Field Theory Approach to Diffusion-Limited Reactions:
1. Models and Mappings

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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 $A + A \rightarrow 0$ 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.
Diffusion-Limited Reactions

One or more species of particles undergoing random walks on a lattice, with reactions occurring for particles on the same lattice site.

\[ \text{A} + \text{A} \rightarrow \text{A} \quad \text{A} + \text{B} \rightarrow \emptyset \]

Example: for \( \text{A} + \text{A} \rightarrow \emptyset \) the density of particles decays as

\[
\rho(t) = \begin{cases} 
Ct^{-1} & \text{for } d > 2 \\
\tilde{A} \ln t / D & \text{for } d = 2 \\
A_d (Dt)^{-d/2} & \text{for } d < 2
\end{cases}
\]

where \( A_d \) and \( \tilde{A} \) are universal numbers!
Diffusion-Limited Reactions

One or more species of particles undergoing random walks on a lattice, with a reactions occurring for particles on the same lattice site.

\[
\begin{align*}
A + A &\rightarrow A \\
A + B &\rightarrow \emptyset
\end{align*}
\]

Example: for \( A + A \rightarrow 0 \) the density of particles decays as

\[
\rho(t) = \begin{cases} 
Ct^{-1} & \text{for } d > 2 \\
\tilde{A} \ln \frac{t}{Dt} & \text{for } d = 2 \\
A_d(Dt)^{-d/2} & \text{for } d < 2 
\end{cases}
\]

where \( A_d \) and \( \tilde{A} \) are universal numbers!
Field Theory Approach to Diffusion-Limited Reactions:
1. Models and Mappings

Master Equation for Lattice Models

Doi Representation

Mapping to Field Theory
Consider a set of lattice sites labeled $i = 1, 2, 3, \ldots$, and each site is occupied by $n_1, n_2, n_3, \ldots$ particles.

Define

- $\alpha$ = a particular state, i.e., $\alpha = \{n_1, n_2, n_3, \ldots \}$
- $P(\alpha, t)$ = the probability of obtaining state $\alpha$ at time $t$. 

\[ n_i \]

\[ i \]
Dynamical processes (hops, reactions, decays) will cause a change of state from $\alpha$ to $\beta$. 

\[
w_{\alpha \rightarrow \beta} = \text{rate of transition from } \alpha \text{ to } \beta, \text{ defines dynamics}
\]

**Master Equation**

\[
\frac{d}{dt} P(\alpha, t) = \sum_{\beta} \left[ w_{\beta \rightarrow \alpha} P(\beta, t) - w_{\alpha \rightarrow \beta} P(\alpha, t) \right]
\]

- $\sum_{\alpha} P(\alpha, t) = 1$ preserved by the master equation
- Initial conditions $P(\alpha, 0)$ need to be specified
Consider a single lattice site that contains some number of identical particles. These particles decay at rate $\lambda$.

The rate for a transition from $n$ to $m$ particles is

$$w_{n \rightarrow m} = \begin{cases} 
0 & \text{for } m \neq n - 1 \\
n\lambda & \text{for } m = n - 1 
\end{cases}$$

and the master equation is

$$\frac{d}{dt} P(n, t) = \lambda \left[ (n + 1)P(n + 1, t) - n P(n, t) \right]$$
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and the master equation is

$$\frac{d}{dt} P(n, t) = \lambda \left[ (n + 1)P(n + 1, t) - n \, P(n, t) \right]$$

Wait! That doesn’t look like exponential decay . . .
Master Equation to Differential Equation

Let $\rho(t) = \langle n \rangle = \sum_n n P(n, t)$ be the average number of particles at time $t$. Then

$$\dot{\rho} = \sum_n n \dot{P}(n, t) = \sum_n n \left[ \lambda (n + 1) P(n + 1, t) - \lambda n P(n, t) \right]$$
Master Equation to Differential Equation

