Phase transition of the one-dimensional coagulation-production process

Géza Ódor

Research Institute for Technical Physics and Materials Science,
H-1525 Budapest, P.O.Box 49, Hungary

Recently an exact solution has been found for the 1d coagulation production process: \( 2A \rightarrow A \), \( AO \rightarrow 3A \) with equal diffusion and coagulation rates. This model evolves into the inactive phase independently of the production rate with \( t^{-1/2} \) density decay law. Here I show that cluster mean-field approximations and Monte Carlo simulations predict a continuous phase transition for higher diffusion/coagulation rates as considered in [1]. Numerical evidence is given that the phase transition universality agrees with that of the annihilation-fission model with low diffusions.

One-dimensional, non-equilibrium phase transitions have been found to belong to a few universality classes, the most robust of them is the directed percolation (DP) class \[2,3\]. According to the hypothesis of \[2,3\] all continuous phase transitions to a single absorbing state in homogeneous systems with short ranged interactions belong to this class provided there is no additional symmetry and quenched randomness present.

Recent studies on the annihilation fission (AF or PCPD) process \( 2A \rightarrow O, 2A \rightarrow 3A \) \[4,5\] found evidence that there is a phase transition in this model that does not belong to any known universality classes. This model without the diffusion of single particles was introduced originally by \[6\]. The renormalization group analysis of the corresponding bosonic field theory was given by \[7\]. This study predicted a non-DP class transition, but it could not tell to which universality class this transition really belongs. An explanation based on symmetry arguments are still missing but numerical simulations suggest \[7]\) that the behavior of this system can be well described (at least for strong diffusion) by coupled sub-systems: single particles performing annihilating random walk coupled to pairs \( (B) \) following DP process: \( B \rightarrow 2B, B \rightarrow O \). The system has two non-symmetric absorbing states: one is completely empty, in the other a single particle walks randomly. Owing to this fluctuating absorbing state this model does not oppose the conditions of the DP hypothesis. Some exponents are close to those of the PC class \[8\] but the order parameter exponent \( (\beta) \) has been found to be very far away from both of the DP and PC class values \[9\]. In fact this system does not exhibit neither a \( Z_2 \) symmetry nor a parity conservation that appear in models with PC class transition. It is conjectured \[9\] that this kind of phase transition appears in models where (i) solitary particles diffuse, (ii) particle creation requires two particles and (iii) particle removal requires at least two particles to meet.

In this paper the following one-dimensional coagulation production processes will be investigated:

a) Spatially symmetric coagulation production processes:

\[
AOA \xrightarrow{f} 3A, \quad (1)
\]
\[
2A \xrightarrow{c/2} AO, \quad 2A \xrightarrow{c/2} OA, \quad (2)
\]
\[
AO \xrightarrow{d} OA \quad (3)
\]

b) Spatially asymmetric coagulation production processes:

\[
AAO \xrightarrow{f/2} 3A, \quad OAA \xrightarrow{f/2} 3A, \quad (4)
\]
\[
2A \xrightarrow{c/2} AO, \quad 2A \xrightarrow{c/2} OA, \quad (5)
\]
\[
AO \xrightarrow{d} OA \quad (6)
\]

Both versions fulfill conditions (i-iii) but Henkel et al. \[10\] show that for \( d = c \) the symmetric version always evolve into the inactive state with \( \rho \propto t^{-0.5} \) scaling law. They argue that the asymmetric version displays a non-equilibrium phase transition. The difference is said to be similar to the hard-core effects observed in one-dimensional models \[11,14\]. Hard-core particle exclusion effects can really change both the dynamic \[12,14\] and static \[12,15\] behavior of one dimensional systems by introducing blockades into the particle dynamics but in this work I argue that not this kind of hard-core effects responsible for the lack of phase transition.

One can quickly check by simulations that for \( d \leq c \) the density in the asymmetric version decays in much the same way – with \( \rho \propto t^{-0.5} \) scaling law – as in case of the symmetric version. Furthermore I shall show that if the coagulation rate is smaller than the diffusion rate particles can escape before removal an active phase will emerge with a continuous phase transition belonging to same class that was found in the AF model for weak diffusion. Therefore both version exhibit qualitatively the same phase diagram.

