APPLICATIONS OF THE CAM TO THE STUDY
OF 1D AND 2D NONEQUILIBRIUM MODELS WITH
SINGLE AND MANY ABSORBING STATES

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ABSTRACT

Nonequilibrium lattice models with absorbing states show continuous phase transitions. These models have been studied by various methods such as Monte-Carlo simulations and series expansions. A different method, based on the consideration of increasing order mean-field approximations, was applied before in the study of the 1D model A proposed by Dickman and Burchuk. The critical exponents and the critical parameter are obtained from the application of the Coherent Anomaly Method (CAM). Here, we study the 2D version of this model. Since for these higher dimensional systems the numerical integration of the mean-field master equation is computationally heavy, a mean-field Monte-Carlo algorithm is proposed. The results for the order-parameter critical exponent are compatible with the corresponding estimates for the 2+1 directed percolation (DP) universality class. We also consider a model, the 1D Pair-Contact-Process, which has infinitely many absorbing states. The results for the mean-field approximations and the CAM are compared with available results obtained by Monte-Carlo simulations.

1. Introduction

Lattice models with absorbing states are being intensively studied by different methods such as Monte-Carlo simulations and series expansions. The models are defined by giving transition rates for creation and annihilation of particles at the lattice sites. A continuous phase transition may occur from an active steady state to a non-active state where the order parameter is zero. For models with a unique type of particles and a single absorbing state, it was conjectured that they belong to the DP universality class. This conjecture was later extended to all systems with a scalar order parameter and a single absorbing state thus including the ZGB model. The numerical estimates of dynamic and static critical exponents are compatible with this conjecture.

Most of these studies were made for one-dimensional systems. The 2+1 DP critical exponents are known with less accuracy than the 1+1 ones because of the inherent increase of computational effort needed to study higher dimensional systems. Moreover, the static critical exponents are more difficult to obtain than the time-dependent ones because of the requirement that finite size effects be included. A direct estimate of the order parameter critical exponent of the 2D version of the model A is given in the present work, in agreement with available results for the 2+1 DP universality.
class.

More recently, models with many absorbing states were also studied\textsuperscript{11,12} using the Monte-Carlo method. While the static critical behaviour was seen to fall on the directed percolation universality class\textsuperscript{11,12}, the time-dependent one depend on the particle density at the near-absorbing initial state. A generalised scaling capable of describing this initial configuration dependence was proposed\textsuperscript{18}. As there is still no field theory available to describe the critical behaviour of these systems, it is important to perform studies of different models by distinct methods in order to compare the results and get reliable estimates of the exponents.

Here we consider a method based on mean-field approximations\textsuperscript{2,19,26}. Mean-field approximations neglect correlations present in the system beyond a given range. Consequently mean-field critical exponents are obtained. Before the proposal of the Coherent Anomaly Method\textsuperscript{4,5,8} mean-field approximations were used to get a qualitative picture of the models phase diagram. Considering increasing order approximations the infinite system behaviour is successively better approximated—the mean-field critical parameter gets closer to the true critical parameter and the mean-field critical amplitudes increases. The CAM allows us, then, to obtain the critical parameter and critical exponents of the system by extrapolation to the infinite order of approximation and the measurement of the divergence exponents of the critical amplitudes.

First we define the mean-field approximations in arbitrary spatial dimension. Particular examples in one and two dimensions are also given. The 2D model A is studied by using a suitable mean-field Monte-Carlo algorithm. Results for a one-dimensional model with many absorbing states, the Pair Contact Process, will also be given. In this case the mean-field master equation is numerically integrated. The results are discussed and compared with available ones obtained by Monte-Carlo simulations\textsuperscript{11,12}.

2. Mean-Field Approximations

We consider some infinite lattice \( \Lambda \) where some variables \( \sigma_{\vec{r}} = 0,1 \) can be associated with the presence or absence of particles. The transition rate, \( w(\sigma_{\vec{r}}|\sigma_{\vec{r}'}\Lambda) \) for the process \( \sigma_{\vec{r}} \rightarrow 1 - \sigma_{\vec{r}} \) depends on the state of the sites near to site \( \vec{r} \). Let us denote these sites by \( \Omega_{\vec{r}} \) and \( \sigma_{\Omega_r} \) their state. More general transitions rates could also be considered. A master equation can be written for the probability, \( P(\sigma_{\Lambda},t) \), of a state of the infinite system, \( \sigma_{\Lambda} = \{\sigma_{\vec{r}}, \vec{r} \in \Lambda\} \), at time \( t \). These probabilities are conditional probabilities dependent upon the initial state.

