Field Theory Approach to Diffusion-Limited Reactions: 3. Applications

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Field Theory Approach to Diffusion-Limited Reactions

$A + A \to A$: One-Species Coalescence Reaction

Mapping of $A + A \to A$ to field theory gives [Peliti, JPA 1986]

$$S = \int d^dx\, dt \left[\tilde\phi(\partial_t - D\nabla^2)\phi + \cancel{2}\lambda_0\tilde\phi\phi^2 + \lambda_0\tilde\phi^2\phi^2 - n_0\tilde\phi\,\delta(t)\right]$$

Diagrammatic expansion and renormalization identical, only the 3-point vertex coefficient is changed.

Rescaling symmetry: [BL, JPA 1994]

Under $\phi \to b\phi$ and $\tilde\phi \to \tilde\phi/b$, action is invariant except

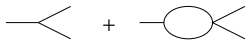
$$\lambda_0\tilde\phi\phi^2 \to b\lambda_0\tilde\phi\phi^2 \qquad n_0\tilde\phi \to (n_0/b)\tilde\phi$$

Choosing $b = 2$ maps $A + A \to A$ into $A + A \to 0$, implying

$$a_{A+A\to A}(t) = 2a_{A+A\to 0}(t)$$

$A + A \to 0$ for $d > 2$

We found for $d > 2$ that loop diagrams made finite, non-universal corrections to the 3-point vertex



Equivalently, the 4-point vertex $\lambda_0\tilde\phi^2\phi^2$ flows to zero under renormalization. For late times, the problem reduces to an effective action [BL & J. Cardy, JSP 1995]

$$S = \int d^dx\, dt \left[\tilde\phi(\partial_t - D\nabla^2)\phi + 2\lambda_0\tilde\phi\phi^2 - n_0\tilde\phi\,\delta(t)\right]$$

This is linear in $\tilde\phi$, so $\int \mathcal{D}\tilde\phi e^{-\tilde\phi(\cdots)}$ gives

$$\partial_t\phi = D\nabla^2\phi - 2\lambda_{\text{eff}}\phi^2 + n_0\delta(t)$$

Reaction-diffusion equation without the noise!

$3A \to \ell A$: Higher Order Reactions

- Rate equation $\partial_t a = -\lambda a^3$ predicts $a \sim t^{-1/2}$, so we expect $d_c = 1$
- Interaction vertices are now 
- Dyson sum of tree diagrams gives

$$a_{\text{tree}} = \frac{n_0}{(1 + 6\lambda_0 n_0^2 t)^{1/2}} \sim \frac{1}{\sqrt{3\lambda_0 t}}$$

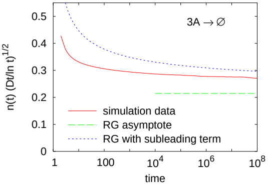
- Full calculation with RG flows yields

$$a_\ell(t) = \left[C_\ell^{(0)} g_R^{-1/2} + C_\ell^{(1)} + C_\ell^{(2)} g_R^{1/2} + \ldots\right](Dt)^{-1/2}$$

with $g_R \sim \dfrac{2\pi}{\sqrt{3}\ln(t/\tau)}$ where the $C_\ell^{(n)}$ are universal coefficients and τ is some non-universal time.

$3A \to \ell A$: Higher Order Reactions [BVL & M. Gildner, PRE 2006]

$$\begin{aligned} a_\ell(t) &= \left[A_\ell \sqrt{\ln(t/\tau)} + B_\ell + C_\ell \frac{1}{\sqrt{\ln(t/\tau)}} + \ldots\right](Dt)^{-1/2} \\ &= \left[A_\ell \sqrt{\ln t} + B_\ell + \left(C_\ell + \tfrac{1}{2}\ln\tau\right)\frac{1}{\sqrt{\ln t}} + \ldots\right](Dt)^{-1/2} \end{aligned}$$



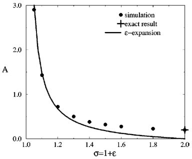
$A + A \to 0$ with Lévy Flights [D. Vernon, PRE 2003]

Allow hops of size ℓ with probability $P \sim \ell^{-d-\sigma}$. For $\sigma < 2$, $x_{\text{rms}} \sim t^{1/\sigma}$ (superdiffusive).

