Cluster Approximation for the Contact Process

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The one-dimensional contact process is analyzed by a cluster approximation. In this approach, the hierarchy of rate equations for the densities of finite length empty intervals are truncated under the assumption that adjacent intervals are not correlated. This assumption yields a first order phase transition from an active state to the adsorbing state. Despite the apparent failure of this approximation in describing the critical behavior, our approach provides an accurate description of the steady state properties for a significant range of desorption rates. Moreover, the resulting critical exponents are closer to the simulation values in comparison with site mean-field theory.

The contact process (CP) is an irreversible lattice model involving nearest neighbor interactions only [1,2]. This model incorporates spontaneous desorption and nearest-neighbor induced adsorption. This stochastic process can be used to mimic epidemic spread as well as catalytic reactions. This model belongs to a general class of nonequilibrium models exhibiting a continuous phase transition. Near the critical point, the system exhibits divergence of spatial and temporal correlations. Such properties, conveniently characterized by critical exponents, can be used to classify different models. The CP belongs to the same universality class as Sclögel's first model [3], Reggeon field theory [4], directed percolation [5], and the ZGB model [6] of catalysis. Field theoretic renormalization group studies [7,8] provide considerable understanding of the critical behavior of the CP. However, the best estimates for the characteristic exponents were found numerically by Monte Carlo simulations [9] and by series expansion analysis [10,11] .

Motivated by the incomplete theoretical understanding, we introduce an approximate approach to the CP. We study the temporal evolution of the density of empty intervals. The corresponding rate equations lead to an infinite hierarchy of equations. By writing the density of pairs of neighboring empty intervals as a product over single interval densities, we obtain a closed set of equations. We use the generating function technique to obtain the steady-state properties of the system. Within this approximation, the system exhibits a discontinuous phase transition from an active state to the empty state. As the system approaches the critical point, the relaxation time, associated with the temporal approach to the final state, diverges. Consequently, at the critical point, an anomalously slow decay towards the final state takes place. We find the corresponding kinetic exponent by scaling techniques, as well as by numeric integration of the rate equations.

We compare the cluster approximation predictions with the results of site mean-field theory and with series analysis of this process. Despite the failure to predict a continuous transition, the cluster approximation provides a good approximation for the final density and the empty interval density for a reasonable range of desorption rates. Moreover, the resulting estimates for the critical exponents are closer to the numeric values in comparison with site mean-field theory. The cluster approach is also applicable to generalizations of the contact process, such as the A model and the N3 model. We verify that the resulting critical behavior of these processes is identical with the contact process. Our approach is advantageous since it can be improved systematically by considering the evolution of higher order empty interval densities.

In the CP, a particle desorbs spontaneously with rate λ. On the other hand, a particle adsorbs at a given site at a rate proportional to the number of neighboring occupied sites. In other words, the adsorption rate at a particular site is given by n_p/n_s, with n_s the total number of neighboring sites and n_p the number of neighboring particles. Since every neighboring particle contributes independently to the adsorption rate, this stochastic process can viewed as an interacting particle system with nearest-neighbor interactions only. The above process possesses an adsorbing "vacuum" state: once the system reaches the empty state, adsorption becomes impossible. In sufficiently high dimensions, neighboring sites are not correlated, and the density follows from $d\rho/dt = \rho(1-\rho) - \lambda\rho$. The adsorption term represents the density of vacant sites that neighbor an occupied site. This site mean-field theory (SMF) gives a steady state concentration equal to $1 - \lambda$. Hence, at $\lambda_c = 1$ this process undergoes a simple continuous transition.

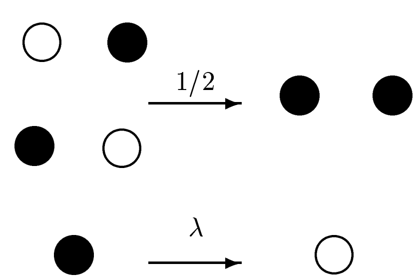

Figure 1. The Contact Process.

