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LETTER TO THE EDITOR

Mean-field approximation with coherent anomaly method for a non-equilibrium model

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Abstract. A mean-field approximation for a 1D non-equilibrium lattice model, known as model A [1], is considered allowing us to compute the probability of a configuration of a given cluster of sites. The mean-field equations are numerically solved in the stationary regime for different cluster sizes L ($\leqslant 15$). From a finite-size analysis and the application of the coherent anomaly method (CAM) [2] we compute the critical parameter of the model, the correlation length critical exponent $\nu_{\perp}$ and the order parameter critical exponent β; the results are in agreement with those obtained by other methods.

In this letter we consider a 1D non-equilibrium lattice model, known as model A; although being a simple model it still exhibits a continuous non-equilibrium phase transition. The model was proposed as a simplification of the ZGB (Ziff, Gulari and Barshad) model [3], preserving, however, some of its important physical features [1]. Single-component models of this type with a unique absorbing state are expected to be in the universality class of Reggeon field theory [4,5] as is also the case for directed percolation [6]. Quite extensive studies of this model have been done using both the Monte Carlo method [1] and the series expansion technique [1,7,8] leading to precise estimates of the critical exponents and the critical parameter. We use here yet a different approach, based on a combination of the mean-field type approximation and the coherent anomaly method (CAM) [2]. Mean-field approximations have been applied before to non-equilibrium lattice models [1,5,9] giving a semi-quantitative picture of the phase diagram. However, as they ignore long-range correlations present at continuous phase transitions they yield the usual mean-field critical exponents. The CAM furnishes a way to obtain the correct critical exponents and entails considering successive approximations, each including more correlations than the previous one. Such a method was successfully applied to various equilibrium models [2, 10–12]. Our main goal here is to see how it works when applied to a 1D non-equilibrium lattice model. In a nutshell our strategy can be summarized as follows. We consider a succession of clusters of increasing size L. The fact that the local dynamics depends only on the state of neighbouring sites allows us to consider the dynamics of a given cluster exactly except that the behaviour of the two boundary sites is included in an approximate way. The critical exponents obtained have mean-field value; the critical parameter and the critical amplitudes depend, however, upon the size L of the cluster.

We then apply the CAM to extract, in a consistent way, the true critical exponents and the critical parameter from a succession of L-dependent parameters. The system of mean-field equations which we use has been described before [13] and a preliminary version of the results of applying CAM to this model has already been given [14]. Recently, a series of general cluster approximations was proposed [15]. It turns out that our mean-field approximation is a special case of these cluster approximations.

Consider a 1D array of sites where particles are deposited at the rate λ with the proviso that the site where deposition occurs is found vacant. A particle leaves its site i with rate 1 if one or both of its neighbouring sites are empty. We can assign an Ising-type variable σ_i to each lattice site such that, if a particle is present, the variable takes value 1 and is zero otherwise. With this notation the transition rates for deposition and evaporation at a specified site i can be written as

$$w_d(\sigma_i) = \lambda(1 - \sigma_i)$$
$$w_e(\sigma_{i-1}, \sigma_i, \sigma_{i+1}) = \sigma_i(1 - \sigma_{i-1}\sigma_{i+1}). \tag{1}$$

The order parameter of the transition is the fraction of vacant sites, ρ, and it becomes zero above the critical parameter value λ_c. We, therefore, expect, for $\lambda \leqslant \lambda_c$,

$$\rho \sim (\lambda_c - \lambda)^\beta. \tag{2}$$

The known best estimates of these parameters, λ_c and β, are given by a series expansion [8] and the values obtained are $\lambda_c = 0.574\,141(2)$ and $\beta = 0.276\,74(2)$. Other quantities associated with other exponents can also be studied but they are not used here. For a discussion of the present best estimates of some of these exponents, see [16].

We can write down the master equation for the time evolution of the probability of a configuration of an L-site cluster $P_L(\sigma_1, \ldots, \sigma_i, \ldots \sigma_L, t)$ in terms of probabilities $P_{L+2}(\sigma_0, \ldots, \sigma_i, \ldots \sigma_{L+1}, t)$ of the configurations of higher order, $(L+2)$, cluster. It should be noted that all the probabilities are conditional probabilities dependent upon the initial configuration. The equation is

$$\frac{d}{dt} P_L(\sigma_1, \ldots, \sigma_L, t)$$
$$= \sum{}' [(w_d(1 - \sigma_k) + w_e(\sigma_{k-1}, 1 - \sigma_k, \sigma_{k+1}))$$
$$\times P_{L+2}(\sigma_0, \ldots, 1 - \sigma_k, \ldots \sigma_{L+1}, t) - (w_d(\sigma_k) + w_e(\sigma_{k-1}, \sigma_k, \sigma_{k+1}))$$
$$\times P_{L+2}(\sigma_0, \ldots, \sigma_k, \ldots \sigma_{L+1}, t)] \tag{3}$$

where the summation $\sum'$ denotes summation over the variables σ_0, σ_{L+1}, and the site index k ($1 \leqslant k \leqslant L$). In order to obtain an equation that contains only the probabilities of configurations of L sites we make the following approximation:

$$P_{L+1}(\sigma_0, \ldots, \sigma_L, t) = \frac{P_L(\sigma_1, \ldots, \sigma_L, t) P_L(\sigma_0, \ldots, \sigma_{L-1}, t)}{P_L(\sigma_0, \ldots, \sigma_{L-1}, t) + P_L(1 - \sigma_0, \ldots \sigma_{L-1}, t)}. \tag{4}$$