To proceed one defines a finite cluster \( \Omega \) of which examples will be given below. For each site \( \vec{r} \) in \( \Omega \) the set \( \partial\Omega_{\vec{r}} \) includes all sites that are members of \( \Omega_{\vec{r}} \) but not of \( \Omega \). Starting with the infinite system master equation we perform a sum over all the
variables $\sigma_\bar{r}$ such that $\bar{r}$ is not contained in $\Omega$. The resulting master equation reads:

$$\frac{dP(\sigma_\Omega, t)}{dt} = \sum_{\sigma_{\partial\Omega}} \sum_{\bar{r} \in \bar{t}} [P(\sigma_{\Omega \cup \partial\Omega_{\bar{r}}}, t)w(1 - \sigma_{\bar{r}}|\sigma_{\Omega_{\bar{r}}}) - P(\sigma_{\Omega \cup \partial\Omega_{\bar{r}}}, t)w(\sigma_{\bar{r}}|\sigma_{\Omega_{\bar{r}}})]$$ (1)

where $\Omega \cup \partial\Omega_{\bar{r}}$ denotes the union of the two sets and $\sigma_{\Omega \cup \partial\Omega_{\bar{r}}}$ is obtained from $\sigma_{\Omega \cup \partial\Omega_{\bar{r}}}$ by changing $\sigma_{\bar{r}}$ into $1 - \sigma_{\bar{r}}$. For some of the sites $\bar{r}$, $\partial\Omega_{\bar{r}}$ is an empty set which means that all the summations could be performed.

In order to close the master equation one writes $P(\sigma_{\Omega \cup \partial\Omega_{\bar{r}}}, t)$ in terms of $P(\sigma_\Omega, t)$,

$$P(\sigma_{\Omega \cup \partial\Omega_{\bar{r}}}, t) = P(\sigma_\Omega, t)P(\sigma_{\partial\Omega_{\bar{r}}}|\sigma_\Omega, t)$$ (2)

where $P(\sigma_{\partial\Omega_{\bar{r}}}|\sigma_\Omega, t)$ is the conditional probability of $\sigma_{\partial\Omega_{\bar{r}}}$ given $\sigma_\Omega$. The simplest of all approximations consists in neglecting the correlation between all the sites:

$$P(\sigma_{\Omega_{\bar{r}}}|\sigma_\Omega, t) \approx \prod_{\bar{r} \in \partial\Omega_{\bar{r}}} P(\sigma_{\bar{r}}, t)$$ (3)

bringing $P(\sigma_\bar{r}, t)$ self-consistently computed from the state probability of the central site, $\bar{r}$ of the cluster $\Omega$. This is the approximation we are going to use to study the 2D system.

Other approximations can be obtained. For example consider a lattice translation of the cluster $\Omega$ giving $\Omega_{\bar{r}}$. This translation is performed in such a way that all the sites of $\partial\Omega_{\bar{r}}$ are members of $\Omega_{\bar{r}}$. Consider the approximation,

$$P(\sigma_{\Omega_{\bar{r}}}|\sigma_\Omega, t) \approx \frac{P(\sigma_{\Omega_{\bar{r}}|\Omega_{\bar{r}}}, t)}{\sum_{\sigma_{\Omega_{\bar{r}}}} P(\sigma_{\Omega_{\bar{r}}|\Omega_{\bar{r}}}, t)}$$ (4)

