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LETTER TO THE EDITOR

Time-dependent perturbation theory for diffusive non-equilibrium lattice models

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Abstract. We recently presented a perturbation theory for the asymptotic survival probability of an interacting particle system which can become trapped in an absorbing state. In this letter we extend the method to a simple diffusive model. Analysis of the resulting series shows that diffusion is an irrelevant perturbation, i.e. it does not change the critical behaviour. Quantitative predictions of the phase boundary are confirmed by results of Monte Carlo simulations.

Non-equilibrium phase transitions have been studied intensively in recent years [1, 2]. However, our theoretical understanding is far from complete, and a general unified description has not yet been achieved. Some progress has been achieved via field-theoretic renormalization group methods [3–6], but while these methods are successful in predicting the possible universality classes, they are not very effective in determining critical parameters. It is thus very important to develop new analytic methods which are also efficient calculational tools. We recently presented a time-dependent perturbation theory which yields precise, detailed predictions of the critical behaviour in an interacting particle system exhibiting a non-equilibrium second-order phase transition to an absorbing state [7]. In this paper we extend the method to include the effects of diffusion.

The system considered in this work is a non-equilibrium stochastic lattice model or *interacting particle system* [8, 9] evolving according to a Markov process with local, intrinsically irreversible transition rules. One of the simplest such models is the *contact process* (CP) [10], which was introduced as a model for the spread of an epidemic. The CP is closely related to Schlögl's (first) model [11] of an autocatalytic chemical reaction, to directed percolation [12], and to Reggeon field theory (RFT) [13, 14]. In the CP each site can be either vacant or occupied by a particle, so that the state of the system can be characterized by occupation variables $\{\sigma_i\}$ ($i \in Z^d$, with $\sigma_i = 0,\ 1$ corresponding to site i vacant or occupied, respectively). The evolution of the system is governed by simple local rules: particles are annihilated at rate λ independent of the states of other sites, and vacancies become occupied at rate n/z, where n is the number of *occupied* neighbours and z is the total number

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of neighbours. As there is no spontaneous creation of particles the vacuum is an absorbing state for the Markov process. In addition to this trivial state the CP has (in the infinite-size limit) for sufficiently small λ a non-trivial ('active') steady state, with a non-zero average particle concentration ρ. The CP is known to exhibit a continuous phase transition from the active state to the absorbing state at a critical value λ_c [15]. This kind of phase transition is also found in more complicated models for catalytic surface reactions [16–18]. As in equilibrium the behaviour of the system near λ_c is characterized by various critical exponents, e.g. the steady state concentration of particles (which is the appropriate order parameter) decays asymptotically as $\rho \propto (\lambda_c - \lambda)^\beta$ as $\lambda \to \lambda_c^-$. Steady state series expansions [19] in $d = 1$ yield $\lambda_c \simeq 0.3032$ and $\beta \simeq 0.277$, and time-dependent series expansions [20] yield $\lambda_c \simeq 0.303\,228$ and $\beta \simeq 0.2769$. This places the CP in the same universality class as RFT [13, 14] and directed percolation [21].

In this work we extend the CP to include diffusion of particles. This is simply done by allowing the hopping of particles to empty nearest neighbour sites at rate D. There are many reasons for wanting to develop series expansions for diffusive models: surface diffusion of ad-atoms plays an important role in catalytic reactions. In the epidemic modelling diffusion comes into play as soon as we consider non-sedentary populations. In population models with 3-particle creation and/or annihilation rules, diffusion can lead to a re-entrant phase diagram [22–24], or change the order of the phase transition [25]. We do not expect diffusion to change the critical behaviour of the CP. A coarse-grained description of the non-diffusive CP will in fact already include a diffusive term, i.e. $\propto \nabla^2\rho$. Thus field-theoretic analysis of the diffusive CP [3] predicts RFT behaviour. Even without coarse graining, an effective hopping process is present in the CP, e.g. through the sequence $\bullet\circ \to \bullet\bullet \to \circ\bullet$ ($\bullet$ and $\circ$ denoting occupied and vacant sites, respectively). Our main reason for studying the diffusive CP is to develop time-dependent perturbative expansions in a context in which we know what to expect. We hope that these methods will prove useful in the study of more complicated models in which diffusion plays a more crucial role [22, 23, 25].