We consider the one-dimensional case only (see Figure 1), where studying the density of empty interval has proven useful in adsorption processes [12], as well as in reaction processes [13]. Denote by $E_n(t)$ the probability that a randomly chosen string of n sites is empty (see Figure 1). We emphasize the fact that the actual empty string might be of length larger than n. Let us also consider $R_n(t)$, the probability that a random string of length $n+1$ has n consecutive vacant sites and a particle at the extreme right site. For symmetric processes, such as the CP, $R_n(t)$ also represent the probability of finding an empty string with a particle at the extreme left. These two interval densities are related by

$$R_n = E_n - E_{n+1} \quad \text{or} \quad E_n = 1 - R_0 \cdots - R_{n-1}, \quad (1)$$

for $n \geq 0$. For $n = 0$, the definition of E_n is trivial, leading to the following conditions satisfied by the empty interval densities,

$$E_0 = 1 \qquad \text{or} \qquad \sum_{n=0}^{\infty} R_n = 1. \qquad (2)$$

The condition for R_n is obtained by using Eq. (1) and noting that the sum over E_n reduces to an alternating series. The above interval densities are useful in describing macroscopic properties; for example, the concentration is given by $\rho(t) = R_0(t)$.

$$E_n = \text{Prob}(\underbrace{\circ \cdots \circ}_{n}) \qquad R_n = \text{Prob}(\underbrace{\circ \cdots \circ}_{n}\bullet)$$

Figure 2. Empty interval densities.

We write the rate equations governing $E_n(t)$ by considering the adsorption and the desorption processes separately. Adsorption can contribute only to loss of empty intervals. Empty intervals of length n can be destroyed when a particle is desorbed at the edge of the interval. This occured only where the empty interval has an occupied site at its edge. By taking into account contributions from adsorption at either boundary, we find $dE_n/dt\big|_{\rm ads} = -R_n$. Desorption, on the other hand, leads only to creation of empty intervals. When a particle desorbs, the two empty intervals it borders create a larger empty interval. We define the pair density $E_{l,m}$ as the density of two neighboring empty intervals, with lengths at least equal to l and m, separated by a single particle. Note that from this definition the relation $E_{0,n} = E_{n,0} = R_n$ is satisfied. In terms of this pair density, the increase in the density of empty intervals of length at least n due to desorption is described by $dE_n/dt\big|_{\rm des} = \lambda \sum_{l=0}^{n-1} E_{l,n-1-l}$. We then approximate the pair density, $E_{l,m}$, by the product $E_{l,m} \cong R_l R_m/R_0$, where the factor $1/R_0$ ensures the normalization condition $E_{0,n} = R_n$. Combining contributions from both adsorption and desorption yields the following rate equation for the empty interval density,

$$\frac{dE_n}{dt} = -R_n + \frac{\lambda}{R_0}\sum_{l=0}^{n-1} R_l R_{n-1-l}, \qquad n > 0. \qquad (3)$$

The steady-state properties can be obtained by requiring that the time derivative in Eq. (3) vanishes. We introduce the generating function $R(z) = \sum_n R_n z^n/R_0$, with R_n being the steady-state interval densities. Dividing Eq. (3) by R_0, summing over all n, and solving the resulting quadratic equation yields

$$R(z) = \frac{1-\sqrt{1-4\lambda z}}{2\lambda z}, \qquad \lambda < 1/4. \qquad (4)$$

The normalization condition of Eq. (2) shows that $\rho = R_0 = 1/R(z)\big|_{z=1}$ and, consequently, the concentration is given by

$$\rho = \frac{1+\sqrt{1-4\lambda}}{2}, \qquad \lambda < 1/4. \qquad (5)$$

For $\lambda > \lambda_c = 1/4$ the system indeed exhibits a transition to the absorbing state, where the concentration vanishes. The nature of this transition is discontinuous, while for the actual CP, the transition is continuous. For the CP, the approach to the critical density is an algebraic one,

$$\rho - \rho_c \sim (\lambda_c - \lambda)^{\beta}. \qquad (6)$$

Note that while for a continuous transition to a vacuum state one has $\rho_c = 0$, the critical density of the cluster approximation is finite, $\rho_c = 1/2$. Extensive power series studies suggest $\beta \cong 0.277$, and $\lambda_c \cong 0.3032$ [10,11]. The corresponding values obtained by the cluster approximation, $\beta = 1/2$ and $\lambda_c = 1/4$, are closer than the SMF values $\beta = \lambda_c = 1$. While the critical point depends heavily on the microscopic definition of the process, the critical exponents are universal. Applying the cluster approximation to variants of the CP always yields $\beta = 1/2$.