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$$\dot{\rho} = \sum_n n \dot{P}(n, t) = \sum_n n \left[ \lambda(n + 1)P(n + 1, t) - \lambda n P(n, t) \right]$$

$$= \lambda \sum_n n(n + 1)P(n + 1, t) - \lambda \sum_n n^2 P(n, t)$$

$$= \lambda \sum_m (m - 1)mP(m, t) - \lambda \sum_n n^2 P(n, t)$$
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$$\dot{\rho} = \sum_n n \dot{P}(n, t) = \sum_n n \left[ \lambda(n + 1)P(n + 1, t) - \lambda n P(n, t) \right]$$

$$= \lambda \sum_n n(n + 1)P(n + 1, t) - \lambda \sum_n n^2 P(n, t)$$

$$= \lambda \sum_m (m - 1)m P(m, t) - \lambda \sum_n n^2 P(n, t)$$

$$= -\lambda \sum_m m P(m, t)$$

$$= -\lambda \rho$$
Again, consider a single lattice site, with the rule that a pair of particles may annihilate each other. The rates are

\[ w_{n \rightarrow m} = \begin{cases} 
0 & \text{for } m \neq n - 2 \\
n(n - 1)\lambda & \text{for } m = n - 2
\end{cases} \]

and the master equation is

\[ \frac{d}{dt}P(n, t) = \lambda \left[ (n + 2)(n + 1)P(n + 2, t) - n(n - 1)P(n, t) \right] \]
Now consider two sites, \( i = 1 \) and 2, with a rate \( \Gamma \) of hopping from site 1 to site 2.

\[
\begin{align*}
\mathcal{W}_{(n_1, n_2) \rightarrow (m_1, m_2)} &= \begin{cases} 
0 & \text{for } m_1 \neq n_1 - 1 \text{ or } m_2 \neq n_2 + 1 \\
n_1 \Gamma & \text{for } m_1 = n_1 - 1 \text{ and } m_2 = n_2 + 1
\end{cases}
\end{align*}
\]

and the master equation is

\[
\frac{d}{dt} P(n_1, n_2, t) = \Gamma \left[ (n_1 + 1) P(n_1 + 1, n_2 - 1, t) - n_1 P(n_1, n_2, t) \right]
\]
Consider a one-dimensional chain of lattice sites $i = 1, 2, \ldots$ and let all particles hop left or right with rate $\Gamma$. The master equation is

\[
\frac{d}{dt} P(\alpha, t) = \Gamma \sum_{\langle ij \rangle} \left[ (n_i + 1)P(n_i + 1, n_j - 1, \ldots, t) - n_iP(\alpha, t) 
+ (n_j + 1)P(n_i - 1, n_j + 1, \ldots, t) - n_jP(\alpha, t) \right]
\]
Consider a one-dimensional chain of lattice sites $i = 1, 2, \ldots$ and let all particles hop left or right with rate $\Gamma$. The master equation is

$$\frac{d}{dt} P(\alpha, t) = \Gamma \sum_{\langle ij \rangle} \left[ (n_i + 1)P(n_i + 1, n_j - 1, \ldots, t) - n_i P(\alpha, t) 
\right. 
\left. (n_j + 1)P(n_i - 1, n_j + 1, \ldots, t) - n_j P(\alpha, t) \right]$$

Define $\rho(x, t) = \sum_{\alpha} n_i P(\alpha, t)$ where $x = i \Delta x$.

For small $\Delta x$ this becomes the diffusion equation:

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} \quad D = \Gamma \Delta x^2 = \text{diffusion constant.}$$
Master Equation for $A + A \rightarrow 0$ Diffusion-Limited Reaction

\[
\frac{d}{dt}P(\{n\}, t) = \frac{D}{\Delta x^2} \sum_{\langle ij \rangle} [(n_i + 1)P(\ldots, n_i+1, n_j-1, \ldots, t) - n_iP(\{n\}, t) \\
+ (n_j + 1)P(\ldots, n_i-1, n_j+1, \ldots, t) - n_jP(\{n\}, t)] \\
+ \lambda \sum_i [(n_i + 2)(n_i + 1)P(\ldots, n_i + 2, \ldots, t) \\
- n_i(n_i - 1)P(\{n\}, t)]
\]

with $P(\{n\}, 0) = \prod_i \frac{n_0^{n_i} e^{-n_0}}{n_i!}$ for random initial conditions.
Master Equation for $A + A \rightarrow 0$ Diffusion-Limited Reaction

\[ \frac{d}{dt}P\{n\}, t) = \]