Before venturing into a description of the time-dependent perturbation theory we review the scaling behaviour of models exhibiting a continuous transition to an absorbing state. Following Grassberger and de la Torre [14] we consider the asymptotic behaviour of the model, starting at $t = 0$ with a single seed particle at the origin. According to the usual scaling hypothesis, one expects that any function of x, t, and Δ ($\Delta = \lambda_c - \lambda$) depends on these variables only through x^2/t^z and $\Delta \cdot t^{1/\nu}$, times some power of x^2, t, or Δ, where ν and z are new critical exponents. For the probability of survival, i.e. the probability that the system has not entered into the vacuum state at time t, one expects

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

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

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

Since the system is in the supercritical region there must be a non-zero chance of survival; were this not the case any configuration would eventually die out, contrary

to our knowledge that the system has an active steady state in this region. Thus since $P_\infty \equiv \lim_{t\to\infty} P(t)$ is finite, $\lim_{y\to\infty} \psi(y)$ is finite too, and we get

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

However, it can be shown [14] that P_∞ and ρ have the same critical exponent, leading to the scaling relation $\beta = \nu\delta$.

Markov processes in many-particle systems may be conveniently described via an operator formalism [26–28], as demonstrated by the successful application of the formalism to non-equilibrium steady states of interacting particle systems [19], the dynamics of random sequential adsorbtion [29], the asymptotic survival probability [7] and related quantities [20]. In this paper we use the formalism of [7, 19] 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 $|\{\sigma_i\}\rangle = \prod_{i\in Z^d} |\sigma_i\rangle$.

Creation and annihilation operators for site i are defined in the obvious manner $A_i^\dagger|\sigma_i\rangle = (1-\sigma_i)|\sigma_i+1\rangle$ and $A_i|\sigma_i\rangle = \sigma_i|\sigma_i-1\rangle$.

The state of the system at time t is

$$|\Psi(t)\rangle = \sum_{\{\sigma_i\}} p(\{\sigma_i\},t)|\{\sigma_i\}\rangle \tag{4}$$

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

$$\frac{\mathrm{d}|\Psi(t)\rangle}{\mathrm{d}t} = S\,|\Psi(t)\rangle \tag{5}$$

which has the formal solution, given that S is time-independent, $|\Psi(t)\rangle = \mathrm{e}^{St}|\Psi(0)\rangle$, where $|\Psi(0)\rangle$ is the initial probability distribution. The evolution operator S for the diffusive CP in one dimension may be expressed as

$$S = \lambda W + V + D\mathcal{D} \tag{6}$$

where

$$W = \sum_i (1 - A_i^\dagger)A_i \tag{7}$$

$$V = \sum_i (1-A_i)A_i^\dagger\left[1 - \tfrac{1}{2}(A_{i-1}A_{i-1}^\dagger + A_{i+1}A_{i+1}^\dagger)\right] \tag{8}$$

and

$$\mathcal{D} = \sum_i [(1 - A_{i-1}^\dagger A_i)A_{i-1}A_i^\dagger + (1 - A_{i+1}^\dagger A_i)A_{i+1}A_i^\dagger]. \tag{9}$$

In this decomposition W annihilates particles, V creates particles, and $\mathcal{D}$ corresponds to nearest-neighbour hopping of particles. S fulfills the conditions required for a probability interpretation, i.e. it preserves positivity and normalization.

In the following we will give a generalized description of the time-dependent perturbation theory derived in [7] and [20]. Assume that we split up the evolution operator S in two parts U and R, $S = U + \kappa R$; we want to treat R perturbatively. Let $|X_0\rangle$ denote the initial distribution which assigns probability 1 to the configuration with the origin occupied, and all other sites vacant. Consider the Laplace transform of $|\Psi(t)\rangle$:

$$|\tilde{\Psi}(z)\rangle = \int_0^\infty e^{-zt}|\Psi(t)\rangle\,dt = (z - S)^{-1}|\Psi(0)\rangle\,. \tag{10}$$

Assuming that $|\tilde{\Psi}(z)\rangle$ can be expanded in powers of κ:

$$|\tilde{\Psi}(z)\rangle = |\tilde{\Psi}_0\rangle + \kappa|\tilde{\Psi}_1\rangle + \kappa^2|\tilde{\Psi}_2\rangle + \cdots \tag{11}$$

we find upon inserting (11) and the expression for S in (10)

$$|\tilde{\Psi}_0\rangle = (z - U)^{-1}|X_0\rangle \tag{12}$$

and

$$|\tilde{\Psi}_n\rangle = (z - U)^{-1}R|\tilde{\Psi}_{n-1}\rangle \qquad n \geqslant 1\,. \tag{13}$$

Letting (r) denote any configuration we have

$$(z - U)^{-1}(r) = z_q[(r) + (z - U)^{-1}\sum_i C_{r_i'}(r_i')] \tag{14}$$

where $z_q \equiv (z + q)^{-1}$, and q is the sum of the coefficients $C_{r'}$ to the new configurations (r') generated from (r) by the application of U. A premise for the applicability of the method outlined above is that the operators $(z-U)^{-1}$ and R create only finitely many new configurations or that the recursive application of $(z - U)^{-1}$, as expressed in (14), may be truncated in a natural way.