where $\Omega_{\bar{r}} \cap (\partial\Omega_{\bar{r}} \cup \Omega)$ denotes the set of sites of $\Omega_{\bar{r}}$ that are also members of $\partial\Omega_{\bar{r}}$ or $\Omega$. The closure of equation (1) is obtained by invoking translation invariance and observing that $\Omega_{\bar{r}}$ and $\Omega$ are just translations of the same cluster. For two and higher dimensional systems the choice of the geometry of the cluster $\Omega$ could be important. In one dimension the above approximation gets quite simple: Choose $\Omega = \Omega^L = \{1, 2, ..., L\}$. Suppose the set $\Omega_{\bar{r}}$ which defines the neighbourhood of the site $\bar{r}$ is given by, $\Omega_{\bar{r}} = \{r - 1, r + 1\}$. Then there are only two non-empty sets $\partial\Omega_{\bar{r}}$: the sets $\partial\Omega_{\bar{1}} = \{0\}$ and $\partial\Omega_{\bar{L}} = \{L + 1\}$. An appropriate translation of $\Omega_{\bar{r}}$ for the case $r = 0$ would be $\Omega_{\bar{r}} = \{0, 1, ..., L - 1\}$ giving the approximation,

$$P(\sigma_0|\sigma_{\Omega_{\bar{r}}}, t) \approx \frac{P(\sigma_{\Omega_{\bar{r}}}, t)}{\sum_{\sigma_0} P(\sigma_{\Omega_{\bar{r}}}, t)}$$ (5)

where $\Omega_{\bar{r}} \cap (\partial\Omega_{\bar{1}} \cup \Omega) = \Omega_{\bar{r}}$ was used. This approximation was previously applied to the study the 1D version of model $A^2$. Appropriate approximations for long-range
systems can be obtained in the same way.

3. The Coherent Anomaly Method and Criticality

The coherent anomaly method (CAM) is based on the assumption that the mean-field approximation gets closer and closer to the infinite system solution as the order of approximation increases. Near criticality the mean-field solution is not expected to reproduce the behaviour of the system as a consequence of the divergence of the correlation length. However, as the order of approximation increases, more and more correlations are properly included, thus shrinking the region where the failure is observed. We denote the order of approximation by \( L \) which is a measure of the size of the cluster used. A complete discussion of the method can be found in the literature.\(^{4,5,6}\)

For the type of models here studied, the mean-field order parameter, \( \bar{\rho} \), can be expanded for \( \lambda < \lambda_c^L \) in powers of \( \lambda - \lambda_c^L \), where \( \lambda \) is the model's parameter and \( \lambda_c^L \) the mean-field critical value,

\[
\bar{\rho} = A_L (\lambda - \lambda_c^L) + \text{higher order terms} \tag{6}
\]

The corresponding mean-field exponent, \( \beta_{MF} \), is equal to one and larger than the infinite system exponent \( \beta \). As the order of approximation gets larger the mean-field critical value is assumed to converge to the infinite system value, \( \lambda_c \):

\[
\lambda_c^L = \lambda_c + aL^{-\omega} + bL^{-\alpha} \tag{7}
\]

where \( \omega \) is the leading exponent of convergence and \( \alpha > \omega \) is the exponent of the first correction term. For the case of the one-dimensional model A studied using the approximation (5) it was found\(^2\) that \( \omega = 1/\nu_L \) and \( \alpha \approx 2 \), being \( \nu_L = 1.101(3) \) the correlation length critical exponent of the 1+1 DP universality class.

The mean-field critical amplitude \( A_L \) shows an anomalous behaviour as \( \lambda_c^L \) approaches \( \lambda_c \),

\[
A_L = a(\lambda_c^L - \lambda_c)^{\beta_{MF}} + b(\lambda_c^L - \lambda_c)^{\beta_{MF} + 1} + \ldots \tag{8}
\]

The work presented here is restricted to the study of the stationary behaviour. However, the time-dependent behaviour can also be studied within CAM\(^{4,19}\).

4. The 2D Model A

The model A is perhaps the simplest model able to show a nonequilibrium continuous phase transition. The transition rates for this model can be written as,

\[
\omega(\sigma_{tr}\mid \sigma_{Otr}) = \lambda(1 - \sigma_{tr}) + \sigma_{tr}(1 - \prod_{r \neq \rho} \sigma_{tr}) \tag{9}
\]

The parameter \( \lambda \) can be interpreted as a rate of deposition of particles. The process of evaporation is independent of the number of neighbours and stops only if all the
Fig. 1. Examples of finite clusters $\Omega^R$ for $R = 3, 5, 7$. The full circles represent the members of $\Omega^R$ and the open circles the members of $\bigcup_{r \in \Omega^R} \partial \Omega_r$.

nearest neighbours of the lattice site $\vec{r}$ are occupied. The order parameter can be defined to be the stationary value of the fraction of vacant sites present in the system.