To prove this first I shall apply cluster mean-field approximations (GMF) \[13,18\], which can predict phase diagrams qualitatively well. The mean-field equation for the steady state of both version is

\[
0 = f(1 - p_A)p_A^2 - \rho p_A^2 \quad (7)
\]
where \( p_A \) is the probability of \( A \)-s at a given site. Note that the diffusion rate \( d \) does not play a role in this approximation. By introducing the parametrization \( c = p(1 - d) \), \( f = (1 - p)(1 - d) \) – that is similar to that of the PCPD model – this has the solution:

\[
\rho = p_A = \frac{2p - 1}{p - 1}
\]  

(8)

for \( p < 1/2 \) and \( \rho = 0 \) if \( p \geq 1/2 \). Therefore an active state appears in the mean-field approximation already.

For higher order cluster mean-field approximations similar scenario can be found, but one has to treat the two versions separately. The density in pair approximation for the symmetric version is:

\[
\frac{(p - 1) p^2 - 2 dp (p^2 + 2 p - 2) + d^2 (p^3 + 5 p^2 + 4 p - 4)}{(p - 1) p^2 - 2 dp (p^2 + 2 p - 2) + d^2 (p^3 + 5 p^2 - 4)}
\]

(9)

One can easily prove that if the coagulation rate is equal to the diffusion rate \( d = p(1 - d)/2 \) this gives a single \( \rho = 0 \) absorbing state solution in agreement with [7]. The steady state solution with positive density is possible if

\[
d > \frac{p^2 - p}{p^2 + 3p - 2}.
\]

(10)

This gives the phase boundary in pair approximation that is a continuous unlike in case of the PCPD model [8] (see Fig.1).

![Phase diagram of the symmetric coagulation-production model. Dotted line: mean-field approximation, dashed line: pair approximation, squares: simulation results. The circles show \( d_c \) as the function of \( c \). Lines connecting symbols are used to guide eyes only.](image1)

**FIG. 1.** Phase diagram of the symmetric coagulation-production model. Dotted line: mean-field approximation, dashed line: pair approximation, squares: simulation results. The circles show \( d_c \) as the function of \( c \). Lines connecting symbols are used to guide eyes only.

The pair density in this approximation

\[
c = \frac{((p - 1) p - d (p^2 + 3 p - 2))^{1} (p - 1)^{-1}}{(p - 1) p^2 - 2 dp (p^2 + 2 p - 2) + d^2 (p^3 + 5 p^2 - 4)}
\]

(11)

has a leading order singularity all along the phase transition line

\[
c \propto (p_c - p)^2
\]

(12)

suggesting one universality class unlike in the case of PCPD model [8].

The GMF solutions for \( N = 3, 4, 5, 6, 7 \) block sizes have been determined numerically at \( d = 0.2 \). The approximation level is constrained by the numerical stability of the fixed point solution in the multi-dimensional space of \( N \)-block probability variables. As Figure 2 shows the \( \rho_N \) density curves of different approximations converge to the simulation results.

![Cluster mean-field approximations in the symmetric coagulation-production model for \( d = 0.2 \). The curves correspond to steady state density solutions as the function of \( p \), for \( N = 2, 3, 4, 5, 6, 7 \) (right to left). The circles with error bars represent simulation results. Insect: Corresponding coherent anomaly amplitudes with a power-law fitting.](image2)

**FIG. 2.** Cluster mean-field approximations in the symmetric coagulation-production model for \( d = 0.2 \). The curves correspond to steady state density solutions as the function of \( p \), for \( N = 2, 3, 4, 5, 6, 7 \) (right to left). The circles with error bars represent simulation results. Insect: Corresponding coherent anomaly amplitudes with a power-law fitting.