In this work we consider how to extend the method outlined above to diffusive models. As diffusion preserves the number of occupied sites it can never be included in U because there would be no natural way to truncate the recursive application of $(z - U)^{-1}$. In the absence of an exact solution for $(z - V - \mathcal{D})(r)$, we are forced to treat the diffusion operator perturbatively. In this letter we have chosen to look at $R = \lambda[W + \overline{D}\mathcal{D}]$ for a fixed numerical value for $\overline{D}$. Thus we derive a series in powers of λ for each value of $\overline{D}$. From this series we then determine the critical value λ_c which then combined with $\overline{D}$ determines the corresponding value of the diffusion rate, $D_c = \lambda_c\overline{D}$. The major drawback of this method is that diffusion enters at different orders in each term of the expansion, i.e. in an expansion to order n the coefficient of λ^k truncates at D^{n-k}.

We can calculate the *extinction* probability $\tilde{p}(z)$, i.e. the probability of having entered the absorbing state. The λ^j term in the expansion for $\tilde{p}(z)$ is simply the coefficient of $|0\rangle$ in $|\tilde{\Psi}_j\rangle$. As each application of W annihilates at most one particle, it follows from (13) that in a calculation of $\tilde{p}(z)$ to $\mathcal{O}(\lambda^n)$ we can discard (j) for $j > n$ in the expression for $|\tilde{\Psi}_0\rangle$. Similarly, we can ignore all configurations with more than $n - k$ occupied sites in $|\tilde{\Psi}_k\rangle$, as none of these contribute to the extinction probability at this order. The algebra involved in the calculation of $\tilde{p}(z)$ rapidly

Table 1. The critical point λ_c and the critical exponent β for various values of the diffusion rate $\overline{D}$. Figures in parentheses indicate the estimated errors.

$\overline{D}$	λ_c	β	$\overline{D}$	λ_c	β
0.0	0.303 229(1)	0.2769(1)	0.75	0.352 22(2)	0.2773(3)
0.001	0.303 298(8)	0.2765(6)	1.0	0.365 83(2)	0.2775(3)
0.005	0.303 597(6)	0.2767(3)	1.5	0.389 75(5)	0.2775(3)
0.01	0.303 967(5)	0.2767(2)	2.0	0.410 7(1)	0.2812(3)
0.02	0.304 709(3)	0.2768(1)	3.0	0.443 52(4)	0.2806(3)
0.05	0.306 912(1)	0.2768(1)	4.0	0.469 2(4)	0.280(1)
0.1	0.310 534(5)	0.2766(4)	5.0	0.490 4(9)	0.279(5)
0.2	0.317 60(1)	0.2768(1)	6.0	0.509(2)	0.283(9)
0.35	0.327 732(5)	0.2769(2)	7.0	0.524(2)	0.284(9)
0.5	0.337 329(6)	0.2768(2)	10.0	0.558(1)	0.275(5)

Table 2. Examples of the values of the poles and corresponding residues as obtained from the various Padé approximants used in estimating the critical points λ_c and the critical exponents β in table 1.

	$\overline{D}=1$		$\overline{D}=5$		$\overline{D}=10$	
Approximant	λ_c	β	λ_c	β	λ_c	β
[10,10]	0.365 882	0.278 25	0.491 886	0.286 22	0.587 655	0.404 24
[10,11]	0.365 837	0.277 50	0.490 203	0.278 20	0.556 511	0.270 20
[10,12]	0.365 832	0.277 42	0.490 222	0.278 30	0.569 830	0.327 82
[11,10]	0.365 834	0.277 45	0.488 503	0.268 77		
[11,11]	0.365 832	0.277 42	0.490 222	0.278 30	0.569 346	0.325 33
[11,12]	0.365 818	0.277 16	0.490 200	0.278 19	0.559 089	0.279 89
[12,10]	0.365 830	0.277 38	0.491 690	0.286 94	0.581 979	0.385 82
[12,11]	0.365 837	0.277 49	0.490 393	0.279 28		

becomes very complex. The steps used to generate the series are, however, simple enough to be codified as a computer algorithm (see [20] for further details). We have derived the series expansion for $\lim_{z\to 0} z\tilde{p}(z)$ to 24th order in λ (it takes a little more than 20 minutes on an IBM3090).