The finite clusters used to study the system have a circular geometry. These clusters are parametrized by the parameter $R$ and can be defined by,

$$\Omega^R \equiv \Omega^R = \{ \vec{r} \in \mathbb{Z}^2 : |\vec{r}| \leq r(R) \}, \quad r(R) = \frac{R - 1}{2} + 0.01, \quad (10)$$

where $\mathbb{Z}$ represents the set of positive and negative integers. Examples of finite clusters of this type are given in Fig. 1.

The parameter $R$ is an odd integer and measures the size of the clusters.

In order to sample the mean-field master equation discussed in the above section we have used the following Monte Carlo algorithm:

1. $N_s$ samples were initialized to the empty configuration. This fixes the single site initial probability distribution to be $P(0, 0) = 1, P(1, 0) = 0$.

2. The dynamic evolution of each sample is performed according to the transition rules of the model. When a site $\vec{r}$ that corresponds to a non-empty set $\partial \Omega_\vec{r}$ is selected the corresponding averaged transition rate is computed and used to evolve the system.

3. After each update $P(\sigma, t)$ is estimated by looking at the state of the central site in each sample.

This algorithm can be used to study both the time-dependent and the stationary properties of the system. However, to compute the stationary properties we can use a different approach: the probability of having vacant sites can be self-consistently adjusted to be equal (within errors) to the time spent (at stationarity) by the central site of a unique sample in the empty state. This reduces the effort of following the evolution of a large number of samples, $N_s$. 
4.1. Results and discussion

Simulations were performed for $R = 3, 5, 7, 11, 21$ and 31. The results for $\bar{\rho}$ can be seen in Fig. 2. The solid line in the figure is the result of the numerical integration of the master equation that could be performed for $R = 3$. These values were used to compute $\lambda_c^R$ and $A_R$. The linear and the quadratic terms in eq. (6) were included. The results are listed in table 1. The results of the application of the coherent anomaly

<table>
<thead>
<tr>
<th>$R$</th>
<th>$\lambda_c^R$</th>
<th>$A_R$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>3.383</td>
<td>0.154</td>
</tr>
<tr>
<td>5</td>
<td>2.973</td>
<td>0.229</td>
</tr>
<tr>
<td>7</td>
<td>2.702</td>
<td>0.311</td>
</tr>
<tr>
<td>11</td>
<td>2.467</td>
<td>0.442</td>
</tr>
<tr>
<td>15</td>
<td>2.376</td>
<td>0.509</td>
</tr>
<tr>
<td>21</td>
<td>2.294</td>
<td>0.633</td>
</tr>
<tr>
<td>31</td>
<td>2.230</td>
<td>0.794</td>
</tr>
</tbody>
</table>
method are the following: fitting the obtained values of $\lambda_c^R$ to equation (7) (without inclusion of the term $E^{-\rho}$) we have obtained $\lambda_c = 2.13$ and $\omega = 1.14$. The value of $\omega$ is far from the 2+1 DP $1/\nu_1$ value, 1.372. It is not clear if this value of $\omega$ represents its asymptotic value---it would be interesting to consider even larger clusters. The results of fitting $A_R$ to eq. (8) with all the parameters adjustable gave $\lambda_c = 2.12$ and $\beta = 0.57$. The value obtained for $\lambda_c$ is very near the corresponding value obtained from $\lambda_c^R$. An additional fit, where $\lambda_c$ was constrained to be 2.13, gives $\beta = 0.584$. The points $(\lambda_c^R - 2.13)$ vs. $R^{-1}$ and $(\lambda_c^R - 2.13) vs. A_R$ are plotted in Fig. 3. The solid lines are the results of the fits.

There are, to our knowledge, no previous results for the critical properties of this model. However, a cellular automata version was previously studied23. For this version the value of $\lambda_c$ reported was 2.95(1) which is larger than the value here obtained. The discrepancy could be explained by the different types of updating considered, although in 1D both updateings give the same critical parameter23.

