Field Theory Approach to Diffusion-Limited Reactions:  
2. Single-Species Annihilation

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The $A + A \to 0$ Annihilation Reaction

- Rate equation: assume particles remain mixed, then $\partial_t a = -\lambda a^2$  
  $\Rightarrow a \sim 1/\lambda t$

- For $d \leq 2$ random walks recurrent: a particle surviving to time $t$ sweeps out a volume $t^{d/2}$,  
  $\Rightarrow a \sim t^{-d/2}$

Anti-correlations cause slower than rate equation decay for $d \leq 2$.

From exact solutions, RG calculations, and simulations we know

$$a \sim \begin{cases} 
  Ct^{-1} & \text{for } d > 2 \\
  \frac{1}{8\pi} \ln t & \text{for } d = 2 \\
  A_d(Dt)^{-d/2} & \text{for } d < 2
\end{cases}$$

with universal amplitudes for $d \leq 2$!

E.g. $A_1 = 1/\sqrt{8\pi}$. 

Field Theory Approach to Diffusion-Limited Reactions

1. Models and Mappings  
   How to turn stochastic particle models into a field theory, with no phenomenology.

2. Single-Species Annihilation  
   Field theoretic renormalization group calculation for $A + A \to 0$ reaction in gory detail.

3. Applications  
   Higher order reactions, disorder, Lévy flights, two-species reactions, coupled reactions.

4. Active to Absorbing State Transitions  
   Directed percolation, branching and annihilating random walks, and all that.
Origin of Universality & Upper Critical Dimension $d_c = 2$

Asymptotically, the spatial separation between surviving particles becomes large.

For $d \leq 2$, a pair of random walkers in a spatial continuum will eventually meet.

- Reaction rate depends on the universal statistics of random walks bringing particles near to each other.
- Lattice effects, capture radius, or reaction probability not relevant

For $d > 2$, point particles undergoing random walks never meet.

- Particles rely on lattice or finite capture radius in order to react
- Effective reaction rate will always depend on these details.

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Critical Behavior in Diffusion-Limited Reactions

Diagrammatic Expansion

Renormalization of Field Theory

RG Equation and Observables

$A + A \rightarrow 0$ Field Theory

Action:

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

($\tilde{\phi}$ $\phi$ diffusion reaction i.c.)

Averages:

$$\langle A(\phi) \rangle = N^{-1} \int \mathcal{D}\tilde{\phi} \mathcal{D}\phi A(\phi) e^{-S[\tilde{\phi},\phi]} \quad N = \int \mathcal{D}\tilde{\phi} \mathcal{D}\phi e^{-S[\tilde{\phi},\phi]}$$

Diffusion part gives gaussian integrals, which is all we know how to do. So we treat the interaction terms perturbatively

- $S = S_D + S_{\text{int}}$

$$\langle A \rangle = N^{-1} \int \mathcal{D}\tilde{\phi} \mathcal{D}\phi A e^{-S_{\text{int}}} e^{-S_D} = \langle A e^{-S_{\text{int}}} \rangle_D$$

Expansion of Interactions

$$S_{\text{int}} = \int d^d x \ dt \left[ 2\lambda_0 \tilde{\phi} \phi^2 + \lambda_0 \tilde{\phi}^2 \phi^2 - n_0 \tilde{\phi} \delta(t) \right]$$

$$e^{-S_{\text{int}}} = 1 - S_{\text{int}} + \frac{1}{2} S_{\text{int}}^2 - \ldots$$

$$= \left( 1 - 2\lambda_0 \int \tilde{\phi}_1 \phi_1^2 + \frac{(2\lambda_0)^2}{2} \int \int \tilde{\phi}_1 \phi_1^2 \tilde{\phi}_2 \phi_2^2 + \ldots \right)$$

$$\times \left( 1 - \lambda_0 \int \tilde{\phi}_1^2 + \frac{\lambda_0^2}{2} \int \int \tilde{\phi}_1 \phi_1^2 \tilde{\phi}_2^2 \phi_2^2 - \ldots \right)$$

$$\times \left( 1 + n_0 \int \tilde{\phi}_1(0) + \frac{1}{2} n_0^2 \int \int \tilde{\phi}_1(0) \phi_1(0) + \ldots \right)$$
Wick’s Theorem

Averages against a gaussian weight equals the product of paired averages, summed over all possible pairings.