Changes propagator in field theory $e^{-Dk^2 t} \to e^{-Dk^\sigma t}$.

Now $d_c = \sigma < 2$ and our expansion is in powers of $\epsilon = \sigma - d$

Allows comparison to $d = 1$ simulations with ϵ small:



$A + B \to 0$ Introduction

Conservation law: Since $n_A - n_B$ unchanged by reaction, $a(t) - b(t) = \text{const}$.

Rate Equations: $\partial_t a = -\lambda ab \qquad \partial_t b = -\lambda ab$

Case I: $a_0 = b_0 \quad \Rightarrow \quad a(t) = b(t) \sim 1/(\lambda t)$

Case II: $a_0 > b_0 \quad \Rightarrow \quad a(t) \to a_0 - b_0$

and $\partial_t b \sim -\lambda(a_0 - b_0)b \quad \Rightarrow \quad b \sim e^{-\lambda(a_0 - b_0)t}$

Reaction-Diffusion Equations:

$$\partial_t a = D_A \nabla^2 a - \lambda ab \qquad \partial_t b = D_B \nabla^2 b - \lambda ab$$

For $a_0 = b_0$ and $d < 4$ particles segregate: [Bramson & Lebowitz, PRL 1988]

$$\langle a(t) \rangle = \tfrac{1}{2}\Big\langle \big(a(t) + b(t)\big) \Big\rangle \sim \tfrac{1}{2}\Big\langle \big|a(t) - b(t)\big| \Big\rangle$$

$A + B \to 0$ Results [Toussaint & Wilczek, JCP 1983]

Consider $D_A = D_B$ and take difference of reaction-diffusion equations:

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

Long-lived mode, decays only by diffusion.

- Initial densities $\langle (a - b) \rangle_0 = 0$, but

$$\Big\langle \big(a(\mathbf{x}) - b(\mathbf{x})\big)\big(a(0) - b(0)\big) \Big\rangle_0 = n_0 \delta(\mathbf{x})$$

- These fluctuations relax by diffusion:

$$\Big\langle \big(a(t) - b(t)\big)^2 \Big\rangle = \frac{n_0}{(8\pi D t)^{d/2}}$$

- Taking into account segregation:

$$a(t) = b(t) = \boxed{\frac{\sqrt{n_0}}{\sqrt{\pi}(8\pi D t)^{d/4}}} \quad \text{for } d < 4$$

$A + B \to 0$ Field Theory [BL & J. Cardy, JSP 1995]

Action has propagators $G_A = e^{-D_A k^2 t}$ and $G_B = e^{-D_B k^2 t}$.

Vertices are

$-\lambda_0\, \tilde{a}\, ab$ $\quad -\lambda_0\, \tilde{b}\, ab$ $\quad -\lambda_0\, \tilde{a}\tilde{b}\, ab$

Diagrams that renormalize the reaction are given by

$\Rightarrow$ everything goes through as before: $d_c = 2$, and for $d < 2$, $\lambda_0 \to g_R \sim O(\epsilon)$.

- What happened to $d = 4$?
- Why don't we see anything special happen in the density at $d = 2$?

$A + B \to 0$: Role of $d_c = 2$ and $d = 4$

$d = 4$ RG predicts for $d > 2$ asymptotic results given by the effective field theory with $\lambda_0 \tilde{a}\tilde{b}\, ab \to 0$. This is equivalent to the reaction-diffusion equations.

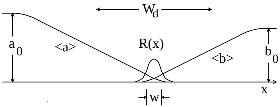
The change from t^{-1} to $t^{-d/4}$ is just a property of fluctuations in the initial conditions surviving to late times or not.

$d_c = 2$ Plenty happens at $d_c = 2$. For $a_0 > b_0$, reaction-diffusion equations predict $b \sim e^{-\lambda_0(a_0 - b_0)t}$, but

$$b \sim \begin{cases} e^{-\Gamma t/\ln t} & \text{for } d = 2 \\ e^{-\Gamma t^{d/2}} & \text{for } d < 2 \end{cases}$$

Reaction zones also exhibit qualitative change at $d = 2$ and not $d = 4$ ...