Several determinations of the exponent $\beta$ for the 2+1 DP universality class are reported in the literature. For some of them the estimates are indirect: $\beta = 0.598 \pm 0.017, 0.592 \pm 0.013$. One direct estimate recently published gives $\beta = 0.578 \pm 0.018$. It was reported for the 2D model A cellular automata an exponent $\beta = 0.52(1)$ different than expected for the 2+1 DP universality class. However, the same authors have found in one dimension DP critical behaviour. Our estimate is, $\beta = 0.584 \pm 0.01$, consistent with the DP estimates given above. Considering the modest sizes studied, an improvement of the error bound can be easily achieved. The proposed method to obtain $\beta$ is seen to be competitive with others mentioned in the literature.

5. The 1D Pair Contact Process

The 1D Pair Contact Process (PCP) is defined by the transition rates shown in table 2. A pair of nearest neighbour particles may annihilate, leaving two empty sites.

Table 2. Transition rates of different processes for the Pair Contact Process (PCP).11 Occupied and vacant sites are denoted respectively by $\bullet$ and $\circ$. The symbol $\times$ represents an arbitrary state. Left-right symmetry is understood.

<table>
<thead>
<tr>
<th>Processes</th>
<th>Rates</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\times \bullet \bullet \times \rightarrow \times \circ \circ \times$</td>
<td>$p$</td>
</tr>
<tr>
<td>$\bullet \bullet \circ \circ \times \rightarrow \bullet \bullet \circ \times$</td>
<td>$(1-p)/2$</td>
</tr>
<tr>
<td>$\bullet \bullet \circ \times \circ \rightarrow \bullet \bullet \times \circ$</td>
<td>$(1-p)/2$</td>
</tr>
<tr>
<td>$\bullet \bullet \circ \bullet \circ \rightarrow \bullet \bullet \bullet$</td>
<td>$(1-p)$</td>
</tr>
</tbody>
</table>

A pair of particles induces the creation of particles at neighbouring sites. The order
parameter is the fraction of pairs of nearest-neighbour sites occupied by particles. The infinite number of configurations where the order parameter vanishes are absorbing states of the system.

Since annihilation occurs at pairs of occupied sites the master equation (1) should be generalised. However, the approximations required can be cast in the same general form as given in equation (4). Thus, the approximation used here is the natural extension of the approximation previously used to study model $A^2$. For example we take,

$$ P(\sigma_{-1}, \sigma_0 | \sigma_{\Omega}, t) \approx \frac{P(\sigma_{\Omega^T}, t)}{\sum_{\sigma_{-1}, \sigma_0} P(\sigma_{\Omega^T}, t)} $$

(11)

where, $\Omega^L = \{1, ..., L\}$ as before and $\Omega^T_1 = \{-1, 0, ..., L - 2\}$.

5.1. Results and discussion

The results obtained from the numerical integration of the mean-field master equation are listed in table 3. The computer code was carefully checked against possible errors, by comparing with the analytic solution for $L = 3$. The equations
for $L = 5$ automatically generated by the computer program were also checked and found to be correct.

Table 3. Results of $p_c^L$ and $A_L$ for the Pair Contact Process

<table>
<thead>
<tr>
<th>$L$</th>
<th>$p_c^L$</th>
<th>$A_L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.138663560</td>
<td>10.6295</td>
</tr>
<tr>
<td>4</td>
<td>0.118449649</td>
<td>10.0616</td>
</tr>
<tr>
<td>5</td>
<td>0.118001564</td>
<td>1.2442</td>
</tr>
<tr>
<td>6</td>
<td>0.102561921</td>
<td>19.9687</td>
</tr>
<tr>
<td>7</td>
<td>0.100589599</td>
<td>18.4156</td>
</tr>
<tr>
<td>8</td>
<td>0.096934568</td>
<td>18.2163</td>
</tr>
<tr>
<td>9</td>
<td>0.093855591</td>
<td>31.8992</td>
</tr>
<tr>
<td>10</td>
<td>0.092141270</td>
<td>34.2092</td>
</tr>
<tr>
<td>11</td>
<td>0.090464422</td>
<td>40.0743</td>
</tr>
<tr>
<td>12</td>
<td>0.089204945</td>
<td>44.8147</td>
</tr>
<tr>
<td>13</td>
<td>0.088167499</td>
<td>49.1127</td>
</tr>
<tr>
<td>14</td>
<td>0.087281006</td>
<td>53.3687</td>
</tr>
</tbody>
</table>

For $L \leq 8$, the expected systematic increase of $A_L$ with $L$ is not seen. This must be attributed to limitations of the approximation itself.

