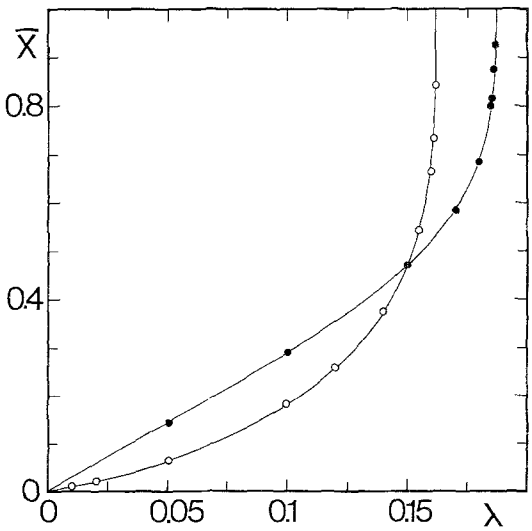


Fig. 5. Occupation fraction $\bar{x}$ versus λ for (●) the A2-model and (○) the N3-model, from Monte Carlo simulations.[30] (—) The series expansion predictions.

Table V. Coefficients in v Expansion for $\bar{x}$ and $c_{(||)}$ for the A2-Model

n	$\bar{x}_n$	$c_{(||)}^{(n)}$
1	1	1/3
2	−1/3	−2/9
3	139/216	25/72
4	0.0654899691	−0.150559416
5	0.5412416811	−0.260070047
6	0.5104784140	0.235710699
7	0.9705235878	−0.248591396
8	1.149277989	−0.012648025

parison between theory and simulation[30] for the N3 and A2-models. In the former case, the prediction for $\bar{x}(\lambda)$ was obtained by integrating the [8, 7] Padé approximant for the logarithmic derivative. For the A2-model $\bar{x}(\lambda)$ was derived using the w series, extended (to $n = 5000$, to ensure convergence), by assuming linear behavior of the ratios a_n for $n \geqslant 9$. The agreement between theory and simulation is excellent.

10. SUMMARY AND DISCUSSION

Using rather straightforward operator and perturbation methods, useful series expansions for nonequilibrium lattice models have been derived. I have illustrated the utility of the method for one-dimensional models with two- and three-site interactions, and with pairwise as well as single-site adsorption. Preliminary results for a diffusive model were also presented. The method is well suited to computer analysis in which the algebra is represented diagrammatically, and should be applicable to a variety of lattice models exhibiting nonequilibrium phase transitions.

The numerical results presented in Section 9 yield a precise β value for the CP/Schlögl-model class in one dimension, and confirm the expectation that the sort of three-body interactions which differentiate the A- and N3-models from the CP are irrelevant to critical behavior. (They also remind one that a rate-equation approach to critical behavior may be quite misleading!)

A natural extension of the present work is to study models with higher-order kinetics, two or more species of particles, and in two or more spatial dimensions. A systematic method for calculating (long-range) correlations would be most valuable, as would a more effective means for studying models with diffusion. A series expansion method for time-dependent behavior also seems to be feasible.

Finally, since sequential interacting particle systems and their corresponding stochastic cellular automata can belong to the same universality class, one may hope that series expansions (applied to sequential IPS) and SCAs (capable of efficient simulation on parallel computers) will together provide a powerful means for studying nonequilibrium critical phenomena.

APPENDIX: STEADY-STATE DISTRIBUTION FOR THE A-MODEL ON A FINITE RING

Consider the A-model on a ring of N sites, with periodic boundary conditions ($\sigma_{N+1} \equiv \sigma_1$). The absorbing state is

$$\begin{aligned} |\Phi\rangle &= \prod_{j=1}^{N} |\phi_{1,j}\rangle \\ &= \prod_{j=1}^{N} [(v-1)\,|\psi_{1,j}\rangle + |\psi_{0,j}\rangle] \\ &= -\sum_{m=0}^{N} (v-1)^m \sum_{\{j_1,\ldots,j_m\}} B_{j_1}^{\dagger} \cdots B_{j_m}^{\dagger}\, |\bar{\Psi}^0\rangle \end{aligned} \tag{A.1}$$

The $m=0$ term is simply $|\bar{\Psi}^0\rangle$. Using (5.2), (5.9), and (5.10), we may write the interaction as

$$V_i = -B_i^{\dagger}(v - B_i)\, A_{i-1}^{\dagger} A_{i-1} A_{i+1}^{\dagger} A_{i+1} \tag{A.2}$$

so that, for a system with periodic boundary conditions,

$$\begin{aligned} V\,|\Phi\rangle &= -\sum_{i} |\psi_{i,1}\rangle \prod_{j(\neq i)} [(v-1)\,|\psi_{1,j}\rangle + |\psi_{0,j}\rangle] \\ &= -\sum_{m=1}^{N} m(v-1)^{m-1} \sum_{\{j_1,\ldots,j_m\}} B_{j_1}^{\dagger} \cdots B_{j_m}^{\dagger}\, |\bar{\Psi}^0\rangle \end{aligned} \tag{A.3}$$

where m denotes the number of excited sites. Using (5.7), one finds that $[S^0]^{-1} V\,|\Phi\rangle$ is given (A.3), with the factor $m(v-1)^{m-1}$ replaced with $(v-1)^m$. Thus, $[S^0]^{-1} V\,|\Phi\rangle = -(|\Phi\rangle - |\bar{\Psi}^0\rangle)$, i.e., we have verified that $(1 + [S^0]^{-1} V)\,|\Phi\rangle = |\bar{\Psi}^0\rangle$ for the A-model on a ring.

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