

# Field Theory Approach to Diffusion-Limited Reactions:

## 4. Active to Absorbing State Transitions

Ben Vollmayr-Lee  
Bucknell University

Boulder School for Condensed Matter and Materials Physics  
July 17, 2009

# A Few More Applications

Particle Source  $0 \rightarrow A$ : Droz & Sasvari, PRE '93; Rey & Droz, JPA '97

Persistence: Cardy, JPA 1995

Quenched Random Velocity Fields: Oerding, JPA 1996; Richardson & Cardy, JPA 1999

Quenched Random Potential: Park & Deem, PRE 1998

Site Occupation Restrictions: van Wijland, PRE 2001

Reversible Reactions: Rey & Cardy JPA 1999

Coupled Reactions: Howard, JPA 1996; Howard & Täuber, JPA 1997;  
and many more

Active to Absorbing State Transitions: subject for today ...

## Absorbing State

- ▶ A state that the system can flow into, but not out of.
- ▶ In reaction-diffusion models, the state with no particles is an absorbing state.
- ▶ A system many have one, two, many, or infinitely many absorbing states

## Active State

- ▶ Not an absorbing state, i.e., a state connected dynamically to all other states
- ▶ Often used to mean a non-equilibrium **steady state**.
- ▶ In reaction-diffusion models, this then requires birth ( $0 \rightarrow A$ ) or branching ( $A \rightarrow kA$ ) processes.

# Field Theory Approach to Diffusion-Limited Reactions:

## 4. Active to Absorbing State Transitions

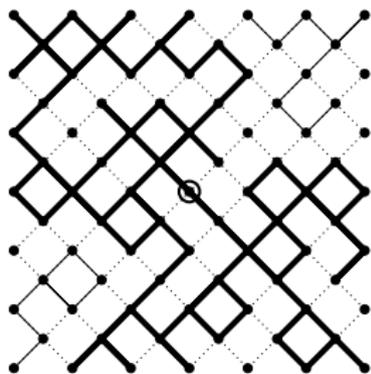
Directed Percolation

Branching and Annihilating Random Walks

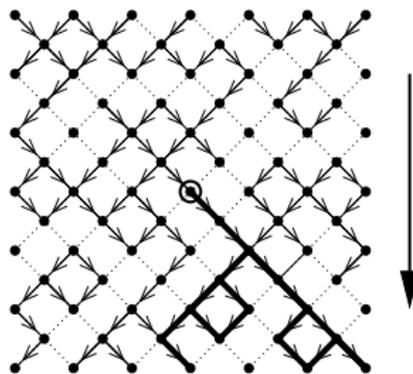
Pair Contact Process with Diffusion

# Directed Percolation Model

Figure from H. Hinrichsen, *Adv. Phys.* **49**, 815 (2000)