In Figure 3, we plot the cluster approximation density *vs.* the series study density. For desorption rates $\lesssim 0.2$ both curves are practically identical and, for example, at $\lambda = 0.2$ the relative difference is less than 0.5%. We conclude that despite the failure near the transition point, the cluster approximation is useful in describing the process for a substantial dynamic range. Another way to determine the accuracy of the approximation is by expanding Eq. (5) as a power series in λ^n, and comparing to the coefficients, obtained by the series expansion study [11]. We find that both expansions are identical to the third order,

$$\rho(\lambda) = \begin{cases} 1-\lambda-\lambda^2-2\lambda^3-5\lambda^4+O(\lambda^5) & \text{CA,} \\ 1-\lambda-\lambda^2-2\lambda^3-4\frac{1}{2}\lambda^4+O(\lambda^5) & \text{CP.} \end{cases} \qquad (7)$$

Since R_n is of order λ^n, we expect similar correspondence between the approximate interval density from our rate equations and the actual contact process densities. To test this, we have performed a Monte-Carlo simulation with 10^5 particles at $\lambda = 0.2$. Indeed, the average over 200 different realizations yields values for R_n that agree with the approximate density to within 0.5%, for $n = 0, 1, 2, 3$. The quality of the approximation gradually decreases as n increases and for example for $n = 4$ the discrepancy is 4%.

The interval density also exhibits an interesting critical behavior. By expanding the generating function of Eq. (4), one finds $R_n = \rho\lambda^n (2n)!/n!(n+1)!$ for $\lambda \le \lambda_c$. This expression shows that for $\lambda < \lambda_c$ the interval density depends exponentially on the interval length,

$$R_n \sim n^{-3/2} \exp\Big(-4\Delta n\Big) \qquad \Delta \ll 1, \tag{8}$$

where $\Delta = \lambda_c - \lambda$. The Stirling formula was used to obtain the above form of the interval density. At the critical point, power-law decay is recovered, $R_n \sim n^{-3/2}$.

These static properties are closely related to the kinetics of the system. Far from the critical point, the density rapidly relaxes to its steady-state value from any initial conditions. As the system approaches the critical point, the relaxation time diverges and a power-law decay of the concentration takes place. We thus expect that for sufficiently large times and close enough to the critical point, the temporal approach to the final state is given by the scaling form [10,14]

$$\rho - \rho_c \sim t^{-\delta} \psi\big(\Delta t^{1/\nu}\big). \tag{9}$$

In other words, the critical exponent δ characterizes the critical kinetics, while the exponent ν characterizes the sub-critical relaxation time. The above scaling form should match the steady-state form of Eq. (6) at large times and hence we conclude that $\psi(x) \sim x^\beta$ for $x \gg 1$. To cancel the temporal dependence, the scaling relation $\beta = \delta\nu$ must be satisfied. Furthermore, Eq. (8) indicates that the relaxation length associated with the steady-state interval density diverges as $1/\Delta$ as the system approaches the critical point. Thus, it is natural to assume that $R_n(t)$ depends on time through a rescaled size, $n \to nt^{-\alpha}$, as well as a rescaled adsorption rate. Noting that $R_0 = \rho$, we postulate the following scaling behavior for $R_n(t)$:

$$R_n(t) \sim \phi\Big(\Delta t^{1/\nu}, nt^{-\alpha}\Big). \tag{10}$$

On the other hand, Eq. (8) indicates that the steady-state density depends on the size and the rate only through the variable $n\Delta$. Hence, $\phi(x,y) \sim \tilde{\phi}(xy)$, and by eliminating the temporal dependence we find the scaling relation $\alpha\nu = 1$.