\[ \frac{D}{\Delta x^2} \sum_{\langle ij \rangle} \left[ (n_i + 1)P(\ldots, n_i+1, n_j-1, \ldots, t) - n_iP\{n\}, t) \right] \]

\[ + (n_j + 1)P(\ldots, n_i-1, n_j+1, \ldots, t) - n_jP\{n\}, t) \]

\[ + \lambda \sum_i \left[ (n_i + 2)(n_i + 1)P(\ldots, n_i + 2, \ldots, t) \right. \]

\[ \left. - n_i(n_i - 1)P\{n\}, t) \right] \]

with $P\{n\}, 0) = \prod_i \frac{n_i^{n_i} e^{-n_0}}{n_i!}$ for random initial conditions.

Yuck!
Field Theory Approach to Diffusion-Limited Reactions:
1. Models and Mappings

Master Equation for Lattice Models

Doi Representation

Mapping to Field Theory
For a single lattice site:

- Introduce a creation operator $\hat{a}^\dagger$ and annihilation operator $\hat{a}$, with commutator $[\hat{a}, \hat{a}^\dagger] = 1$.

- Represent the state of zero particles by $|0\rangle$, defined via $\hat{a}|0\rangle = 0$.

- Represent a state of $n$ particles by $|n\rangle = \hat{a}^\dagger n |0\rangle$. (Note: normalization differs from usual QM.)

- For this state

\[
\hat{a}^\dagger |n\rangle = |n + 1\rangle \quad \hat{a} |n\rangle = n |n - 1\rangle \quad \hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle
\]
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- For this state

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\hat{a}^\dagger |n\rangle = |n + 1\rangle \quad \hat{a} |n\rangle = n |n - 1\rangle \quad \hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle
\]

For multiple lattice sites: introduce a pair $\hat{a}_i$, $\hat{a}_i^\dagger$ at each site

\[
\{n\} = (n_1, n_2, \ldots) \quad \Leftrightarrow \quad |\{n\}\rangle = \prod_i \hat{a}_i^\dagger n_i |0\rangle
\]
We can pack the probability $P$ into a Fock space state:

$$|\phi(t)\rangle = \sum_{\{n\}} P(\{n\}, t) |\{n\}\rangle = \sum_{\{n\}} P(\{n\}, t) \prod_i \hat{a}_i^{n_i} |0\rangle$$

and re-write the master equation in Schrödinger-like form:

$$\frac{d}{dt} |\phi(t)\rangle = -\hat{H} |\phi(t)\rangle$$
We can pack the probability $P$ into a Fock space state:

$$|\phi(t)\rangle = \sum_{\{n\}} P(\{n\}, t) |\{n\}\rangle = \sum_{\{n\}} P(\{n\}, t) \prod_i \hat{a}_i^{n_i} |0\rangle$$

and re-write the master equation in Schrödinger-like form:

$$\frac{d}{dt} |\phi(t)\rangle = -\hat{H} |\phi(t)\rangle$$

Why do this? Because it is a simpler description of the dynamics. For $A + A \rightarrow 0$ diffusion-limited reaction we get

$$\hat{H} = \Gamma \sum_{\langle ij \rangle} (\hat{a}_i^\dagger - \hat{a}_j^\dagger)(\hat{a}_i - \hat{a}_j) - \lambda \sum_i (1 - \hat{a}_i^{2\dagger})\hat{a}_i^2$$

and formal solution $|\phi(t)\rangle = \exp(-\hat{H}t)|\phi(0)\rangle$. 
A + A \rightarrow 0 on a Single Site

Master equation:

\[ \frac{d}{dt} P(n, t) = \lambda \left[ (n + 2)(n + 1)P(n + 2, t) - n(n - 1)P(n, t) \right] \]

Multiply by \( |n\rangle \) and sum over \( n \):

\[ \frac{d}{dt} \langle \phi(t) \rangle = \lambda \sum_n P(n+2, t) (n + 2)(n + 1)|n\rangle - \lambda \sum_n P(n, t) n(n - 1)|n\rangle \]
\[ A + A \rightarrow 0 \text{ on a Single Site} \]