*isotropic bond percolation*

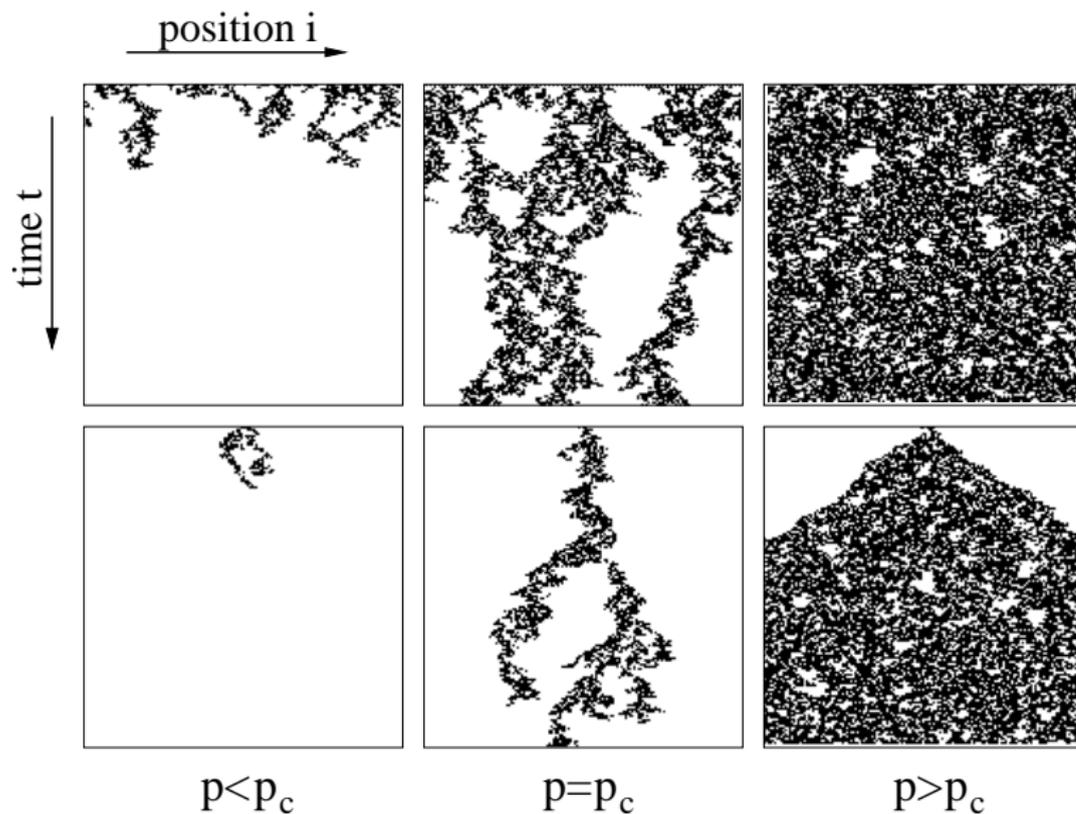


*directed bond percolation*

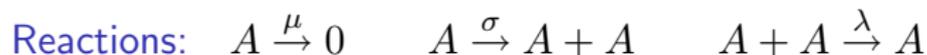
## Reaction-Diffusion Model:



plus diffusion



# Rate Equations



$$\partial_t a = (\sigma - \mu)a - \lambda a^2 \quad a(t) \rightarrow \begin{cases} a_\infty = \frac{\sigma - \mu}{\lambda} & \sigma > \mu \\ 0 & \sigma \leq \mu \end{cases}$$

- ▶ For  $\sigma > \mu$ , steady state approached exponentially fast:

$$|a(t) - a_\infty| \sim e^{-(\sigma - \mu)t}$$

- ▶ For  $\sigma = \mu$  it is like  $A + A \rightarrow A$ , and  $a(t) \sim 1/(\lambda t)$ .

# Critical Exponents

## Reaction-Diffusion Equation

Let  $r = (\mu - \sigma)/D$  (active state  $r < 0$ ), then

$$\partial_t a = -D(r - \nabla^2)a - \lambda a^2$$

Characteristic length:  $\xi \sim |r|^{-1/2}$  and time:  $\tau \sim \xi^2/D \sim |r|^{-1}$

## Critical Exponents

$$\langle a_\infty \rangle \sim (-r)^\beta \quad (r < 0) \quad \langle a(t) \rangle \sim t^{-\alpha} \quad (r = 0)$$

$$\xi \sim |r|^{-\nu} \quad (r \neq 0) \quad \tau \sim \xi^z \quad (r \neq 0)$$

## Mean-Field Exponents

$$\beta = 1 \quad \alpha = 1 \quad \nu = 1/2 \quad z = 2$$

# Directed Percolation Conjecture [Janssen '81, Grassberger '82]

A model should belong to the DP universality class if the following conditions are met

1. The model displays a continuous phase transition from a fluctuating active phase into a unique absorbing state.
2. The transition is characterized by a positive, one-component order parameter.
3. The dynamic rules involve only short-range processes.
4. The system has no special attributes such as additional symmetries or quenched randomness.

# Directed Percolation Field Theory

Reactions:  $A \xrightarrow{\mu} 0$      $A \xrightarrow{\sigma} A + A$      $A + A \xrightarrow{\lambda} A$

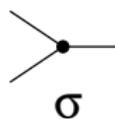
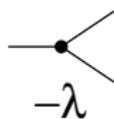
$$\hat{H}_{\text{reaction}} = \mu(\hat{a}^\dagger \hat{a} - \hat{a}) + \sigma(\hat{a}^\dagger \hat{a} - \hat{a}^\dagger \hat{a}^2) + \lambda(\hat{a}^\dagger \hat{a}^2 - \hat{a}^\dagger \hat{a}^2)$$

Action:

$$S = \int d^d x dt \left\{ \tilde{\phi} [\partial_t + D(r - \lambda^2)] \phi - \sigma \tilde{\phi}^2 \phi + \lambda \tilde{\phi} \phi^2 + \lambda \tilde{\phi}^2 \phi^2 \right\}$$

Propagator:  $G_0(\mathbf{k}, \omega) = \frac{1}{-i\omega + D(r + k^2)}$

Vertices:



# Effective Field Theory

Since the three point vertices appear in tandem, it is helpful to rescale the fields to make their coefficients match. Take

$$\tilde{\phi} \rightarrow \tilde{s}\sqrt{\sigma/\lambda} \quad \phi \rightarrow s\sqrt{\lambda/\sigma}$$

giving for  $u = \sqrt{\sigma\lambda}$

$$S = \int d^d x dt \left\{ \tilde{s}[\partial_t + D(r - \lambda^2)]s - u(\tilde{s}^2 s - \tilde{s}s^2) + \lambda\tilde{s}^2 s^2 \right\}$$

