The Trapping Reaction with Mobile and Reacting Traps

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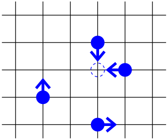
Reaction-Diffusion Models

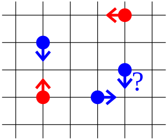
- classical particles hop randomly on lattice
- one-species or multi-species
- react when occupying the same site

Examples:

$A+A \to A$



$A+B \to \varnothing$



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 $d > 2$.

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

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

Reacting Traps

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

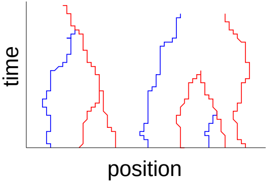
Fluctuations: again important for $d \leq 2$. RG techniques give

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

with universal amplitude [Peliti '86, BL '94]

The Trapping Reaction with Reacting Traps

The decaying trap density increases the survival probability of particles



Rate Equation: $\dot{b} = -\lambda' ab \sim \dfrac{\lambda'}{(2-p)\lambda t}\, b \quad \Rightarrow \quad b \sim t^{-\theta}$

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 $\theta = \dfrac{d}{2-p}\left(\dfrac{1+\delta}{2}\right)^{d/2}$ for $d < 2$.

Renormalization Group Calculation

- RG techniques describe fluctuation dominated case $d \leq 2$.
- Uses Doi-Peliti mapping from master equation to a field theory.
- Gives $b \sim t^{-\theta}$ with

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

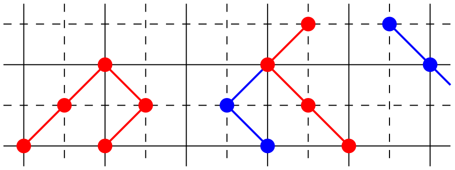
  where $\epsilon = 2 - d$. [Howard '96, Krishnamurthy, Rajesh, & Zaboronski '03, Rajesh, & Zaboronski '04]
- Demonstrates universality!

Straightforward Monte Carlo

Randomly populate a lattice with A and B particles, randomly hop them, and remove particles when they land on the same site.

Random Sequential Update: choose a particle at random, hop and react, then update time by the inverse of the density

Parallel Update: hop all particles simultaneously. Can be done without bias when all particles occupy even sites at the same time.



Improved Monte Carlo

The B particle distribution remains locally Poissonian at all times!

This is because each update consists of

1. On each site, splitting the particles into groups determined by their hopping destination
2. Combining the particles hopping to the same site
3. Removing the particles with probability r if the destinaton site is occupied by a trap.

. . . so local distribution specified by local mean.

Improved Monte Carlo: Update Rules for Local Mean

- The traps (A particles) are still treated via Monte Carlo.
- For a given realization of the trap dynamics, the entire B particle distribution is obtained via simple floating point update rules

  Diffusion: $\tilde{b}_{i,t+1} = z^{-1} \sum_j b_{j,t}$

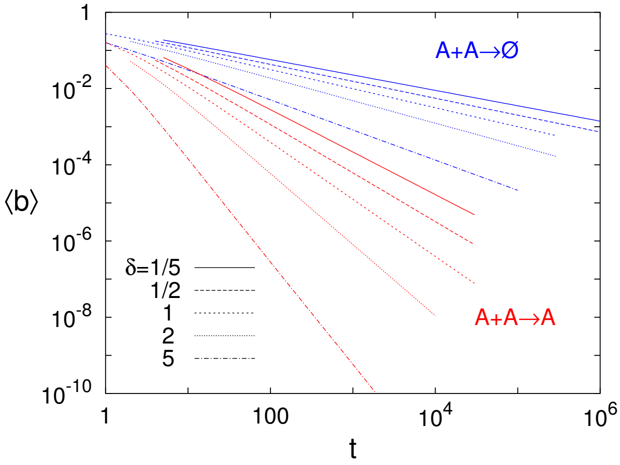
  Reaction: $b_{i,t+1} = (1-r)^{n_{i,t+1}} \, \tilde{b}_{i,t+1}$

  where $n_{i,t}$ is the number of traps on site i at time t.
- $D \neq D'$ by taking multiple A or B steps
- Benefit is much better statistics for little extra effort