Ordinary Gaussian Example:

\[
\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 p_\sigma(x) \, dx = \sigma^2 \quad \Rightarrow \quad \langle x^4 \rangle = 3\langle x^2 \rangle^2 = 3\sigma^4
\]

because

\[
\langle \vdash \vdash \rangle = \begin{array}{c} \vdash \vdash \vdash \vdash \end{array} = 3(\begin{array}{c} \vdash \end{array})^2
\]

Field Theory Example:

\[
\langle \tilde{\phi}_1 \phi_2 \tilde{\phi}_3 \phi_4 \rangle_D = \langle \tilde{\phi}_1 \tilde{\phi}_3 \rangle_D \langle \phi_2 \phi_4 \rangle_D + \langle \tilde{\phi}_1 \phi_4 \rangle_D \langle \phi_2 \tilde{\phi}_3 \rangle_D
\]

Feynman Diagrams

\[
\langle \phi_7 \left( \left( \frac{-2\lambda_0}{2} \right)^2 \int \tilde{\phi}_6 \phi_6^2 \int \tilde{\phi}_5 \phi_5^2 \right) \left( -\lambda_0 \int \tilde{\phi}_4 \phi_4^2 \right) \left( \frac{n_0^3}{3!} \int \int \int \tilde{\phi}_3 \phi_2 \phi_1 \right) \rangle
\]

Propagator

Fourier transform fields: 

\[
\phi(k, \omega) = \int d^d x \, dt \, e^{-i \mathbf{k} \cdot \mathbf{x} + i \omega t} \, \phi(x, t),
\]

action becomes

\[
S_D = \int \frac{d^d k}{(2\pi)^d} \frac{d\omega}{2\pi} \phi(-\mathbf{k}, -\omega)(-i \omega + Dk^2) \phi(k, \omega)
\]

Propagator is Green’s function for diffusion:

\[
G_D(x, t) = \langle \phi(x, t) \tilde{\phi}(0, 0) \rangle_D \quad \Rightarrow \quad G_D(k, \omega) = \frac{1}{-i \omega + Dk^2}
\]

Back into the time domain:

\[
G_D(k, t) = \int \frac{d\omega}{2\pi} \frac{e^{-i \omega t}}{-i \omega + Dk^2}
\]

\[
= \theta(t) e^{-Dk^2 t}
\]

\[
\Rightarrow \quad G_D(x, t > 0) = \frac{e^{-x^2/(4Dt)}}{(4\pi D t)^{d/2}}
\]

Feynman rules — Fourier Space

- only allow diagrams with all interaction vertices connected, earlier \( \tilde{\phi} \) to later \( \phi \) (time flows left)
- each vertex gets a factor:
- vertices connected by propagators \( G_D = e^{-Dk^2 t} \)
- \( k \) conserved at each vertex:
- integrate vertices over time, integrate internal \( k \) over \( \int \frac{d^d k}{(2\pi)^d} \)

\[
\begin{array}{c}
\text{versus}
\end{array}
\]

\[
\begin{array}{c}
\text{versus}
\end{array}
\]
Example 1

Let’s practice a bit (recall \( G_D = e^{-Dk^2t} \))

\[
\int_0^t dt_1 G_D(0, t-t_1) (-2\lambda_0)G_D(0,t_1)^2 n_0^2
\]

\[
= -2\lambda_0 n_0^2 \int_0^t dt_1 = -2\lambda_0 n_0^2 t
\]

… and you thought this would be hard!

Example 2

\[
\int_0^t dt_2 \int_0^{t_2} dt_1 \int \frac{d^d k}{(2\pi)^d} G_D(0, t-t_2)(-2\lambda_0)
\]

\[
\times 2 G_D(k, t_2-t_1) G_D(-k, t_2-t_1) (-\lambda_0) G_D(0, t_1)^2 n_0^2
\]

\[
= 4\lambda_0^2 n_0^2 \int_0^t dt_2 \int_0^{t_2} dt_1 \int \frac{d^d k}{(2\pi)^d} e^{-2Dk^2(t_2-t_1)}
\]

\[
= \frac{4\lambda_0^2 n_0^2}{(8\pi D)^{d/2}} \int_0^t dt_2 \int_0^{t_2} dt_1 (t_2-t_1)^{-d/2} = \frac{16\lambda_0^2 n_0^2}{(8\pi D)^{d/2}} \frac{t^{2-d/2}}{(2-d)(4-d)}
\]

Diagrammatic Expansion for the Density

\[\langle \phi \rangle = \quad + \quad + \quad + \quad + \quad + \quad + \quad \]

\[+ \quad + \quad + \quad + \quad \]

\[+ \quad \]

\[\]

Diagrams have a physical interpretation, in terms of the history of a surviving particle at time \( t \)