Power counting:

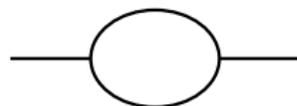
$$[\sigma] = \ell^{-2}, [\lambda] = \ell^{d-2} \quad \Rightarrow \quad [u] = \ell^{d-4} \text{ and } d_c = 4.$$

For perturbation theory around  $\epsilon = 4 - d$ , four-point vertex is irrelevant, so we'll drop it.

$$S_{\text{eff}} = \int d^d x dt \left\{ \tilde{s}[\partial_t + D(r - \lambda^2)]s - u(\tilde{s}^2 s - \tilde{s}s^2) \right\}$$

# Renormalization

The one-loop correction to the propagator requires a shift in the critical point ( $\tau \equiv r - r_c$ ) and renormalization of



1. the fields  $s$  and  $\tilde{s}$  (which renormalize identically)
2. the diffusion constant
3. the true distance from the critical point  $\tau$
4. the coupling  $u$

Coupling  $v = u^2$  flows to  $O(\epsilon)$  fixed point  $v^*$ , which feeds back via the method of characteristics to determine the critical exponents.

To one-loop order

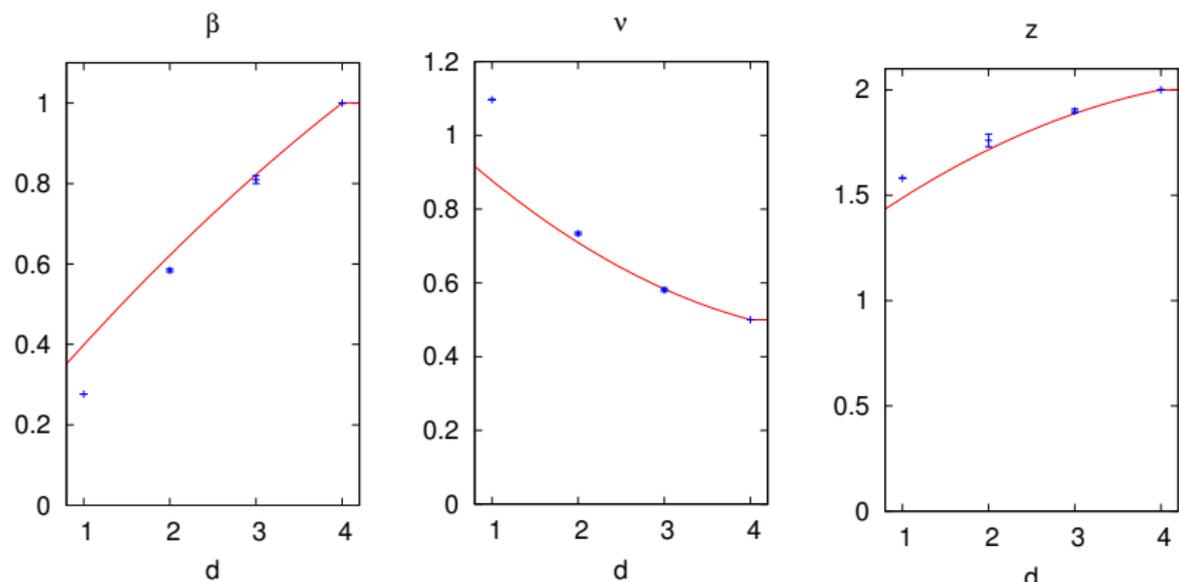
$$\beta = 1 - \frac{\epsilon}{6} + O(\epsilon^2)$$

$$\alpha = 1 - \frac{\epsilon}{4} + O(\epsilon^2)$$

$$\nu = \frac{1}{2} + \frac{\epsilon}{16} + O(\epsilon^2)$$

$$z = 2 - \frac{\epsilon}{12} + O(\epsilon^2)$$

# DP Critical Exponents



2-loop RG: Bronzan & Dash, Phys. Lett. B, 1974

Series expansions: Jensen, JPA 1999; Voigt & Ziff, PRE 1997;  
Jensen, PRE 1992

# Field Theory Approach to Diffusion-Limited Reactions:

## 4. Active to Absorbing State Transitions

Directed Percolation

Branching and Annihilating Random Walks

Pair Contact Process with Diffusion

# Branching and Annihilating Random Walks (BARW)

Consider the processes



## Rate Equation

$$\partial_t a = \sigma m a - 2\lambda a^2 \quad \text{which implies} \quad a(t) \rightarrow a_\infty = \frac{\sigma m}{2\lambda}$$

For  $d < 2$ , fluctuations can change this result, so  $a(t) \rightarrow 0$ .

