Field Theory Approach to Diffusion-Limited Reactions:

2. Single-Species Annihilation

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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.

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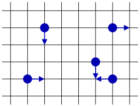
Critical Behavior in Diffusion-Limited Reactions

Diagrammatic Expansion

Renormalization of Field Theory

RG Equation and Observables

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 suriving 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

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

with universal amplitudes for $d \leq 2$!

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

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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$A + A \to 0$ Field Theory

Action:

$$S = \int d^d x\, dt \left[\underbrace{\tilde{\phi}(\partial_t - D\nabla^2)\phi}_{\text{diffusion}} + \underbrace{2\lambda_0 \tilde{\phi}\phi^2 + \lambda_0 \tilde{\phi}^2\phi^2}_{\text{reaction}} - \underbrace{n_0 \tilde{\phi}\,\delta(t)}_{\text{i.c.}}\right]$$

Averages:

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

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

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

Expansion of Interactions

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

$$\begin{aligned} e^{-S_{\text{int}}} &= 1 - S_{\text{int}} + \tfrac{1}{2} S_{\text{int}}^2 - \dots \\ &= \left(1 - 2\lambda_0 \int \tilde{\phi}_1\phi_1^2 + \tfrac{(2\lambda_0)^2}{2} \iint \tilde{\phi}_1\phi_1^2\, \tilde{\phi}_2\phi_2^2 + \dots\right) \\ &\quad \times \left(1 - \lambda_0 \int \tilde{\phi}_1^2\phi_1^2 + \tfrac{\lambda_0^2}{2} \iint \tilde{\phi}_1^2\phi_1^2\, \tilde{\phi}_2^2\, \phi_2^2 - \dots\right) \\ &\quad \times \left(1 + n_0 \int' \tilde{\phi}_1(0) + \frac{1}{2} n_0^2 \int'\!\!\int' \tilde{\phi}_1(0)\tilde{\phi}_2(0) + \dots\right) \end{aligned}$$

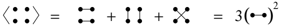
Wick's Theorem

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

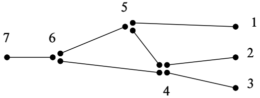


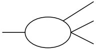
Field Theory Example:

$$\langle \phi_1\phi_2\tilde\phi_3\tilde\phi_4\rangle_D = \langle\phi_1\tilde\phi_3\rangle_D\langle\phi_2\tilde\phi_4\rangle_D + \langle\phi_1\tilde\phi_4\rangle_D\langle\phi_2\tilde\phi_3\rangle_D$$

Feynman Diagrams

$$\left\langle \phi_7 \left(\frac{(-2\lambda_0)^2}{2} \int \tilde\phi_6\phi_6^2 \int \tilde\phi_5\phi_5^2 \right) \left(-\lambda_0 \int \tilde\phi_4^2\phi_4^2 \right) \left(\frac{n_0^3}{3!} \int' \!\! \int' \!\! \int' \tilde\phi_3\, \tilde\phi_2\, \tilde\phi_1 \right) \right\rangle$$





Propagator

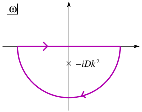
Fourier transform fields: $\phi(\mathbf{k},\omega) = \int d^dx\, dt\, e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t}\,\phi(\mathbf{x},t)$, action becomes

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

Propagator is Green's function for diffusion:

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

Back into the time domain:



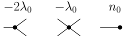
$$G_D(\mathbf{k},t) = \int \frac{d\omega}{2\pi}\,\frac{e^{-i\omega t}}{-i\omega + Dk^2}$$

$$= \boxed{\theta(t)\, e^{-Dk^2 t}}$$

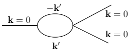
$$\Rightarrow \quad G_D(\mathbf{x},t>0) = \frac{e^{-x^2/(4Dt)}}{(4\pi Dt)^{d/2}}$$

Feynman rules — Fourier Space

- only allow diagrams with all interaction vertices connected, earlier $\tilde\phi$ to later ϕ (time flows left)
- each vertex gets a factor:

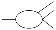


- vertices connected by propagators $G_D = e^{-Dk^2 t}$
- $\mathbf{k}$ conserved at each vertex:



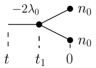
- integrate vertices over time, integrate internal $\mathbf{k}$ over $\int \frac{d^dk}{(2\pi)^d}$
- symmetry factors:

versus



Example 1

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

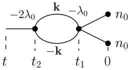


$$\int_0^t dt_1\, G_D(0, t-t_1)(-2\lambda_0) G_D(0,t_1)^2 n_0^2$$

$$= -2\lambda_0 n_0^2 \int_0^t dt_1 = \boxed{-2\lambda_0 n_0^2 t}$$

…and you thought this would be hard!