Reaction Zones: Initially Segregated Particles



Reaction-diffusion eqs give [Gálfi & Rácz, PRA 1988]

Depletion zone: $W_d \sim t^{1/2}$ width: $w \sim t^{\beta}$

Interparticle spacing in reaction zone: $\ell_{rz} \sim t^{\gamma}$

$$\beta = \begin{cases} \frac{1}{6} & d > 2 \\ \frac{1}{2(1+d)} & d < 2 \end{cases} \qquad \gamma = \begin{cases} \frac{1}{3d} & d > 2 \\ \frac{1}{2(1+d)} & d < 2 \end{cases}$$

The Trapping Reaction

Two-species reaction-diffusion system $A + B \to A$

- $A =$ "traps" with diffusion constant D
- $B =$ "particles" with diffusion constant D'. $\delta \equiv D'/D$

Rate Equation: $\dot{b} = -\lambda' a_0 b \quad \Rightarrow \quad b \sim \exp(-a_0 \lambda' t)$

Static Traps: case $D = 0$ special, dominated by rare regions
$b \sim \exp(-\Gamma t^{d/(d+2)})$ [Donsker & Varadhan '75]

Fluctuations: rate equation valid only for $d > 2$. For $d \leq 2$ take
$a_0 \to a_0 t^{d/2}$, $\lambda' \to g^*$ $(d < 2)$ or $1/\ln t$ $(d = 2)$

$$b \sim \begin{cases} \exp(-\Gamma t/\ln t) & d = 2 \\ \exp(-\Gamma t^{d/2}) & d < 2 \end{cases}$$

[Exact: Bramson & Lebowitz '88, Bray & Blythe '02]

Reacting Traps

Now consider the case where the trap density also decays due to

$$A + A \to \begin{cases} A & \text{coalescence, probability } p \\ \emptyset & \text{annihilation, probability } 1 - p, \end{cases}$$

a well-studied one-species reaction.

Rate Equation: $\dot{a} = -(2-p)\lambda a^2 \quad \Rightarrow \quad a \sim \dfrac{1}{(2-p)\lambda t}$

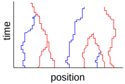
RG Calculation: fluctuations important for $d \leq 2$:

$$a \sim \begin{cases} \tilde{A}_p \dfrac{\ln t}{Dt} & d = 2 \\ A_p (Dt)^{-d/2} & d < 2 \end{cases}$$

with universal amplitude

The Trapping Reaction with Reacting Traps

The decaying trap density increases the survival probability of particles



Rate Equation: $\dot{b} = -\lambda' a b \sim \dfrac{\lambda'}{(2-p)\lambda t} b \quad \Rightarrow \quad b \sim t^{-\theta}$
with nonuniversal $\theta = \frac{\lambda'}{(2-p)\lambda}$.

Exponential decay replaced by a power law!

Fluctuations: give a universal decay exponent $\theta(p, \delta)$ for $d < 2$.
Theoretical results include exact solutions, RG calculations, and Smoluchowski theory.

Exact Solutions for Decay Exponent $\theta(p, \delta)$ in $d = 1$

Persistence: For $D' = 0$, the B particles measure locations not visted by a trap.

$$\theta = \frac{2}{\pi^2} \arccos\left(\frac{-p}{\sqrt{2}(2-p)}\right)^2 - \frac{1}{8} \quad \text{[Derrida \textit{et al.} '95]}$$

3 Walker Problem: For $p = 1$ $(A + A \to A)$, a B particle sees only its left and right neighbors. Recall $\delta = D'/D$.

$$\theta = \frac{\pi}{2\arccos[\delta/(1+\delta)]} \quad \text{[Fisher \& Gelfand '88]}$$

B is a Tagged A: for $\delta = 1$ (equal diffusion constants) and $p = 0$ $(A + A \to \emptyset)$. Gives $\theta = 1/2$.

Smoluchowski Theory

Correlation function mean field theory:

1. attach the origin of a coordinate system to a particle
2. solve for the diffusion field exterior to the particle, $r > R$. BC's:
   - $n(R,t) = 0$ at particle boundary
   - $n(r \to \infty, t) = n(t)$: uniform density at infinity
3. use the resulting flux toward the particle to define an effective rate constant
4. solve rate equation with time-dependent rate constant

Surprisingly effective for one-species reactions.

Gives $b \sim t^{-\theta}$ with $\theta = \frac{d}{2-p}\left(\frac{1+\delta}{2}\right)^{d/2}$ for $d < 2$.