We have obtained $p_c$ by fitting the results for $p_c^L$ to the equation $p_c^L = p_c + cL^{-\omega}$. The results for $L \geq 10$ are listed in Table 4—for smaller values of $L$ the values of $p_c^L$ could not be adjusted to this equation.

Table 4. Estimates of $p_c$ and $\omega$ for the PCF model including data points in the interval $[L_1, L_2]$

<table>
<thead>
<tr>
<th>$[L_1, L_2]$</th>
<th>$p_c$</th>
<th>$\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[10, 12]</td>
<td>0.0830</td>
<td>2.137</td>
</tr>
<tr>
<td>[11, 13]</td>
<td>0.0789</td>
<td>1.321</td>
</tr>
<tr>
<td>[13, 14]</td>
<td>0.0762</td>
<td>1.040</td>
</tr>
</tbody>
</table>

The values of $p_c$ obtained should be compared with the value obtained by Monte-Carlo simulation. The $p_c = 0.0771(1)$. For the largest values of $L$, the $p_c$ value obtained is smaller than 0.0771 which is not compatible with convergence to this value. Fits performed by separately including even and odd values of $L$, do not improve the
estimates. We have also tried to include a correction term, \( L^{-\omega} \) without success. The obtained values of \( \omega \) are consistent with convergence to the value \( 1/\nu_L = 0.903 \), corresponding to DP in 1+1 dimensions, being however far from this value. An additional fit where \( p_c \) was constrained to be 0.0771 was performed. For the largest sizes studied (\( L=13,14 \)) we have obtained \( a = 0.1954 \) and \( \omega = 1.119 \).

In order to obtain the exponent \( \beta \) we have fitted the values of \( A_L \) to equation (8). Using the value \( p_c = 0.0771 \) we have obtained \( \beta = 0.238 \) including data points in the interval [12,14]. Inclusion of higher order terms was again not possible. The value obtained is still far from the known 1+1 DP value\(^{24} \) 0.2769(2). In the Fig. 4 we plot \( L^{-1} \) and \( A_L \) vs \( p_c^L - p_c \) using for \( p_c \) the value 0.0771. The solid lines are the results of fits. The erratic behaviour of \( A_L \) and \( p_c^L \) for the smaller values of \( L \) is clearly seen.

![Graph showing L^{-1} vs. A_L and p_c^L - p_c](image)

**Fig. 4.** Plot of \( L^{-1} (\triangledown) \) and \( A_L (\bigcirc) \) vs. \( p_c^L - p_c \) taking \( p_c = 0.0771 \). The solid lines are the fits: \( (a=0.1954, \omega = 1.119) \) and \( (\beta = 0.238, a=1.9825, b=33.386) \).

6. Conclusion

We have presented a general class of mean-field approximations. A particularly simple one was applied to a 2D model. The corresponding mean-field master equation was sampled using the Monte-Carlo method. The value obtained for the exponent \( \beta \) was seen to be compatible with the corresponding value of the directed percolation universality class. The method proposed can be used to improve the available error
bounds for this exponent in 2D.

The results of the application to the 1D, Pair Contact Process gave poor results when compared with others previously obtained for the 1D model $A^2$. This may be explained by the bigger range of interaction present in the PCP model — the largest cluster size studied ($L = 14$) is too small to obtain the asymptotic convergence properties. Other approximations, combined with the Monte-Carlo method are under consideration.

7. Acknowledgements

It is a pleasure to thank Dr. M C Marques, Dr. J C Lopes and Dr. T P Gasche for their critical reading of an earlier version of this manuscript.

8. References

22. N. Ito e M. Suzuki, *Computer Simulation Studies in Condensed Matter*