## Doi Hamiltonian

$$H_{\text{reaction}} = \lambda(\hat{a}^{\dagger 2} \hat{a}^2 - \hat{a}^2) + \sigma(\hat{a}^{\dagger} a - \hat{a}^{\dagger m+1} \hat{a})$$

Note symmetry under  $(\hat{a}, \hat{a}^{\dagger}) \rightarrow (-\hat{a}, -\hat{a}^{\dagger})$  for  $m$  even.

$$S = \int d^d x dt \left\{ \phi^* (\partial_t - D\nabla^2) \phi + \sigma(1 - \phi^{*m}) \phi^* \phi - \lambda(1 - \phi^{*2}) \phi^2 \right\}$$

- ▶ Note that we're avoiding the field shift  $\phi^* \rightarrow 1 + \tilde{\phi}$  to maintain the parity symmetry for  $m$  even. (Initial and final terms unimportant.)
- ▶ In addition to  $A \rightarrow (m+1)A$ , all lower order branching processes are generated:

$$A \rightarrow (m-1)A, \quad A \rightarrow (m-3)A, \quad \dots$$

- ▶ Power counting:  $m=1$  or  $m=2$  will dominate, so all theories will  $m$  odd or  $m$  even will be in the same universality class.
- ▶ For  $m$  odd, the reaction  $A \rightarrow 0$  is also generated.

Effective Field Theory describes processes

$$A + A \rightarrow 0 \quad A \rightarrow A + A \quad A \rightarrow 0$$

which was our starting point for directed percolation.

**Conclusion:** BARW with odd number of offspring is in the DP universality class

... provided that the induced  $A \rightarrow 0$  transition is capable of driving the system to the absorbing state.

- ▶ within perturbative RG, this requires  $d \leq 2$
- ▶ NPRG finds evidence for inactive phase and DP criticality in higher dimensions [Canet, Delamotte, Deloubrière, & Wschebor, PRL 2004]

## Case of Even $m$

Becomes effectively  $A + A \xrightarrow{\lambda} 0$  and  $A \xrightarrow{\sigma} 3A$

- ▶ Branching rate  $\sigma$  renormalization:  $\beta_\sigma = -y\sigma + O(\sigma^2)$
- ▶ For  $d > 2$ , annihilation controlled by gaussian ( $g_R \rightarrow 0$ ) fixed point, power counting gives  $y = 2$ 
  - ⇒ branching is relevant, mean-field active phase.
- ▶ For  $d < 2$  then  $y = 2 - 3\epsilon + O(\epsilon^2)$ , which is negative for  $d < d' = 4/3$ .
  - ⇒ branching is relevant for  $d > 4/3$ , active phase.
  - ⇒ for  $d < 4/3$ , active to absorbing state transition, controlled by value of  $\sigma$ .

New parity-conserving (PC) universality class!

[Originally discovered by Zhong & ben-Avraham, Phys. Lett. A 1995]

# Field Theory Approach to Diffusion-Limited Reactions:

## 4. Active to Absorbing State Transitions

Directed Percolation

Branching and Annihilating Random Walks

Pair Contact Process with Diffusion

# A Cautionary Tale

Instead of branching, consider a pair-contact process:



with site occupation restrictions, or an additional  $3A \rightarrow 0$  reaction to keep the active phase density finite.

With diffusion this is called the **pair contact process with diffusion** (PCPD) [Janssen, van Wijland, Deloubrière, & Täuber, PRE 2004]

- ▶ Action is straightforward, but under renormalization, the couplings don't flow to fixed points (strong coupling fixed point).
- ▶ Numerical evidence is inconclusive, but this could be in the DP universality class.
- ▶ A qualitatively different effective action is required.

# Open Problems

- ▶  $A + B \rightarrow 0$ : full analysis of  $a_0 = b_0$  for  $d < 2$  still lacking. Role of topological constraints in  $d = 1$ .
- ▶ BARW with  $m$  even are poorly understood in  $d = 1$ . New methods for probing the parity-conserving universality class needed.
- ▶ Finding an appropriate field theory for PCPD to determine its universality class.
- ▶ General classification of scale-invariant behavior in reaction-diffusion systems still far from complete.
- ▶ Rate disorder appears to have a large impact on active to absorbing state transitions. Very little is known.
- ▶ Method: Doi-Peliti approach, or variants, may prove useful in rare event statistics, obtaining full generating functions, ...