Renormalization Group Calculation

- Gives $b \sim t^{-\theta}$ with

$$\theta = \frac{1+\delta}{2-p} + f(p,\delta)\epsilon + O(\epsilon^2)$$

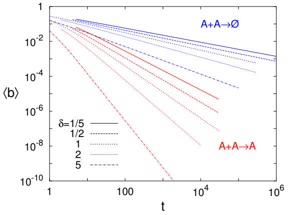
where $\epsilon = 2 - d$. [Howard '96, Krishnamurthy, Rajesh, & Zaboronski '03, Rajesh, & Zaboronski '04]

- Demonstrates universality!

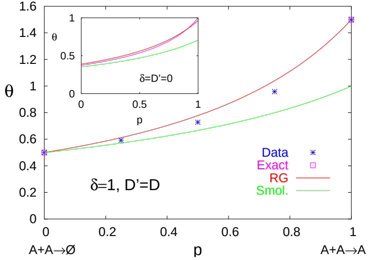
Particle Density Decay [R. Rhoades & BVL]

Simulated $p = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1$ and $\delta = \frac{1}{5}, \frac{1}{3}, \frac{1}{2}, 1, 2, 3, 5$ in $d = 1$

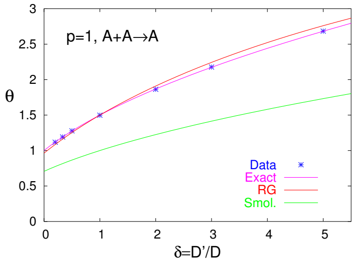
A density known, confirmed. B density power-law in all cases.



Decay Exponent θ versus p



Decay Exponent θ versus $\delta = D'/D$



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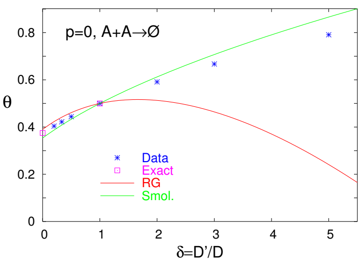
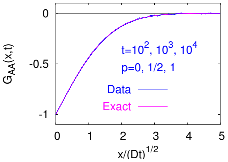


Trap-Trap Correlation Function

Simply scales with the diffusion length:

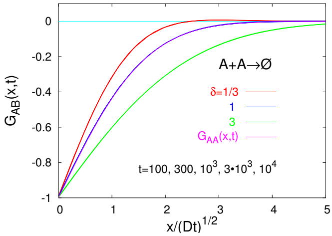
$$C_{AA}(x,t) = \frac{\langle a(x,t)a(0,t)\rangle - \langle a(t)\rangle^2}{\langle a(t)\rangle^2} \sim f_{AA}(x/t^{1/2})$$



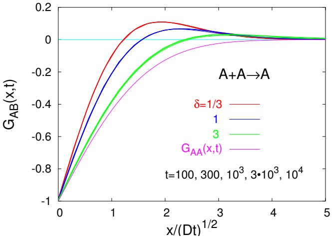
Exact: [Masser & ben-Avraham '01]

Trap-Particle Correlation Function: $p = 0$

$$C_{AB}(x,t) = \frac{\langle a(x,t)b(0,t)\rangle - \langle a(t)\rangle\langle b(t)\rangle}{\langle a(t)\rangle\langle b(t)\rangle} \sim f_{AB}(x/t^{1/2})$$

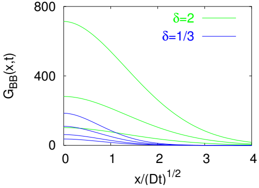


Trap-Particle Correlation Function: $p = 1$



Particle-Particle Correlation Function

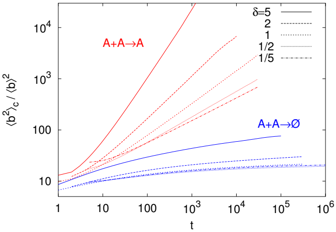
$$C_{BB}(x,t) = \frac{\langle b(x,t)b(0,t)\rangle - \langle b(t)\rangle^2}{\langle b(t)\rangle^2} \sim f_{BB}(x/t^{1/2})?$$



Case $p = 1$. No simple scaling!