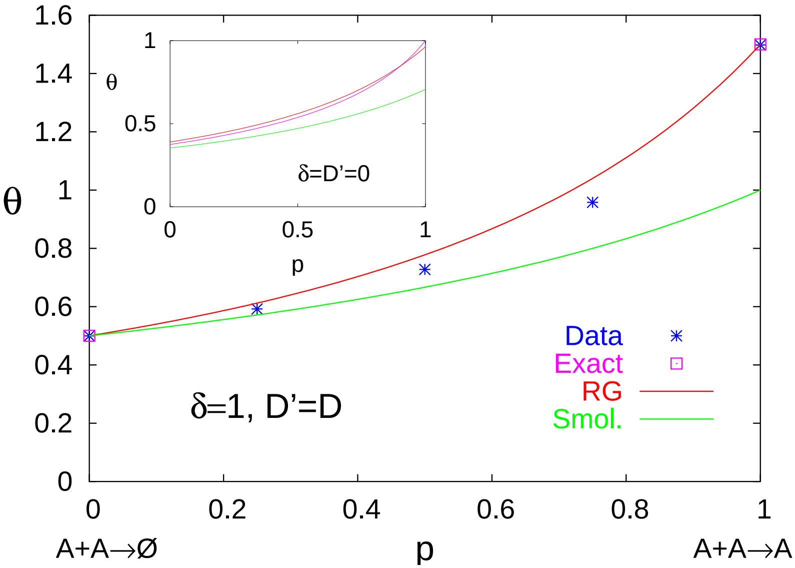
Particle Density Decay

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 $d = 1$

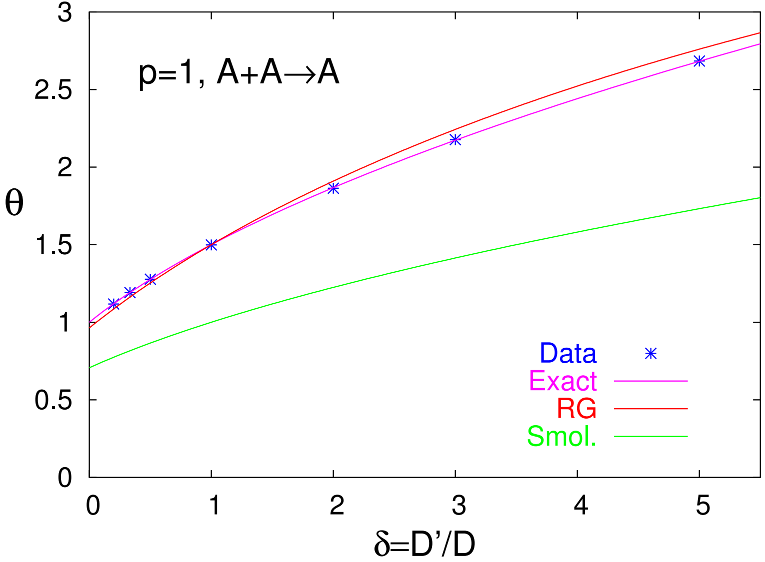
A density known, confirmed. B density power-law in all cases.



