The role of diffusion in branching and annihilating random walk models

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- Overview of nonequilibrium universality classes of reaction-diffusion systems
- The dynamical cluster mean-field method
- Perturbatively unexpected results for simple reaction-diffusion systems with competing reactions
Example 1: Branching and annihilating random walks (BARW) in 1+1 d

$A \rightarrow (n+1)A, \quad 2A \rightarrow A, \quad A \rightarrow 0$

$\langle\text{-- 1+1 d realization --}\rangle$

For $n=1$ directed percolation (DP), contact process, epidemic spreading
$\sim$ BARW1 $\sim$ BARWodd (no $A \rightarrow 0$)

Phase transition with DP class universal behavior:

$\rho_\infty \propto (\sigma - \sigma_c)^\beta \quad \rho(t) \propto t^{-\alpha}$

$\xi_\infty \propto (\sigma - \sigma_c)^{-\nu} \quad R \propto \xi \propto t^{z/2}$

Well known exponents, field theory
Robust universality class, still lacks experimental realization
$\langle\text{-- sensitivity to disorder}\rangle$
Example 2: Binary production (PCPD) model

1D PCPD reaction–diffusion model

- Two absorbing states without symmetry, one of them is diffusive. Carlon, Henkel, Schollwock (PRE 2001).
- Bosonic field theory ('97) failed to describe critical behavior. In the bosonic model diverging active phase.
- Fermionic model shows different critical behavior but field theory is too hard. Numerical methods show new exponents.
- No extra symmetries or conservation laws has been found to explain unexpected critical behavior.
Space-time evolution of universal nonequilibrium spreading models with absorbing states in 1+1d

- **Unary** production spreading without and with *parity conservation*:
  \[ A \rightarrow (m+1)A, \quad 2A \rightarrow 0 \]

- **Binary** production spreading coupled to slave modes without and with *diffusion*:
  \[ 2A \rightarrow (m+2)A, \quad 2A \rightarrow 0 \]

Reactive and diffusive sectors, changing exponents by varying the diffusion rate: 

Critical universality classes

• One of the primary goals of stat. phys. is to explore nonequilibrium universality classes like in equilibrium

• 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: $nA \rightarrow (n+k)A$, $mA \rightarrow (m-l)A \rightarrow /$.
  6) For competing dynamics (diffusion) $\rightarrow /$.

Mean-field classes of site restricted, one-component reaction-diffusion systems

- General, reaction-diffusion systems:

\[ nA \xrightarrow{\sigma} (n+k)A \quad mA \xrightarrow{\lambda} (m-l)A \quad 0A \Leftrightarrow A0 \]

\[ \partial \rho / \partial t = a k \sigma \rho^n (1-\rho)^k - a l \lambda \rho^m \]

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

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

\[ \rho (t) \propto t^{-\alpha} \quad \rho (\infty) \propto \epsilon^\beta \]

\[ \sigma_c = l/(k+l) \quad \sigma_c = 0 \]

The dynamical, $N$-cluster mean-field method (GMF)

- Master equation for $n$-point configuration probabilities of $s_i$
  \[
  \frac{\partial P_n(s_i)}{\partial t} = f(P_n(s_i)), \quad (1)
  \]

- Bayesian extension process ($n>N$ correlations are neglected)
  \[
  P_n(s_1, \ldots, s_n) = \frac{\prod_{j=0}^{j=n-N} P_N(s_{1+j}, \ldots, s_{N+j})}{\prod_{j=1}^{j=n-N} P_{N-1}(s_{1+j}, \ldots, s_{N-1+j})}. \quad (2)
  \]

- Reduction of parameters due to symmetries, conservations
  \[
  P_n(s_1, \ldots, s_n) = \sum_{s_{n+1}} P_{n+1}(s_1, \ldots, s_n, s_{n+1}),
  \]
  \[
  P_n(s_1, \ldots, s_n) = \sum_{s_0} P_{n+1}(s_0, s_1, \ldots, s_n).
  \]

- If we apply GMF for one-dimensional, site restricted lattice version of BARWe. For $N=10$ we have 528 independent variables
Cluster mean-field for BARW($m>n$)

(site MF: $m>n$: $\beta = 1/(m-n)$, $\alpha = 1/(m-1)$, $\sigma_c = 0$)

1) $A \rightarrow 2A$, $2A \rightarrow 0$ :

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

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

ERG field theoretical reminder
(B. Delamotte et al.)

General reactions: \( A \rightarrow mA, kA \rightarrow 0 \)  
(Cardy & Tauber)

\[
S[\phi, \dot{\phi}] = \int d^d x \, dt \left\{ \dot{\phi}(x, t) \left( \partial_t - D \nabla^2 \right) \phi(x, t) - \lambda_k \left( 1 - \dot{\phi}(x, t)^k \right) \phi(x, t)^k + \sigma_m \left( 1 - \dot{\phi}(x, t)^m \right) \dot{\phi}(x, t) \phi(x, t) \right\}
\]

\( A \rightarrow 2A, 2A \rightarrow 0 \)

Perturbative RG

NPRG

(Canet, Chaté, Delamotte, _PRL 2004, NPRG_)
$A \rightarrow 2A, \, 4A \rightarrow 0$ : Reentrant phase diagram

N-cluster approximation

Simulations:
2d: $L^2 = 4000^2$, 1d: $L = 10^5$

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 (and high d) the $A \rightarrow 2A \rightarrow 3A \rightarrow 4A \rightarrow 0$ process becomes relevant! Unexpected by perturbative RG.
Cluster approximations for: 2A -> 3A, 2A -> 0 model

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

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

$\beta = 1/2$
$\beta = 1$

Perturbative RG expectations
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:
G. Ódor, PRE 69, 036112 (2004)

Unexpected by perturbative RG

For low diffusions the $: 2A\rightarrow3A\rightarrow4A\rightarrow0$ process becomes relevant !
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.

$L = 5 \times 10^5$, $t_{\text{max}} = 5 \times 10^8$ 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 $\sigma_c=0.26715$

$L = 7000, t_{\text{max}} = 2 \times 10^6$ 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!
Summary

- In \( nA \rightarrow (n+k) \), \( mA \rightarrow (m-l)A \) type 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:
  - R. Dickman: \( A \rightarrow 2A, 3A \rightarrow 0 \), \( \text{PRA}42, 6985 \ (1990) \)
  - M. Paessens, G. Schütz: bosonic PCPD, \( \text{JPA}37, 4709 \ (2004) \)
  - N. Menyhárd, G. Ódor: NEKIM-A, \( \text{PRE}68, 056106 \ (2003) \)

- Perturbative RG results may not hold for low Diffusion and high dim!

- References: G. Ódor: \( \text{PRE} 67, \ (2003) \ 056114 \)
  G. Ódor: \( \text{PRE} 67, \ (2003) \ 016111 \)
  G. Ódor: \( \text{PRE} 69, \ (2004) \ 036112 \)
  G. Ódor: \( \text{PRE} 70, \ (2004) \ 026119 \)
  G. Ódor: \( \text{PRE} 70, \ (2004) \ 066122 \)