Sum of All Tree Diagrams

Dyson Equation

\[= \quad + \quad + \quad + \quad + \quad + \quad + \quad \]

\[= \quad + \quad \]

\[a_{\text{tree}}(t) = n_0 + \int_0^t dt_1 G_D(0, t-t_1)(-2\lambda_0)a_{\text{tree}}(t_1)^2
\]

gives

\[\frac{d a_{\text{tree}}}{dt} = -2\lambda_0 a_{\text{tree}}^2 \quad \text{with i.c.} \quad a_{\text{tree}}(0) = n_0
\]

Rate Equation! With solution: \( a_{\text{tree}}(t) = \frac{n_0}{1 + 2\lambda_0 n_0 t} \)
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Calculate One-Loop Corrections

\[\begin{align*}
\text{Diagram} & + \text{Diag} = -2\lambda_0 n_0^2 t \left[1 - c_d \frac{\lambda_0 t^{1-d/2}}{D^{d/2}}\right]
\end{align*}\]

For \(d > 2\)
- exponent negative, loop correction blows up for \(t\) small (UV)
- not a problem since it is regulated \(t^{1-d/2} \rightarrow (\frac{\Delta x^2}{d^2} + t)^{1-d/2}\)
- Loops “renormalize” interaction vertex a finite, nonuniversal amount, giving \(\dot{\phi} \sim -2\lambda_{\text{eff}} \phi^2 \leq \text{Rate equation!}\)

For \(d < 2\)
- exponent positive, loop correction blows up for \(t\) large (IR).
- “Bare” expansion is worthless! Need renormalization group.

\(d_c = 2\) is the upper critical dimension.

The Renormalization Group Method is . . .

- A method for curing divergences (our long-time problem)
- A method for finding the unique continuum limit
- The systematic removal of short-distance degrees of freedom resulting in an effective theory for the long-distance degrees of freedom (Wilson)
- Useful near criticality, where the long-distance physics exhibits scale invariance
- Generally only possible perturbatively, so a small parameter is needed
- A resummation of an apparently divergent series to give a convergent series

Renormalization Group Recipe

1. identify primitive divergences via power counting
2. use a normalization point to define renormalized couplings (and renormalized fields, but we won’t need that here)
3. exchange the bare expansion for a renormalized expansion
4. use the RG flow equations to let renormalized couplings flow to their fixed points
5. treat yourself to some Ben and Jerry’s
**Primitive Divergences**

We need to identify which subgraphs contain IR divergences for \( d \leq 2 \):

- **Power counting** shows that only subgraphs with two incoming lines are primitively divergent.
- Our interactions cannot increase the number of lines, so there are no diagrams that “dress” the propagator ⇒ no field renormalization required
- There are no interactions with zero lines coming out ⇒ the only two subgraphs needing renormalization are \( \lambda^{(1,2)} \) and \( \lambda^{(2,2)} \)

**Vertex Function Sum**

\( \lambda^{(1,2)} \) and \( \lambda^{(2,2)} \) contain the same diagrams:

\[
\begin{align*}
\lambda^{(1,2)}(s) &= + + + + \cdots \\
\lambda^{(2,2)}(s) &= + + + + \cdots
\end{align*}
\]

They renormalize identically because of probability conservation and they can be summed exactly!

\[
\lambda^{(2,2)}(t,0) = \lambda_0 \delta(t) - \lambda_0^2 I(t) + \lambda_0^3 \int_0^t dt_1 I(t-t_1) I(t_1) + \cdots
\]

with loop integral \( I(t) = 2(8\pi Dt)^{-d/2} \). Now Laplace transform:

\[
\lambda^{(2,2)}(s) = \lambda_0 - \lambda_0^2 I(s) + \lambda_0^3 I(s)^2 - \lambda_0^4 I(s)^3 + \cdots = \lambda_0 \left[ \frac{1}{1 + \lambda_0 I(s)} \right]
\]

**Renormalized Couplings**

**Normalization point:** choose an arbitrary time \( t_0 \) (to avoid IR)

- Define dimensionless bare coupling \( g_0 \), which is invariant under rescaling:
  \( g_0 \equiv \frac{\lambda_0 t_0}{(Dt_0)^{d/2}} \)
- Define the renormalized coupling \( g_R \) via
  \[
  g_R = \left. \frac{\lambda^{(2,2)}(s) t_0}{(Dt_0)^{d/2}} \right|_{s=t_0^{-1}} = \frac{\lambda_0 t_0}{(Dt_0)^{d/2}} \left[ \frac{1}{1 + \lambda_0 I(s)} \right]_{s=t_0^{-1}}
  \]
  \[
  = \frac{g_0}{1 + g_0/g^*} \quad \text{where} \quad g^* = \frac{(8\pi)^{d/2}}{2\Gamma(1-d/2)} \sim 2\pi(2 - d)
  \]
- Invert to get
  \[
  g_0 = \frac{g_R}{1 - g_R/g^*} = g_R + \frac{g_R^2}{g^*} + \frac{g_R^3}{g^*^2} \cdots
  \]
The $\beta$ Function