With this approximation the set of equations (3) can be reduced to a closed set of nonlinear coupled equations. The solution can be obtained algebraically for

small clusters and numerically for bigger clusters. The solution gives both the time-dependent and the stationary behaviour. From the solutions of increasingly large cluster sizes we construct a series of approximations in the CAM spirit. It should be noted that in the mean-field approximation even finite clusters have true critical behaviour in the sense that the order parameter is zero above a certain critical value λ_c^L, which, however, depends upon the cluster size L. This parameter is expected to approach the true λ_c with increasing L in a manner typical of finite systems [17]:

$$\lambda_c^L = \lambda_c + a L^{-1/\nu_\perp} \tag{5}$$

$\nu_\perp$ being the critical exponent of the correlation length. The order parameter ρ_L vanishes at λ_c^L as

$$\rho_L(\lambda) \sim A_L (\lambda_c^L - \lambda)^{\beta_{mf}} \tag{6}$$

where β_{mf} is the mean-field exponent. The central assumption of CAM is that the true critical behaviour $\rho(\lambda)$ is the envelope function of the family of $\rho_L(\lambda)$ curves. It is then concluded [2, 11] that the amplitude A_L should increase with the cluster size L with a given exponent. This exponent is, however, related to the mean-field and the true exponent in the following manner:

$$A_L \sim (\lambda_c^L - \lambda_c)^{(\beta - \beta_{mf})} \tag{7a}$$

$$A_L \sim L^{(\beta_{mf} - \beta)/\nu_\perp}. \tag{7b}$$

The value of β_{mf} can be seen to be unity by solving the equations in the stationary regime for small clusters (up to $L = 4$, in our case) exactly. The order parameter ρ_L is, in general, a quotient of two polynomials which can be expanded in power series around λ_c^L. Equations (7a) and (7b) can be used to obtain the exponent β either by considering A_L as a function of L or as a function of $(\lambda_c^L - \lambda)$. Sometimes it is necessary to include first-order corrections [11, 12] to the A_L behaviour, not included in (7). Such corrections will modify (7) to

$$A_L \sim a(\lambda_c^L - \lambda_c)^{\beta - \beta_{mf}} + b(\lambda_c^L - \lambda_c)^{\beta - \beta_{mf}+1} \tag{8a}$$

$$A_L \sim a L^{(\beta_{mf} - \beta)/\nu_\perp} + b L^{(\beta_{mf} - \beta - 1)/\nu_\perp}. \tag{8b}$$

The method we have used to obtain λ_c^L and A_L numerically is the following. First we approximately locate the critical point. For this we numerically solve the equations for several λ values. For each value of λ, the time integration is stopped when the order parameter does not change by more than 10^{-10} in a single step. Near the critical point, the λ values scanned were chosen to differ from each other by 5×10^{-5}. The first estimate of λ_c^L and A_L is then obtained, following equation (6), by linear extrapolation from pairs of (λ, ρ) values. As we have mentioned before, the second- (and higher) order powers of $(\lambda_c^L - \lambda)$ are important when we are not extremely close to the critical point. Therefore the first estimates of λ_c^L and A_L were improved by taking into account the second-order term; the final estimates are listed in table 1. The estimated error in λ_c^L and A_L are, respectively, 2×10^{-6} and 10^{-3}. Comparison with the exact solution for small clusters shows that the λ_c^L values tend, systematically, to be slightly overestimated and the A_L values slightly

underestimated. This is due to the approximation involved in the criterion used to check that the stationary regime has been reached. The critical parameter value could, in principle, be obtained using equation (5). However, since we have corrections that show up as an additional term of the form bL^{-x} on the right-hand side, we have to be careful. In order to obtain λ_c we have used equation (5) including such a correction term. Here, to start with we have used the $\nu_\perp$ value obtained in [18], i.e. $\nu_\perp = 1.101(3)$. From the data corresponding to four successive cluster sizes we obtain the parameters, as shown in the first three columns of table 2. As can be seen the λ_c values obtained are slightly lower than those obtained in [8]. The exponent x was found to be near 2, as is also observed in other finite systems [19, 20]. Better results are obtained using a constant value of x ($= 2$), thus reducing the number of free parameters. Therefore, starting with either a fixed value of $\nu_\perp$ ($\nu_\perp = 1.101$) or a fixed value of λ_c ($\lambda_c = 0.574\,141$) we obtain, respectively, λ_c and $\nu_\perp$. The results are shown in the last three columns of table 2 and they are in very good agreement with the previous estimates [8, 18]. An independent determination of both λ_c and $\nu_\perp$, however, requires better precision for the data listed in table 1.