Example 2



okay, that was a little bit hard

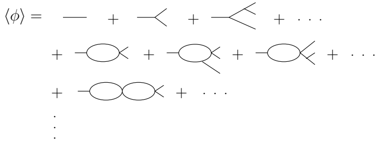
$$\int_0^t dt_2 \int_0^{t_2} dt_1 \int \frac{d^d k}{(2\pi)^d}\, G_D(0, t-t_2)(-2\lambda_0)$$

$$\times\, 2\, G_D(\mathbf{k}, t_2 - t_1) G_D(-\mathbf{k}, t_2 - t_1)(-\lambda_0) G_D(0,t_1)^2 n_0^2$$

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

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

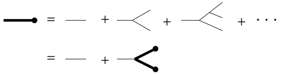
Diagrammatic Expansion for the Density



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

Sum of All Tree Diagrams

Dyson Equation



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

gives

$$\frac{da_{\text{tree}}}{dt} = -2\lambda_0 a_{\text{tree}}^2 \qquad \text{with i.c.} \qquad a_{\text{tree}}(0) = n_0$$

Rate Equation!

With solution: $a_{\text{tree}}(t) = \dfrac{n_0}{1 + 2\lambda_0 n_0 t}$

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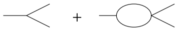
Calculate One-Loop Corrections



$$+ \quad = -2\lambda_0 n_0^2 t \left[1 - c_d \frac{\lambda_0 t^{1-d/2}}{D^{d/2}}\right]$$

For $d > 2$

- exponent negative, loop correction blows up for t small (UV)
- not a problem since it is regulated $t^{1-d/2} \rightarrow (\frac{\Delta x^2}{D} + t)^{1-d/2}$
- Loops "renormalize" interaction vertex a finite, nonuniversal amount, giving $\dot{\phi} \sim -2\lambda_{\text{eff}}\phi^2 \quad \Leftarrow$ 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

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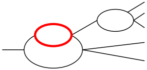
Renormalization Group Recipe

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 $d \leq 2$:



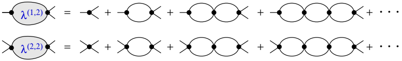
Power counting shows that only subgraphs with two incoming lines are primitively divergent.

Our interactions cannot increase the number of lines, so

- there are no diagrams that “dress” the propagator
  $\Rightarrow$ no field renormalization required
- there are no interactions with zero lines coming out
  $\Rightarrow$ the only two subgraphs needing renormalization are

Vertex Function Sum

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



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

$$\lambda^{(2,2)}(t,0) = \lambda_0\delta(t) - \lambda_0^2 I(t) + \lambda_0^3\int_0^t dt_1\, I(t-t_1)I(t_1)$$
$$-\lambda_0^4\int_0^t dt_2\int_0^{t_2} dt_1\, I(t-t_2)I(t_2-t_1)I(t_1) + \dots$$

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

$$\lambda^{(2,2)}(s) = \lambda_0 - \lambda_0^2 I(s) + \lambda_0^3 I(s)^2 - \lambda_0^4 I(s)^3 + \dots = \boxed{\frac{\lambda_0}{1+\lambda_0 I(s)}}$$

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

$$g_R \equiv \left.\frac{\lambda^{(2,2)}(s)\, t_0}{(Dt_0)^{d/2}}\right|_{s=t_0^{-1}} = \frac{\lambda_0 t_0}{(Dt_0)^{d/2}}\left[\frac{1}{1+\lambda_0 I(s)}\right]_{s=t_0^{-1}}$$

$$= \frac{g_0}{1+g_0/g^*} \quad \text{where } g^* = \frac{(8\pi)^{d/2}}{2\,\Gamma(1-d/2)} \sim 2\pi(2-d)$$

- Invert to get

$$g_0 = \frac{g_R}{1-g_R/g^*} = g_R + \frac{g_R^2}{g^*} + \frac{g_R^3}{g^{*2}}\dots$$