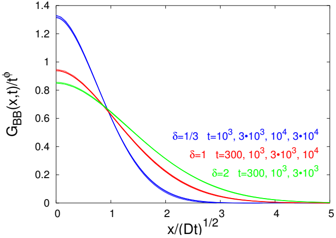
Anomalous Dimension

$$\frac{\langle a^2\rangle_c}{\langle a\rangle^2} \sim \frac{\langle ab\rangle_c}{\langle a\rangle\langle b\rangle} \sim \text{constant, but } \frac{\langle b^2\rangle_c}{\langle b\rangle^2} \sim t^{\phi}$$



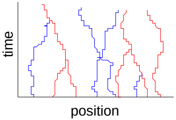
BB Correlations

Now we find $C_{BB}(x,t) \sim t^{\phi} f_{BB}(x/t^{1/2})$ case $p = 1$:

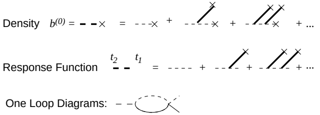


4 Walker Problem

In $d = 1$ for $p = 1$ ($A + A \to A$): exponent ϕ a property of a particular 4 walker problem:



RG Calculation for Particles



Proceeding naively to particle calculation:

$$b(t) \sim t^{-g'_R/(2-p)g_R} \left[A + \frac{B}{\epsilon} g'_R f(g'_R/g_R) + O(g_R^2) \right]$$

Something is wrong.

RG Calculation for Particles

$$b(t) \sim t^{-g'_R/(2-p)g_R} \left[A + \frac{B}{\epsilon} g'_R f(g'_R/g_R) + O(g_R^2) \right]$$

- Howard '96: regulate the $a_0 \to \infty$ limit, removes the $1/\epsilon$, adds logarithmic time dependence: resum.
- KRZ '03: Since bare $b(t)$ diverges as $\ln t$ for small t ($d = 2$), renormalize the initial density b_0
- RZ '04: Or instead do bare expansion of $t\partial_t \ln b(t)$ and renormalize exponent directly.

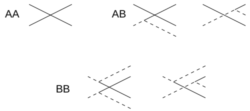
All approaches give the same θ. Can we use one to calculate our anomalous dimension ϕ?

RG Calculation for For Anomalous Dimension

Simplest approach:

$$C_{BB}(\mathbf{k} = 0, t) = \int d^d x \, e^{i\mathbf{k}\cdot\mathbf{x}} C_{BB}(\mathbf{x}, t) \sim t^{d/2+\phi}$$

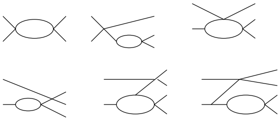
Tree level:



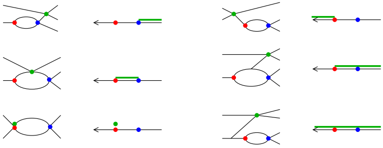
Gives $\phi = 0 + O(\epsilon)$. So we need to look at 1-loop correlations.

Trap-Trap 1-Loop Correlations

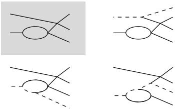
6 diagrams:



Trap Correlation Function — Topology/Causality



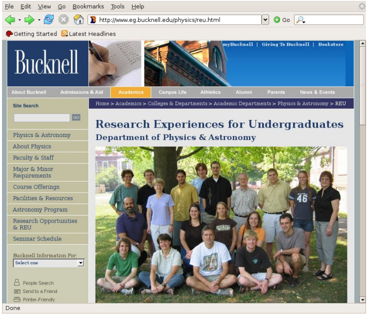
AB and BB Correlation Function — Many Diagrams



Number of one-loop diagrams:

- AA: 6
- AB: 42
- BB: 59

Would be hopeless, except . . .



Summary and Conclusions

- RG methods and exact solutions are complementary. RG justifies the application of reaction-diffusion equations for $d > 2$.
- Many problems can be "solved" by inserting RG flows
  - $n_0 \to n_0 t^{d/2}$
  - $\lambda_0 \to g^*$ for $d < 2$ or $\lambda_0 \to 1/\ln t$
  - $t \to t_0$ and overall $(Dt)^{-d/2}$
- In $A + B \to 0$, the upper critical dimension is $d_c = 2$. Can be seen in unequal initial conditions or reaction zones.
- Many new challenges and Feynman diagrams await...

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: tomorrow.

Exercises (on board during lecture)

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