Table 1. The parameters λ_c^L and A_L as obtained for different cluster sizes.

L	λ_c^L	A_L
1	2	0.5
2	1	2
3	$\sqrt{2/3}$	3
4	0.740 686 2...	4.081...
5	0.700 943 5	5.097
6	0.676 598 1	6.053
7	0.660 194 3	6.953
8	0.648 403 1	7.808
9	0.639 520 6	8.624
10	0.632 587 7	9.406
11	0.627 024 2	10.159
12	0.622 459 4	10.883
13	0.618 644 7	11.587
14	0.615 408 2	12.270
15	0.612 626 9	12.933

The determination of the exponent β could, in principle, be done using equations (7a) and (7b). For this we have to use previous estimates of λ_c and $\nu_\perp$, respectively. The results are shown in the second and third columns of table 3 where each β estimate follows from a pair of A_L data points. These estimates increase with cluster size, approaching the expected value, although here they are seen not to converge. The results for the exponent, however, can be considerably improved by including the corrections to the leading behaviour as shown in equations (8a) and (8b). The results of implementing this procedure are shown in the last two columns of table 3. We have made, here, a series of least-squares fits each including sets of six data points corresponding to successively larger clusters. We verified that including a lower number of data points in each fit results in fluctuating estimates of the exponent for large clusters. These fluctuations are already seen in our six data point fits, reflecting the uncertainty in the determination of the exponent. We believe this to be a consequence of not having sufficient precision in the determination of

Table 2. In the second and third columns we list the λ_c and x estimates as obtained by using equation (5) with a correction term bL^{-x}. Here we have used a constant value for $\nu_\perp$ ($= 1.101$). Starting with a constant value for x ($= 2$) we have also used the same equation to obtain λ_c and $\nu_\perp$. When determining λ_c we use $\nu_\perp = 1.101$ and when determining $\nu_\perp$ we use $\lambda_c = 0.574\,141$ [8, 18]. Corresponding results are listed in the last two columns. The columns under the label $[L_1, L_2]$ indicate the set of points used for the corresponding parameter estimation.

x variable			$x = 2$		
$[L_1, L_2]$	λ_c	x	$[L_1, L_2]$	λ_c	$\nu_\perp$
[4,7]	0.573 00	2.16	[5,7]	0.575 09	1.125
[5,8]	0.573 67	2.11	[6,8]	0.574 69	1.117
[6,9]	0.573 81	2.09	[7,9]	0.574 48	1.112
[7,10]	0.573 88	2.08	[8,10]	0.574 35	1.109
[8,11]	0.573 89	2.08	[9,11]	0.574 26	1.106
[9,12]	0.574 01	2.05	[10,12]	0.574 21	1.104
[10,13]	0.573 81	2.11	[11,13]	0.574 15	1.101
[11,14]	0.574 00	2.05	[12,14]	0.574 12	1.100
[12,15]	0.574 15	1.99	[13,15]	0.574 13	1.100

Table 3. The exponent β as obtained using equations (7a), (7b), (8a) and (8b). Whenever needed we have used the best known estimates of the parameters λ_c and $\nu_\perp$ [8, 18]. As in table 2 the columns labelled $[L_1, L_2]$ list the data point intervals used for a given exponent determination.

$[L_1, L_2]$	β (7.1)	β (7.2)	$[L_1, L_2]$	β (8.1)	β (8.2)
[6,7]	0.2051	0.0094	[2,7]	0.1499	0.2201
[7,8]	0.2134	0.0442	[3,8]	0.2284	0.2442
[8,9]	0.2194	0.0704	[4,9]	0.2481	0.2571
[9,10]	0.2258	0.0931	[5,10]	0.2593	0.2617
[10,11]	0.2309	0.1113	[6,11]	0.2646	0.2684
[11,12]	0.2366	0.1279	[7,12]	0.2724	0.2779
[12,13]	0.2381	0.1381	[8,13]	0.2762	0.2766
[13,14]	0.2415	0.1491	[9,14]	0.2752	0.2732
[14,15]	0.2458	0.1602	[10,15]	0.2771	0.2773

A_L and λ_c^L. The results are, however, consistent with the precise estimate given in [8].

In conclusion, we have developed a numerical algorithm that enables us to obtain the solution of the problem using the mean-field approximation for reasonably large clusters. From a finite-size relation, equation (5), we have computed the critical parameter λ_c and the exponent $\nu_\perp$, and the results are in agreement with previous estimates. We have verified that a correction term should be included corresponding to an exponent x (≈ 2). The application of CAM furnishes us estimates of the order parameter exponent β, which are also in agreement with the results obtained with other methods. As we have access to the time-dependent solution of the mean-field equations, we can obtain other (dynamic) exponents.

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