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 $0 \to A$: 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 ...

Active to Absorbing State Transition

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 ($0 \to A$) or branching ($A \to kA$) processes.

Field Theory Approach to Diffusion-Limited Reactions: 4. Active to Absorbing State Transitions

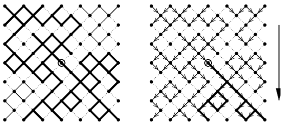
Directed Percolation

Branching and Annihilating Random Walks

Pair Contact Process with Diffusion

Directed Percolation Model

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



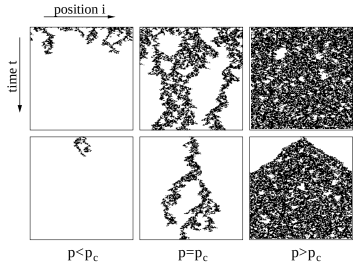
isotropic bond percolation *directed bond percolation*

Reaction-Diffusion Model:

$$\begin{aligned} A &\to 0 && \text{rate } \mu \\ A &\to A + A && \text{rate } \sigma \\ A + A &\to A && \text{rate } \lambda \end{aligned}$$

plus diffusion

Directed Percolation Demo [H. Hinrichsen, 2000]



Rate Equations

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

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

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

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

- For $\sigma = \mu$ it is like $A + A \to A$, 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

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

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

Mean-Field Exponents

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

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

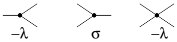
$$\hat{H}_{\text{reaction}} = \mu(\hat{a}^\dagger \hat{a} - \hat{a}) + \sigma(\hat{a}^\dagger \hat{a} - \hat{a}^{\dagger 2}\hat{a}) + \lambda(\hat{a}^{\dagger 2}\hat{a}^2 - \hat{a}^\dagger \hat{a}^2)$$

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

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

$$\tilde{\phi} \to \tilde{s}\sqrt{\sigma/\lambda} \qquad \phi \to s\sqrt{\lambda/\sigma}$$

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:

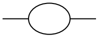
$[\sigma] = \ell^{-2}$, $[\lambda] = \ell^{d-2} \quad \Rightarrow \quad [u] = \ell^{d-4}$ and $d_c = 4$.

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 τ
4. the coupling u

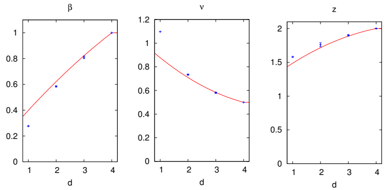
Coupling $v = u^2$ flows to $O(\epsilon)$ fixed point v^*, which feeds back via the method of characteristics the determine the critical exponents.

To one-loop order

$$\beta = 1 - \frac{\epsilon}{6} + O(\epsilon^2) \qquad \alpha = 1 - \frac{\epsilon}{4} + O(\epsilon^2)$$

$$\nu = \frac{1}{2} + \frac{\epsilon}{16} + O(\epsilon^2) \qquad z = 2 - \frac{\epsilon}{12} + O(\epsilon^2)$$

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

$$A + A \xrightarrow{\lambda} 0 \qquad A \xrightarrow{\sigma} (m+1)A$$

Rate Equation

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

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

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 $(\hat{a}, \hat{a}^\dagger) \to (-\hat{a}, -\hat{a}^\dagger)$ for m even.

BARW Field Theory [J. Cardy & U.C. Täuber, PRL '96, JPA '98]

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

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

$$A \to (m-1)A, \quad A \to (m-3)A, \quad \ldots$$

- 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 $A \to 0$ is also generated.

Case of Odd m

Effective Field Theory describes processes

$$A + A \to 0 \qquad A \to A + A \qquad A \to 0$$

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 $A \to 0$ 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 σ renormalization: $\beta_\sigma = -y\sigma + O(\sigma^2)$
- For $d > 2$, annihilation controlled by gaussian ($g_R \to 0$) fixed point, power counting gives $y = 2$

  $\Rightarrow$ branching is relevant, mean-field active phase.
- For $d < 2$ then $y = 2 - 3\epsilon + O(\epsilon^2)$, which is negative for $d < d' = 4/3$.

  $\Rightarrow$ branching is relevant for $d > 4/3$, active phase.

  $\Rightarrow$ for $d < 4/3$, active to absorbing state transition, controlled by value of σ.

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:

$$A + A \xrightarrow{\lambda} 0 \qquad A + A \xrightarrow{\sigma} (m+2)A$$

with site occupation restrictions, or an additional $3A \to 0$ 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

- $A + B \to 0$: 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, . . .