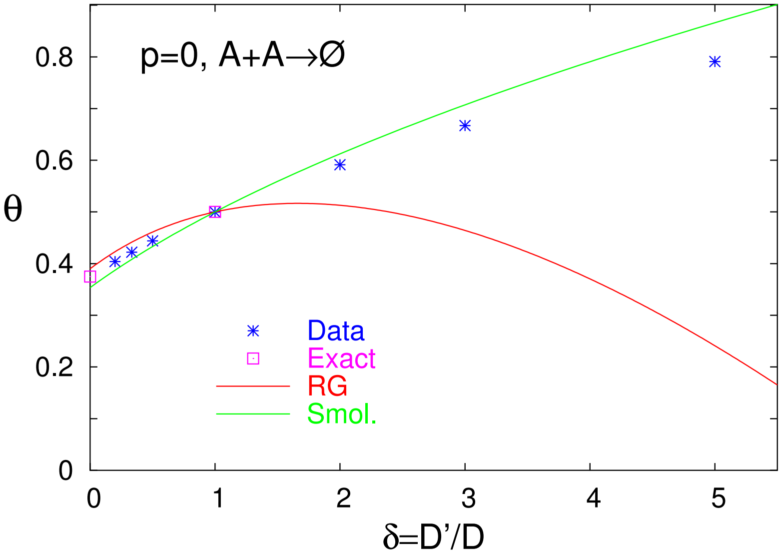
Decay Exponent θ versus p



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



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



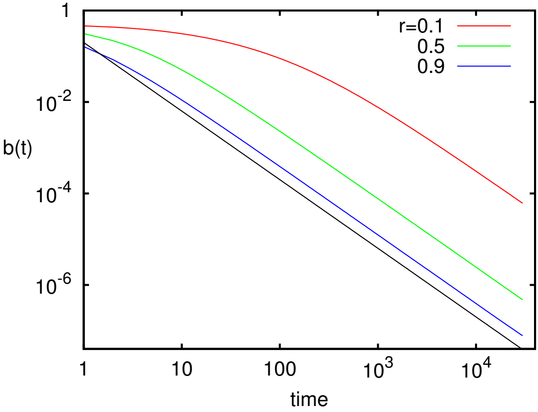
Nonuniversal Amplitude

$A + B \to A$ with probability r when they share a site.

Exponent is universal with respect to microscopic rate, but amplitude isn't.

$A + A \to A$, with $D = D'$.

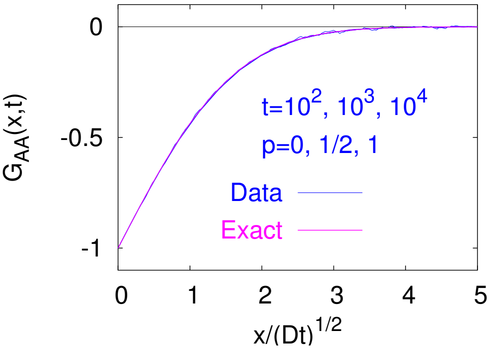
Slope $-3/2$ for reference.



Trap-Trap Correlation Function

Simply scales with the diffusion length:

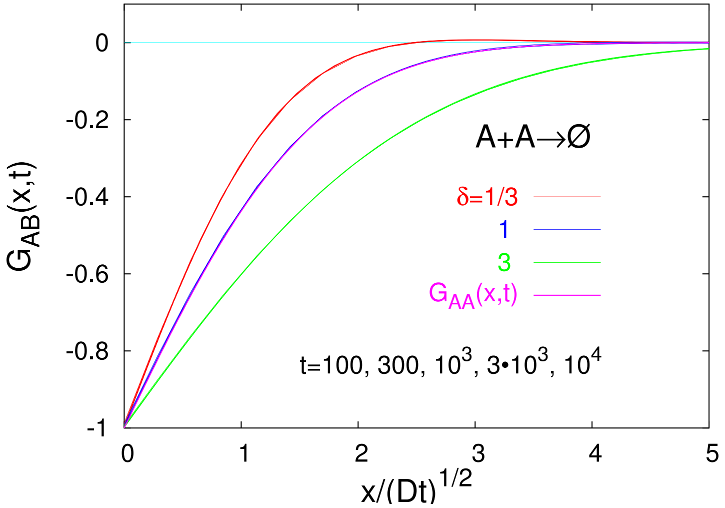
$$C_{AA}(x,t) = \frac{\langle a(x,t)a(0,t)\rangle - \langle a(t)\rangle^2}{\langle a(t)\rangle^2} \sim f_{AA}(x/t^{1/2})$$