Since $\lambda_0 = \lambda_0(g_R, D, t_0)$, we can write the density

$$a(t, n_0, D, \lambda_0) = a(t, n_0, D, g_R, t_0)$$

But our choice of $t_0$ is arbitrary, so

$$0 = t_0 \frac{d a}{d t_0} = \left[ t_0 \frac{\partial a}{\partial t_0} - \beta(g_R) \frac{\partial a}{\partial g_R} \right]$$

where

$$\beta(g_R) = -t_0 \left( \frac{\partial g_R}{\partial t_0} \right)_{\lambda_0, D} = \left( -\frac{2 - d}{2} \right) g_R + \frac{\Gamma(2 - d/2)}{2(8\pi)^{d/2}} g_R^2$$

$\beta \overset{d>2}{=} \beta \overset{d<2}{\sim} \beta$

Method of Characteristics

$$\left[ t \frac{\partial}{\partial t} - \frac{n_0 d}{2} \frac{\partial}{\partial n_0} + \beta(g_R) \frac{\partial}{\partial g_R} + \frac{d}{2} \right] a(t, n_0, g_R, t_0) = 0$$

Make a total derivative $d/dt$ via the “running couplings” $\tilde{n}_0$ and $\tilde{g}_R$

$$t \frac{d \tilde{n}_0}{d t} = -\frac{d}{2} \tilde{n}_0 \quad \text{with i.c.} \quad \tilde{n}_0(t) = n_0$$

$$t \frac{d \tilde{g}_R}{d t} = \beta(\tilde{g}_R) \quad \text{with i.c.} \quad \tilde{g}_R(t) = g_R$$

Solutions:

$$\tilde{n}_0(t/b) = n_0 b^{d/2} \quad \tilde{g}_R(t/b) = g^* \left( 1 + \frac{g^* - g_R}{g_R b^{1-d/2}} \right)$$

For large $b$ we have $\tilde{g}_R(b) \to g^*$ (good), but $\tilde{n}_0 \to \infty$ (bad).

Solution to RG Equation

$\overset{\beta \overset{d>2}{=} \beta \overset{d<2}{\sim} \beta}{\Rightarrow}$

$$a(t, n_0, g_R, t_0) = b^{-d/2} a \left( t/b, n_0 b^{d/2}, \tilde{g}_R(b), t_0 \right) \sim (t/t_0)^{-d/2} a \left( t_0, n_0(t/t_0)^{d/2}, g^*, t_0 \right)$$

- Compares the density at time $t$ to an earlier density with rescaled size and renormalized coupling.

- We can safely calculate the right-hand side in bare perturbation theory, since it is an early time expansion

- **Recipe**: In bare expansion,
  - sub in $n_0 \to n_0(t/t_0)^{d/2}$, $g_R \to g^* \sim O(2 - d)$, and $t \to t_0$
  - multiply by $(t/t_0)^{-d/2}$. 

From dimensional analysis

$$a(t, n_0, D, g_R, t_0) = (D t_0)^{-d/2} f \left( t/t_0, n_0(D t_0)^{d/2}, g_R \right)$$

and so

$$t_0 \frac{d a}{d t_0} = \left[ -\frac{d}{2} - t \frac{\partial f}{\partial t} + \frac{n_0 d}{2} \frac{\partial f}{\partial n_0} \right] a$$

Recall that $t_0 \frac{\partial a}{\partial t_0} = \beta(g_R) \frac{\partial a}{\partial g_R}$.

Combining these gives the RG equation

$$\left[ t \frac{\partial}{\partial t} - \frac{n_0 d}{2} \frac{\partial}{\partial n_0} + \beta(g_R) \frac{\partial}{\partial g_R} + \frac{d}{2} \right] a(t, n_0, g_R, t_0) = 0$$
\( \epsilon = 2 - d \) Expansion — Tree Level

- \( g_R \rightarrow g^* = 2\pi\epsilon + O(\epsilon^2) \) is a small parameter
- But \( n_0 \rightarrow n_0(t/t_0)^{d/2} \) flows to infinity, so we can’t use perturbation theory unless we can re-sum to all orders of \( n_0 \).

