The role of diffusion in nonequilibrium phase transitions

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• One of the primary goals is to explore universality classes like in equilibrium statistical physics

• Due to the lack of Gibbs distribution phase transitions (PT) may occur in low dimensions

• Which factors determine the PT universality class of a model of short range interactions? Besides the spatial dimensions, boundaries, inhomogenities:
  1) Symmetries, conservation laws like in equilibrium (BAW2 ...)
  2) Initial conditions (temporal boundary condition) (PCP ...)
  3) Topological effects in low dimensions (multi-comp systems...)
  4) Dynamically generated long range memory (coupled systems...)
  5) Mean-field classes of RD: \( nA \rightarrow (n+k)A \), \( mA \rightarrow (m-l)A \) --> /
  6) For competing dynamics (diffusion) --> /

See also: G. Ódor, Rev. Mod. Phys. 76 (2004) no. 3.
Mean-field classes of site restricted, one-component reaction-diffusion systems

- General, reaction-diffusion systems:
  \[ nA \xrightarrow{\sigma} (n+k)A \quad mA \xrightarrow{\lambda} (m-l)A \quad 0A \xrightarrow{D} A0 \]
  \[ \partial \rho / \partial t = a k \sigma \rho^n (1-\rho)^k - a l \lambda \rho^m \]

  - \( n = m \) : \( \beta = 1, \alpha = 1/n \)
  - \( n < m \) : \( \beta = 1/(m-n), \alpha = 1/(m-1) \)
  - \( n > m \) : First order transition

  \( n \) és \( m \) determine the mean-field class!
  Diffusion does not play a role.

\[ G. \text{Ódor: PRE 67, 056114 (2003)} \]
The dynamical cluster mean-field method

Master equations for \( N=1,2,... \) block probabilities:

\[
\frac{\partial P_N(s_i)}{\partial t} = f(P_N(s_i)), \quad s_i = 0, 1
\]

\[
P_{\text{abcde}} \approx P_{\text{abcd}} P_{\text{bcde}} / P_{\text{bcd}}
\]

Example 4-Blocks:

Conf. 1

\[1 1 1 1 1 1\]

Taking into account symmetries for \( N=8 \) case 136 independent variables (block probabilities)
Cluster approximations for: $2A \rightarrow 3A, 4A \rightarrow 0$

Steady state density for $N \geq 2$ (diffusion dependence).
Unexpected phase transitions for $\sigma > 0$, with $\beta=1$ (for $n < m$ MF: $\sigma_c = 0$)

For $N=5$ steady state density for $D = 0.5, 0.4, 0.35, 0.3, 0.2, 0.1, 0.005, 0.001$

$\beta = 2$
Critical endpoint

$\beta = 1/2$
$\beta = 1$
Cluster approximations for: \(2A \rightarrow 3A, 4A \rightarrow 0\) model

Density decay solution for \(N = 3\) at \(D=0.05\) near \(\sigma_c > 0\) critical point with exponent \(\alpha = 0.5\) \((2A \rightarrow 3A, 2A \rightarrow 0\) (PCPD) behavior\)

Simulations in 1 and 2 dimension support \(N\)-cluster results:

\[ \text{G. Ódor, PRE 69, 036112 (2004)} \]

\[ \text{G. Ódor: cond-mat/0403562} \]

Unexpected by perturbative RG

For low diffusions the \(2A \rightarrow 3A \rightarrow 4A \rightarrow 0\) process becomes relevant!
Lattice simulations

One dimension

- Random sequential update of occupied sites
- Full or random half filled initial conditions
- \( L \leq 500000 \) in 1d,
  \( L \leq 7000 \times 7000 \) in 2d
- Periodic boundary conditions
- \( t_{\text{max}} \leq 5 \times 10^8 \) MCS
- Master-slave parallel algorithms on international computing GRIDS (~ 100 - 500 CPU-s)

Two dimensions

- Production: \( \sigma : (1-p)(1-D)/2 \)
- Annihilation: \( \lambda = p(1-D) \)
- Diffusion rate: \( D \)
Simulation results for the 2A -> 3A, 4A -> 0 model in 1 dimension

Density decay local exponents with: $\alpha = 0.21(2)$ (~PCPD), at $D = 0.5$, $\sigma_c = 0.42075$.

Steady state local exponents near $\sigma_c = 0.42$ for $D = 0.5, 0.2$, with $\beta = 0.40(2)$ (~PCPD).

For $D = 0.9$: only mean-field with $\beta = 1/2$. 2A -> 0 process becomes irrelevant!

$L = 5 \times 10^5, t_{\text{max}} = 5 \times 10^8 \text{ MCS}$
Simulation results for the 2A $\rightarrow$ 3A, 4A $\rightarrow$ 0 model in 2 dimensions

Density decay local exponents with: $\alpha = 0.50(1)$ (MF-PCPD) at $\sigma_c = 0.26715$

$L = 7000, t_{\text{max}} = 2 \times 10^6 \text{ MCS}, D = 0.05$

Steady state local exponents at $D = 0.05$ with $\beta = 0.98(2)$ (MF-PCPD).
For $D=0.9$: only mean-field with $\beta=1/2$. 2A $\rightarrow$ 0 process becomes irrelevant!
Cluster mean-field for BARW(unary)

1) $A \to 2A, 2A \to 0$: (Canet, Chaté, Delamotte, cond-mat/0403432, NPRG)

   Exact relation: $(\lambda_c/D)_{tr} = 2/(N-1)$ found. For 1d: $(\lambda_c/D)_{tr} \to 0$ as $N \to \infty$.

2) $A \to 2A, 4A \to 0$: $(\lambda_c/D)_{tr} \to \sim 1.2$ as $N \to \infty$.

   $MF: m > n: \beta = 1/(m-n), \alpha = 1/(m-1), \sigma_c = 0$
A -> 2A, 4A -> 0: Reentrant phase diagram

N-cluster approximation

Simulations:
2d: L = 4000x4000, 1d: L = 100000
Critical point decay at $\sigma_c > 0$
in (a): one and (b): two dimensions

DP class value in 1d: $\alpha = 0.159464(6)$ (I. Jensen)
2d: $\alpha = 0.4505(10)$ (Voigt and Ziff)

For low diffusions the $A \rightarrow 2A \rightarrow 3A \rightarrow 4A \rightarrow 0$ process becomes relevant!
Summary

- In general (site restricted) reaction-diffusion systems the mean-field universality class is determined by the number of reacting particles (n,m).

- Diffusion may become relevant in case of competing reactions by changing the phase diagram and introducing nontrivial fixed points.

- Diffusion dependence has been found in similar systems:
  - M. Paessens, G. Schütz: bosonic PCPD, JPA37, 4709 (2004)

- Perturbative RG results should be revised!

  G. Ódor: Rev. Mod. Phys. 76 (2004), cond-mat/0205644
  G. Ódor: cond-mat/0403562, to appear in PRE
  G. Ódor: cond-mat/0406247