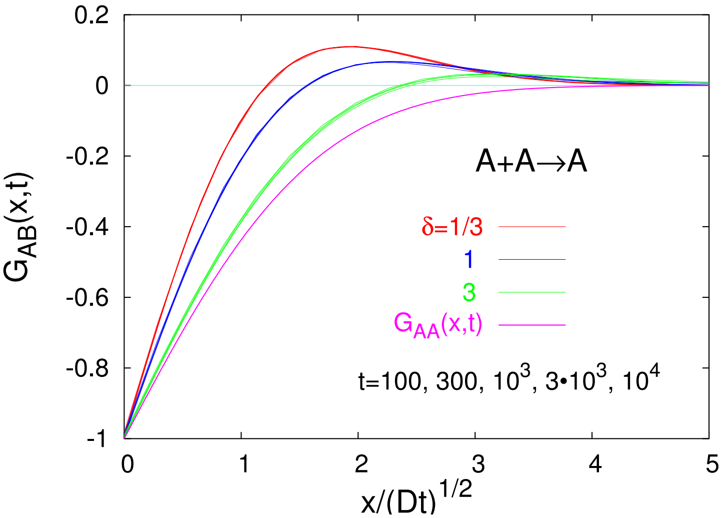
Exact: [Masser & ben-Avraham '01]

Trap-Particle Correlation Function: $p = 0$

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

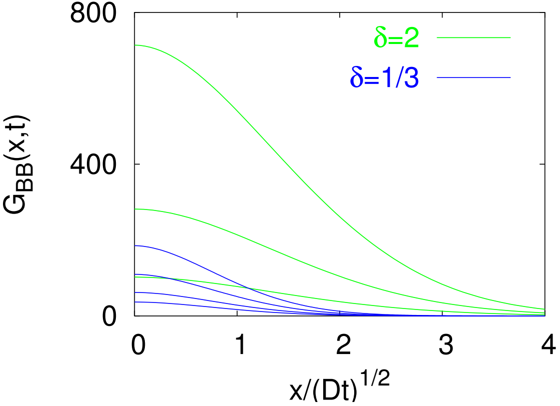


Trap-Particle Correlation Function: $p = 1$



Particle-Particle Correlation Function

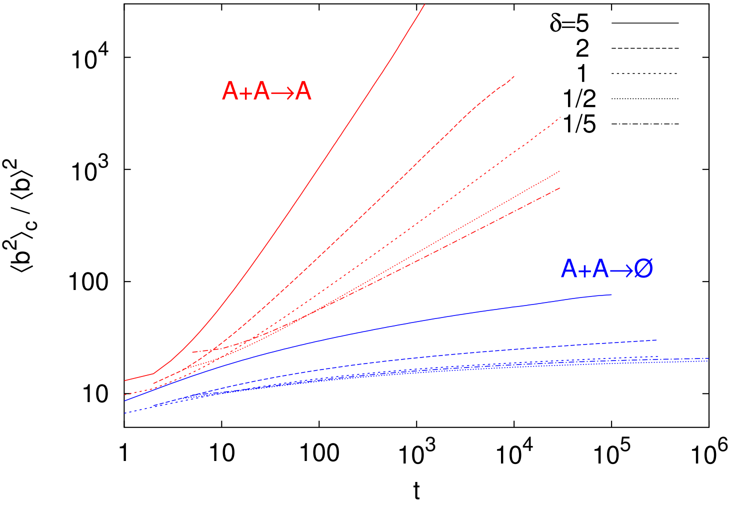
$$C_{BB}(x,t) = \frac{\langle b(x,t)b(0,t)\rangle - \langle b(t)\rangle^2}{\langle b(t)\rangle^2} \sim f_{BB}(x/t^{1/2})?$$