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The β Function

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

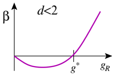
$$a(t, n_0, D, \lambda_0) = a(t, n_0, D, g_R, t_0)$$

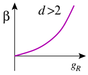
But our choice of t_0 is arbitrary, so

$$0 = t_0 \frac{da}{dt_0} = \left[t_0 \frac{\partial}{\partial t_0} - \beta(g_R) \frac{\partial}{\partial g_R} \right] a$$

where

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





RG Equation

From dimensional analysis

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

and so

$$t_0 \frac{\partial a}{\partial t_0}\bigg|_{g_R} = \left[-\frac{d}{2} - t\frac{\partial}{\partial t} + \frac{n_0 d}{2} \frac{\partial}{\partial n_0} \right] a$$

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

Combining these gives the RG equation

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

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 $\tilde{g}_R$

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

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

Solutions:

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

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

Solution to RG Equation

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

$$\sim (t/t_0)^{-d/2}\, a\Big(t_0,\ n_0 (t/t_0)^{d/2},\ g^*,\ t_0\Big)$$

- 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 $(t/t_0)^{-d/2}$.

$\epsilon = 2 - d$ Expansion — Tree Level

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

Tree Diagrams

$$a^{(0)} = \frac{n_0}{1 + 2\lambda_0 n_0 t} \quad \to \quad \frac{1}{2\lambda_0 t} = \frac{1}{2 g_0 (D t_0)^{d/2} t_0^{-1} t}$$

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

$$a^{(0)} \sim \frac{(t/t_0)^{-d/2}}{2 g_R (D t_0)^{d/2} t_0^{-1} t_0} + O(g_R^0) = \boxed{\frac{1}{2g^*}(Dt)^{-d/2} + O(g_R^0)}$$

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

$\epsilon = 2 - d$ Expansion — Loops

Topology: diagrams of order $n_0^j \lambda_0^k$ have $n = k + 1 - j$ loops, which implies the sum of all n-loop diagrams has the form

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

Calculation: infinite sums of diagrams with n loops are order $O(1)$ in the $n_0 \to \infty$ 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:

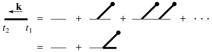
$$a \sim \left[\frac{1}{4\pi\epsilon} + \frac{2\ln 8\pi - 5}{16\pi} + O(\epsilon)\right] \frac{1}{(Dt)^{d/2}}$$

Sum of All n-Loop Diagrams

Define the tree-level response function:

$$G(\mathbf{k}, t_2, t_1)_{\text{tr}} = F.T. \langle \phi(\mathbf{x}_2, t_2) \tilde{\phi}(\mathbf{x}_1, t_1) \rangle_{\text{tree}}$$

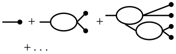
This obeys a Dyson eq:



which yields

$$G(\mathbf{k}, t_2, t_1)_{\text{tr}} = e^{-Dk^2(t_2 - t_1)} \left[\frac{1 + 2\lambda_0 n_0 t_1}{1 + 2\lambda_0 n_0 t_2}\right]^2 \sim e^{-Dk^2(t_2 - t_1)} \left(\frac{t_1}{t_2}\right)^2$$

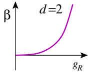
All loop diagrams can be constructed from G_{tr} and a_{tree}



$d = d_c = 2$

The β-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:

$$a \sim \frac{1}{2g_R} \frac{1}{Dt} \sim \boxed{\frac{1}{8\pi} \frac{\ln t}{Dt} + O\left(\frac{1}{Dt}\right)}$$

Matches exact solution!

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.

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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 $\lambda_0^k n_0^j$ have $n = k + 1 - j$ loops.
   (b) Show that this implies that the sum of all n-loop diagrams has the form $\lambda_0^{n-1} f(\lambda_0 n_0)$.

Exercises

4. Calculating the tree-level response function
   (a) Show that the Dyson equation for the tree-level response function gives

$$G(\mathbf{k}, t_2, t_1)_{\text{tr}} = e^{-Dk^2(t_2-t_1)} + \int_{t_1}^{t_2} dt'\, e^{-Dk^2(t_2-t_1)}(-2\lambda_0)2a_{\text{tree}}(t')G(\mathbf{k}, t', t_1)_{\text{tr}}$$

   (b) Plug in the hypothesis $G_{\text{tr}} = e^{-Dk^2(t_2-t_1)} f(t_2, t_1)$ 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.