We have analysed the series for the various values of $\overline{D}$ using Padé approximants to the series for $(\mathrm{d}/\mathrm{d}\lambda)\ln P_\infty$, thus obtaining unbiased estimates for λ_c, the first pole on the positive-λ axis, and β, the residue of the Padé approximant at this pole. Each Padé approximant yields an estimate for λ_c and β. By averaging over several approximants, usually all the approximants $[n,m]$ with $n,m = 10,11$ or 12, we obtain our final estimates. The results of this analysis are summarized in table 1. Our results strongly support the notion of universality, confirming that diffusion does not change the critical behaviour of the CP. In table 2 we have listed the estimates for λ_c and β as obtained from various Padé approximants for three values of $\overline{D}$. The λ_c, β estimates for $\overline{D} = 1$ and 5 are stable, yielding quite accurate final estimates for λ_c and β. However for $\overline{D} = 10$ the estimates from various approximants do not agree very well. In this case we based our final estimate only on the [10,11] and [11,12] approximants, as these yielded β-estimates close to the expected value. For higher values of $\overline{D}$ we could not obtain estimates for the critical parameters. Thus the results for large values of $\overline{D}$ are quite unstable, as reflected in the uncertainties on the estimates for λ_c and β. This is not really surprising considering the approximate

way in which diffusion is treated in this approach. It should also be noted that for small values of $\overline{D}$ the series are very well behaved as all terms are negative and increase in numerical value, whereas for larger values of $\overline{D}$ consecutive terms eventually begin to alternate in sign. In figure 1 we show the phase diagram of the diffusive CP as predicted by the results reported in table 1. Here we clearly see how an increasing diffusion rate leads to an increasing critical annihilation rate. This is what one would intuitively expect as diffusion tends to break up clusters of particles, opening up additional sites for creation and thus making survival easier. We know that for $D \to \infty$, $\lambda_c \to 1$, since mean field theory is correct in the limit $D \to \infty$. The present results seem to be consistent with this limit.

As a check on the accuracy of our results, we performed time-dependent Monte Carlo simulations [5] to determine the critical points of the diffusive contact process for various diffusion rates. Our simulations follow the evolution of the process defined by (8) over many (10^4–10^5) independent realizations, all starting from the same initial state: a single particle at the origin. For details on the simulation procedure, see [23] and [25]. To determine λ_c and some of the critical exponents, we analyse the survival probability, P_t, the mean particle number, n_t, and the mean-square distance of particles from the origin, x_t^2, up to some pre-determined maximum time, t_m. One unit of time corresponds to one attempted update per site, on average. The lattice is taken sufficiently large that particles never reach the boundary during a run. The hallmark of critical behaviour in this sort of process is asymptotic power-law evolution, with P_t, n_t, and $x_t^2 \propto t^{-\delta}, t^{\eta}$, and t^z, respectively. Off-critical evolution is characterized by exponential decay (for $\lambda > \lambda_c$), or saturation (for P_t), or more rapid growth (for n and x^2), when $\lambda < \lambda_c$. By analysing the local slopes of the logarithmic plots [14, 18, 23], we obtain precise exponent values. Our results for the critical point and exponents are summarized in table 3. The simulation results confirm the accuracy of the series expansion predictions, and lend further support to universality, i.e. the exponents are in good agreement with the accepted values for directed percolation in 1+1 dimensions: $\delta = 0.162(4)$, $\eta = 0.308(9)$, and $z = 1.263(8)$ from computer simulations [14] or $\delta = 0.160(3)$, $\eta = 0.317(2)$, and $z = 1.272(7)$ from high-temperature series expansions [13]. The Monte-Carlo simulations typically required 10–30 CPU hours on an IBM3090, for each value of $\overline{D}$. So series expansions are a much more efficient method for determining the phase diagram.

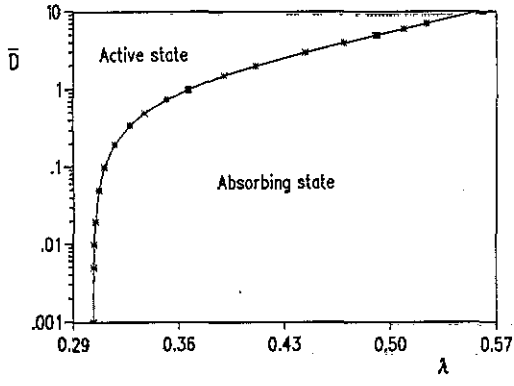

Figure 1. Phase diagram for the diffusive CP. The diffusion rate $\overline{D}$ versus the annihilation rate λ results from series expansions (*) and simulations (■).

Table 3. Results of Monte Carlo simulations of the diffusive contact process. Figures in parentheses indicate uncertainties.

$\overline{D}$	t_m	λ_c	δ	η	z
1	2000	0.3660(1)	0.157(2)	0.315(5)	1.25(2)
5	5000	0.4912(3)	0.155(6)	0.318(4)	1.25(2)
10	5000	0.561(1)	0.15(1)	0.31(1)	1.24(1)

In this work we have presented one method for treating diffusion in time-dependent perturbation expansions for the CP. Our results confirm that diffusion is an irrelevant perturbation of the evolution operator, and thus does not change the critical behaviour of the CP.

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