Tree Diagrams

\[
\alpha^{(0)} = \frac{n_0}{1 + 2\lambda_0 n_0 t} \rightarrow \frac{1}{2\lambda_0 t} = \frac{1}{2g_0(Dt_0)^{d/2}t_0^{-1}t}
\]

Recall \( g_0 = g_R + O(g_R^2) \), so

\[
\alpha^{(0)} \sim \frac{(t/t_0)^{-d/2}}{2g_0(Dt_0)^{d/2}t_0^{-1}t_0} + O(g_0^0) = \frac{1}{2g^*(Dt)^{-d/2} + O(g_R^0)}
\]

We find expected time dependence, and a universal amplitude. But what about the other diagrams?

\( d = d_c = 2 \)

The \( \beta \)-function becomes

\[
\beta(g_R) = \frac{1}{16\pi} g_R^2
\]

Running coupling flows to zero as

\[
\tilde{g}_R(t/b) \sim \frac{4\pi}{\ln t}
\]

It’s still a small parameter, so loop expansion still useful. But now tree diagrams give asymptotic result:

\[
a \sim \frac{1}{2g_R} \frac{1}{Dt} \sim \left( \frac{1}{8\pi Dt} + O\left( \frac{1}{Dt} \right) \right)
\]

Matches exact solution!

\( \epsilon = 2 - d \) Expansion — Loops

**Topology:** diagrams of order \( n_k \lambda_k^k \) have \( n = k + 1 - j \) loops, which implies the sum of all \( n \)-loop diagrams has the form

\[
a^{(n)}(t, n_0, \lambda_0) = \lambda_0^{n-1} f(t, \lambda_0 n_0)
\]

**Calculation:** infinite sums of diagrams with \( n \) loops are order \( O(1) \) in the \( n_0 \rightarrow \infty \) limit. (Shown on the next slide . . .)

Recall that the \( t \)-dependence comes from \( n_0 \) and the overall \( t^{-d/2} \) factor.

**Conclusion:** loop expansion gives \( a^{(n)} \sim g^*(n-1)t^{-d/2} \) to all orders:

\[
a \sim \left[ \frac{1}{4\pi \epsilon} + \frac{2\ln 8\pi - 5}{16\pi} + O(\epsilon) \right] \frac{1}{(Dt)^{d/2}}
\]
Summary and Observations

- Whew!
- Reaction-diffusion field theory for decay processes yield controlled RG calculations, relatively rare in nonequilibrium (compare KPZ, Cahn-Hilliard)
- And can be renormalized to all orders in the loop expansion, relatively rare anywhere!
- For $d < 2$, all orders of diagrams contribute to the $t^{-d/2}$ decay, but the universal amplitude is obtained perturbatively
- RG calculation confirms exact results (for $d = 2$) and demonstrates universality.

Bibliography

$A + A \rightarrow 0$ Renormalization Group Calculation

$A + A \rightarrow 0$ Exact Solutions

Field Theory and RG Techniques

Exercises

1. Loop integrals
   - (a) Confirm that $I(t) = 2(8\pi Dt)^{-d/2}$. Laplace transform this to find $I(s)$.
   - (b) From the definitions of $g_R$, $g_0$, and $g^*$, confirm $g_R = g_0/(1 + g_0/g^*)$.
2. The sum of all 2-loop diagrams can be given by six “skeleton” diagrams. One of these was given. Identify the other five.
3. Order of loop diagrams
   - (a) Confirm that diagrams of order $\lambda_0^kn_j$ have $n = k + 1 - j$ loops.
   - (b) Show that this implies that the sum of all $n$-loop diagrams has the form $\lambda_0^{n-1}f(\lambda_0n_0)$.
4. Calculating the tree-level response function
   - (a) Show that the Dyson equation for the tree-level response function gives
     $$G(k, t_2,t_1)_{tr} = e^{-Dk^2(t_2-t_1)} + \int_{t_1}^{t_2} dt' e^{-Dk^2(t_2-t_1)}(-2\lambda_0)2\alpha_{tree}(t')G(k, t', t_1)_{tr}$$
   - (b) Plug in the hypothesis $G_{tr} = e^{-Dk^2(t_2-t_1)}f(t_2, t_1)$ and derive a differential equation for $f(t_2, t_1)$.
   - (c) Integrate this equation to confirm the result for $G_{tr}$ quoted in the talk.