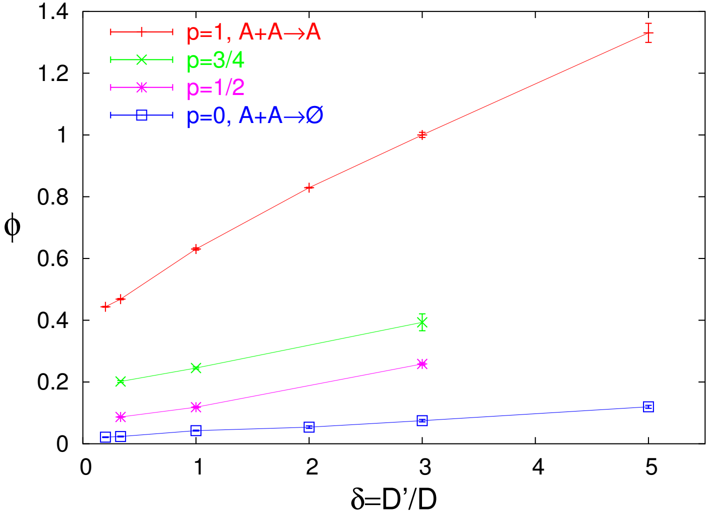
Case $p = 1$. No simple scaling!

Anomalous Dimension

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

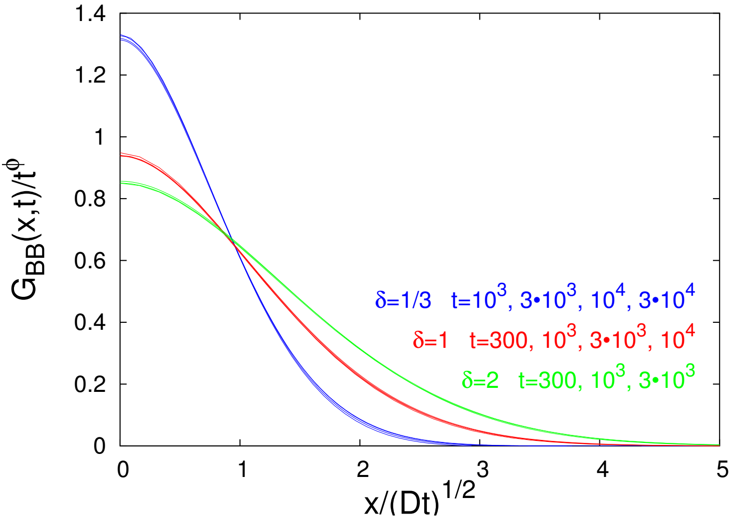


ϕ versus $\delta = D'/D$



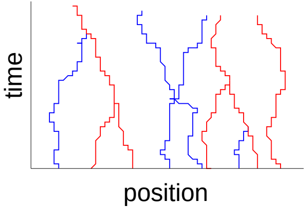
BB Correlations

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 $p = 1$: exponent ϕ a property of a particular 4 walker problem:



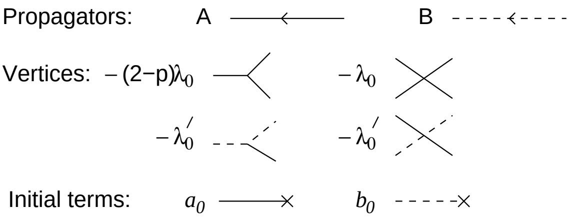
Field Theory

Classical particle model can be mapped to a field theory with $S = S_D + S_R + S_i$:

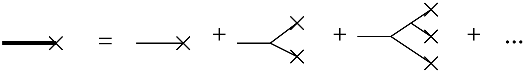
$$S_D = \int d^dx dt \left[\bar{a}(\partial_t - D\nabla^2)a + \bar{b}(\partial_t - D'\nabla^2)b \right]$$

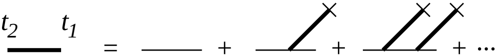
$$S_R = \int d^dx dt \left[(2-p)\lambda_0 \bar{a} a^2 + \lambda_0 \bar{a}^2 a^2 + \lambda_0' \bar{b} ab + \lambda_0' \bar{a}\bar{b} ab \right]$$

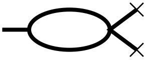
$$S_i = -\int d^dx \left[a_0 \bar{a}(t=0) + b_0 \bar{b}(t=0) \right]$$



Loop Expansion

Density $a^{(0)}$ = 

Response Function 

One Loop Diagrams: 