Using these data an estimate can be given for the order parameter density exponent \( \rho \propto |p - p_c|^{\beta} \) using the Coherent anomaly method (CAM) [19], which has been proven to give precise estimates for the DP [20] and PC [21] classes. According to CAM the amplitudes \( a(N) \) of the cluster mean-field singularities scale in such a way that

\[
a(N) \propto |p_c(N) - p_c|^{\beta - \beta_{MF}}
\]

(13)

the exponent of true singular behavior can be estimated. From the mean-field solution [8] one read-off that \( \beta_{MF} = 1 \). The critical point \( p_c \) can be estimated either by extrapolating on the GMF results or by simulations. Linear extrapolation at \( d = 0.2 \) for \( p_c(1/N \to 0) \) gives: \( p_c = 0.182(2) \). Monte Carlo simulations on large systems – discussed below – give a more precise estimate: \( p_c = 0.17975(8) \). The amplitudes \( a(N) \) near \( p_c(N) \) are determined by linear fitting from the \( \rho_N(p) \) data and shown in inset of Fig.2 as the function of \( p_c(N) - p_c \). A
power-law with exponent $\beta - \beta_{MF} = -0.43(3)$ can fairly well applied for points corresponding to $N > 2$ approximations giving an estimate: $\beta = 0.57(3)$, which agrees well with former results for the AF model with small diffusion rates \[3\].

Monte-Carlo simulations of the symmetric process started from fully occupied lattices of size $L = 40000$ show a phase transition for $d = 0.2$ and $p_c = 0.17975(10)$ (see Fig.3). The local slopes of the density decay:

$$
\alpha_{eff}(t) = -\frac{\ln[\rho(t)/\rho(t/m)]}{\ln(m)}
$$

(14)

(where we use $m = 8$ usually) at the critical point go to exponent $\alpha$ by a straight line, while in sub(super)-critical cases they veer down(up) respectively.

For the critical point ($p_c = 0.17975(8)$) one can estimate that the effective exponent tends to $\alpha = 0.263(9)$, which agrees with results for the AF model \[3\] again. For other $d$-s similar results have been found.

In the supercritical region the steady states have been determined for different $\epsilon = p - p_c$ values. Following level-off the densities were averaged over $10^4$ MCS and 1000 samples. By looking at the effective exponent defined as

$$
\beta_{eff}(\epsilon_i) = \frac{\ln \rho(\epsilon_i) - \ln \rho(\epsilon_{i-1})}{\ln \epsilon_i - \ln \epsilon_{i-1}},
$$

(15)

one can read-off: $\beta_{eff} \rightarrow \beta \simeq 0.57(1)$, which is in good agreement with the exponent of the AF model for weak diffusion determined by coherent anomaly method and simulations \[3\].

The simulations and the cluster mean-field approximations show that if the diffusion rate is lowered this phase transition disappears and the system will decay with the $\rho \propto t^{-0.5}$ law independently of $f$ in both versions. As expected the asymmetric version exhibits a phase transition with the same universal properties as the symmetric version. Example for $d = 0.2$ the transition point is at $c = 0.359(1), f/2 = 0.4409(1)$ with the decay exponent $\alpha = 0.27(1)$.

In conclusion coagulation production models exhibit a phase transition if the diffusion is fast enough. The spatial symmetry of the production process has been found to be irrelevant as in case of the AF model \[3\]. The critical behavior agrees well with that of the AF model in its weak diffusion rate region. An open question is that why one can see the cyclically coupled behavior in this model similarly as in the PCPD model as $d \rightarrow 1$. The corrections to scaling are getting very strong in this limit that make numerical solutions very confusing, but one has to realize that the $B \rightarrow 0$ process of pairs (present in AF) is missing in this model. Therefore a single universality class in this model and two distinct classes in the AF model is likely. This conjecture is strengthened by the pair mean-field results: one obtains analytically the same singular behavior here and two distinct singular behavior in case of the PCPD model along the phase transition line.

\begin{table}[h]
\centering
\caption{Summary of results}
\begin{tabular}{|c|c|c|c|c|}
\hline
$d$ & 0.1 & 0.2 & 0.4 & 0.7 \\
\hline
$p_c$ & 0.1129(1) & 0.17975(8) & 0.2647(1) & 0.3528(2) \\
$\alpha$ & 0.263(9) & 0.268(8) & 0.275(8) & \\
$\beta$ & 0.57(1) & 0.58(1) & 0.57(1) & \\
$\beta_{CAM}$ & 0.57(3) & - & - & \\
\hline
\end{tabular}
\end{table}
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