Thus far, our scaling analysis involved matching the anticipated kinetic behavior to the exact steady-state properties. To determine the critical temporal decay, $\rho - \rho_c \sim t^{-\delta}$, we study the rate equations at $\lambda_c = 1/4$. Using the duality relations between E_n and R_n (see Eq. (1)), the rate equations for $\lambda = \lambda_c$ can be rewritten in terms of R_n only,

$$\sum_{l=0}^{n-1} \frac{dR_l}{dt} = \frac{1}{4R_0} \sum_{l=0}^{n-1} R_l R_{n-1-l} - R_n. \tag{11}$$

To analyze this equation by scaling techniques, we match the leading asymptotic terms in both sides of the above equation. The left hand side is governed by n terms of order R_n. Hence, by taking into account the time derivative, we conclude that the left hand side is proportional to nR_n/t. The right hand side is dominated by the first few terms in the expansion, namely $l \ll n$ and $n - l \ll n$. Therefore, we approximate the sum by $2R_n(R_0 + R_1 + \cdots)/R_0 = 2R_n/R_0$, using the normalization condition of Eq. (2). Finally, we write the resulting expression $R_n\,(1 - 1/2R_0(t))$ in terms of the concentration,

$$\frac{n}{t} R_n \propto R_n(\rho - \rho_c). \tag{12}$$

We conclude that $nt^{-1} \sim t^{\alpha-1} \sim t^{-\delta}$, or equivalently $\alpha + \delta = 1$. The three scaling relations yield the following exponents, $\delta = 1/3$, $\nu = 3/2$ and $\alpha = 2/3$. Numerical integration of the rate equation at $\lambda = \lambda_c$ confirms the scaling prediction for δ (see Figure 4). In Table 1, we compare the exponents, that result from our cluster approximation (CA), with the corresponding series expansion and the SMF values. We conclude that the CA exponents provide significant improvement in comparison with those from SMF.

Table 1 Static and Critical decay exponents obtained by series studies (CP), Cluster Approximations (CA) and Site Mean-Field (SMF).

	β	δ	ν
CP	0.277	0.160	1.735
CA	1/2	1/3	3/2
SMF	1	1	1

Recently, several variants of the CP where introduced and it was shown that they belong to the same universality class as the original model. In these models, the adsorption process is modified while the desorption process remains unchanged. The adsorption rate is set to $\theta/2$ if only one neighboring site is occupied, while the rate remains unity in the case when both neighboring sites are occupied. The empty interval method can be easily generalized to this case and we merely quote the resulting subcritical steady state density

$$\rho = \frac{\theta + \sqrt{\theta^2 - 4\lambda(\theta - \eta)}}{2(\theta - \eta)}, \quad \eta = \frac{\lambda(1-\theta)(\theta - 2\lambda)}{\theta^2 + (1-\theta)(\theta - 2\lambda)}. \tag{13}$$

For the basic CP, $\theta = 1$, we recover Eq. (5). Clearly, the discontinuous nature of the transition is independent of the microscopic details of the model and the exponent $\beta = 1/2$ is indeed robust. The critical point, however, depends on θ and can be found by equating the square root in Eq. (13) to zero. If the adsorption rates are independent of the number of neighboring particles, $\theta = 2$, the predicted critical point is $\lambda_c \cong 0.4608$, while series studies yield $\lambda_c \cong 0.574$ for this so-called A model. In the case where $\theta = 1/2$ (the N3 model), the critical point is $\lambda_c = 0.1366$, while series studies yield $\lambda_c = 0.162$. For the general θ case, the cluster approach yields less accurate estimates for the concentration than for basic CP.

In summary, we have presented an approximate approach to the contact process. Based on the assumption that neighboring empty intervals are not correlated, we solved for the steady state properties. In addition, the kinetic approach towards the steady state was found by scaling techniques. The above approximation is valid for a significant subcritical range. The cluster approximation predicts a discontinuous transition but gives improved exponents in comparison with simple site mean-field theory.

The cluster approximation can be systematically improved by considering higher order interval densities. Indeed, our preliminary results indicate that the second order cluster approximation yields a continuous phase transition. Moreover, the approximation appears to be valid over a significantly larger range of desorption rates.

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FIGURE CAPTIONS

Figure 1. The Contact Process.
Figure 2. Empty interval densities.
Figure 3. The cluster approximation density (solid) *vs.* the actual CP density (dashed). The latter density represent the [12,12] Padé approximant obtained from the perturbation study of ref [11].
Figure 4. The critical approach towards the steady-state. Numeric solution to the rate equations (dots) for the case $\lambda = \lambda_c = 1/4$ is plotted. For comparison a line of slope $-1/3$ is also shown (solid).