Density: $a^{(0)}(t) = \dfrac{a_0}{1 + a_0(2-p)\lambda_0 t}$

Response Function:

$$G_{AA}^{(0)}(p, t_2, t_1) = e^{-Dp^2(t_2 - t_1)} \left(\frac{1 + a_0(2-p)\lambda_0 t_1}{1 + a_0(2-p)\lambda_0 t_2} \right)^2$$

RG Calculation for Traps

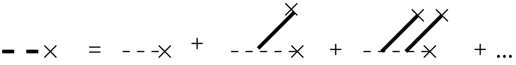
- To renormalize bulk for $d \leq 2$, only coupling constant renormalization needed:

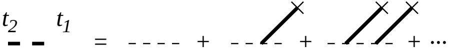
- Under renormalization $\lambda_0 \to$ const.g^*, where $g^* = O(\epsilon)$ fixed point coupling.

- However: $a_0 \to a_0 t^{d/2}$, so a_0 must be summed to all orders $\Rightarrow$ loop expansion.

$$a(t) = (Dt)^{-d/2} \left[\frac{A}{\epsilon} + B + O(\epsilon) \right]$$

RG Calculation for Particles

Density $b^{(0)} =$ 

Response Function 

One Loop Diagrams: 

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.

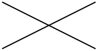
All approaches give the same θ. Can we use one to calculate our anomalous dimension ϕ?

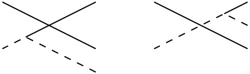
RG Calculation for For Anomalous Dimension

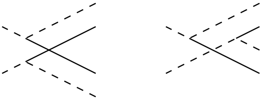
Simplest approach:

$$C_{BB}(p=0,t) = \int d^dx\, e^{ip\cdot x} C_{BB}(x,t) \sim t^{d/2+\phi}$$

Tree level:

AA 

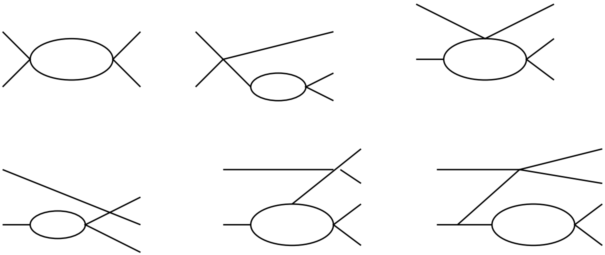
AB 

BB 

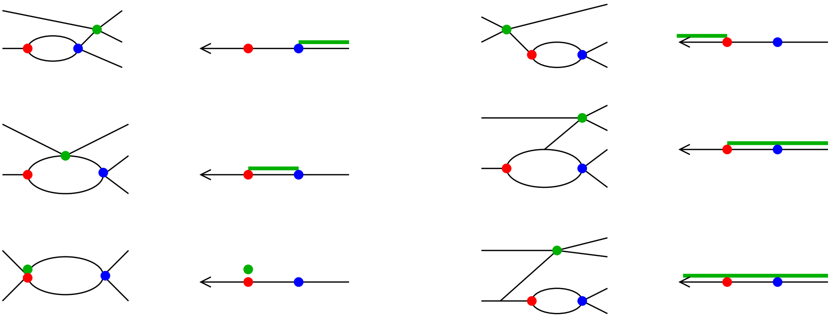
Gives $\phi = 0 + O(\epsilon)$. So we need to look at 1-loop correlations.

Trap-Trap 1-Loop Correlations

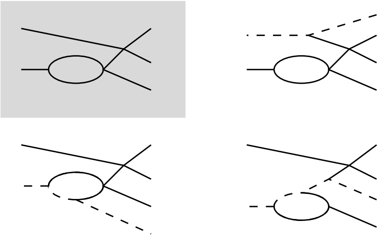
6 diagrams:



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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Summary

- New simulation technique gives high quality data for modest effort.
- Could demonstrate the universality of the correlation functions, nonuniversality of the density amplitude.
- We have learned that the particle-particle correlations do not obey simple scaling: anomalous dimension.
- A tedious but reasonably simple calculation should give us an $O(\epsilon)$ value for ϕ.