Master equation:
\[
\frac{d}{dt} P(n, t) = \lambda \left[ (n + 2)(n + 1)P(n + 2, t) - n(n - 1)P(n, t) \right]
\]

Multiply by \(|n\rangle\) and sum over \(n\):
\[
\frac{d}{dt} |\phi(t)\rangle = \lambda \sum_n P(n+2, t) (n + 2)(n + 1)|n\rangle - \lambda \sum_n P(n, t) n(n - 1)|n\rangle
\]
\[
= \lambda \sum_n P(n + 2, t) \hat{a}^2 |n + 2\rangle - \lambda \sum_n P(n, t) \hat{a}^{\dagger 2} \hat{a}^2 |n\rangle
\]
\[
= \lambda (\hat{a}^2 - \hat{a}^{\dagger 2} a^2) \sum_n P(n, t) |n\rangle
\]
\[
= \lambda (1 - \hat{a}^{\dagger 2}) \hat{a}^2 |\phi(t)\rangle = -\hat{H} |\phi(t)\rangle
\]
Hop from Site 1 to Site 2

Master Equation

\[ \frac{d}{dt} P(n_1, n_2, t) = \Gamma \left[ (n_1+1)P(n_1+1, n_2-1, t) - n_1 P(n_1, n_2, t) \right] \]

Multiply by \(|n_1, n_2\rangle\) and sum over \(n_1\) and \(n_2\):

\[ \frac{d}{dt} |\phi(t)\rangle = \Gamma \sum_{n_1, n_2} P(n_1+1, n_2-1, t) (n_1+1)|n_1, n_2\rangle \]

\[ - \Gamma \sum_{n_1, n_2} P(n_1, n_2, t) n_1|n_1, n_2\rangle \]

\[ = \Gamma \sum_{n_1, n_2} P(n_1+1, n_2-1, t) \hat{a}_2^\dagger \hat{a}_1 |n_1+1, n_2-1\rangle \]

\[ - \Gamma \sum_{n_1, n_2} P(n_1, n_2, t) \hat{a}_1^\dagger \hat{a}_1 |n_1, n_2\rangle \]

\[ = \Gamma (\hat{a}_2^\dagger - \hat{a}_1^\dagger) \hat{a}_1 |\phi(t)\rangle \]
Diffusion

- Hop from site 1 to site 2:
  \[ \hat{H}_{1\rightarrow 2} = \Gamma (\hat{a}^\dagger_1 - \hat{a}^\dagger_2) a_1 \]

- Allow for the reverse hop with the same rate:
  \[ \hat{H}_{1\leftrightarrow 2} = \Gamma (\hat{a}^\dagger_1 - \hat{a}^\dagger_2)(\hat{a}_1 - \hat{a}_2) \]

- For hops between all neighboring lattice sites:
  \[ \hat{H}_D = \frac{D}{(\Delta x)^2} \sum_{\langle i,j \rangle} (\hat{a}^\dagger_i - \hat{a}^\dagger_j)(\hat{a}_i - \hat{a}_j) \]
With two species reactions, such as $A + B \rightarrow 0$ reaction, the master equation is defined in terms of $A$-particle and $B$-particle occupation numbers

$$P(\{m\}, \{n\}, t)$$

For the Doi representation, we introduce distinct creation and annihilation operators for each species: $\hat{a}_i, \hat{a}^\dagger_i, \hat{b}_i, \text{ and } \hat{b}^\dagger_i$, and define state

$$|\phi(t)\rangle = \sum_{\{m\}, \{n\}} P(\{m\}, \{n\}, t) \prod_i \hat{a}^\dagger_{mi} \hat{b}^\dagger_{ni} |0\rangle$$
Each process contributes two terms to $\hat{H}$, of the form

$$(\text{rate}) \left[ (\text{reactants}) - (\text{reaction}) \right]$$

$(\text{reactants}) = \text{creation and annihilation operator for each reactant, normal ordered}$

$(\text{reaction}) = \text{annihilation operator for each reactant, creation operator for each product, normal ordered}$

Examples:

- $A + A \rightarrow 0 \quad \lambda[\hat{a}^\dagger 2 \hat{a}^2 - \hat{a}^2]$  
  $A + A \rightarrow A \quad \lambda[\hat{a}^\dagger 2 \hat{a}^2 - \hat{a}^\dagger \hat{a}^2]$  
- $A \rightarrow A + A \quad \lambda[\hat{a}^\dagger \hat{a} - \hat{a}^\dagger 2 \hat{a}]$  
  $A + B \rightarrow C \quad \lambda[\hat{a}^\dagger \hat{b}^\dagger \hat{a} \hat{b} - \hat{c}^\dagger \hat{a} \hat{b}]$
- Hop $1 \rightarrow 2 \quad \Gamma[\hat{a}_1^\dagger a_1 - \hat{a}_2^\dagger a_1]
For our classical particle system, averages are given by

$$\langle A(t) \rangle = \sum_{\{n\}} A(\{n\}) \ P(\{n\}, t)$$

To map this to the Doi representation, we need a projection state

$$\langle \mathcal{P}| = \langle 0|e^{\sum_i \hat{a}_i}, \text{ which has properties}$$

$$\langle \mathcal{P}|0\rangle = 1 \quad \langle \mathcal{P}|\hat{a}_i^\dagger \rangle = \langle \mathcal{P}| \Rightarrow \langle \mathcal{P}|n\rangle = 1$$

Then, for the operator $\hat{A} = A(\{n_i \rightarrow \hat{a}_i^\dagger \hat{a}_i\})$ we get

$$\langle A(t) \rangle = \langle \mathcal{P}|\hat{A}|\phi(t)\rangle = \langle \mathcal{P}|\hat{A} e^{-\hat{H}t}|\phi(0)\rangle$$

*Note:* for Poisson initial conditions, $|\phi(0)\rangle = \prod_i e^{-n_0+n_0\hat{a}_i^\dagger}|0\rangle$
Probability Conservation

Check Normalization

For some initial state \( P(\{n\}, 0) \) we average the identity operator:

\[
\langle \mathcal{P} | \hat{1} | \phi(0) \rangle = \langle \mathcal{P} | \sum_{\{n\}} P(\{n\}, 0) | \{n\} \rangle = \sum_{\{n\}} P(\{n\}, 0) = 1 \; \checkmark
\]

Check Probability Conservation

What is the condition on \( \hat{H} \)? We need

\[
1 = \langle \mathcal{P} | \hat{1} e^{-\hat{H}t} | \phi(0) \rangle = \langle \mathcal{P} | (1 - \hat{H}t + \frac{1}{2} t^2 \hat{H}^2 - \ldots) | \phi(0) \rangle
\]

for all \( t \), so we require \( \langle \mathcal{P} | \hat{H} = 0 \). Equivalently, \( \hat{H} \to 0 \) as \( \hat{a}_i^\dagger \to 1 \).

Note: \( \hat{H} \) need not be hermitian!
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Doi Representation

Mapping to Field Theory
The coherent state \( |\phi\rangle = \exp(-\frac{1}{2}|\phi|^2 + \phi a^\dagger)|0\rangle \) with complex \( \phi \) has properties

\[
\hat{a}|\phi\rangle = \phi|\phi\rangle, \quad \langle \phi|\hat{a}^\dagger = \langle \phi|\phi^* \]

and the overlap relation

\[
\langle \phi_1|\phi_2 \rangle = \exp(-\frac{1}{2}|\phi_1|^2 - \frac{1}{2}|\phi_2|^2 + \phi_1^*\phi_2) \]

Can construct a resolution of the identity operator

\[
\hat{1} = \sum_n \frac{1}{n!}|n\rangle\langle n| \]
Coherent States

The coherent state $|\phi\rangle = \exp(-\frac{1}{2}|\phi|^2 + \phi a^\dagger)|0\rangle$ with complex $\phi$ has properties

$$\hat{a}|\phi\rangle = \phi|\phi\rangle, \quad \langle \phi|\hat{a}^\dagger = \langle \phi|\phi^*$$

and the overlap relation

$$\langle \phi_1|\phi_2\rangle = \exp(-\frac{1}{2}|\phi_1|^2 - \frac{1}{2}|\phi_2|^2 + \phi_1^*\phi_2)$$

Can construct a resolution of the identity operator

$$\hat{1} = \sum_n \frac{1}{n!}|n\rangle\langle n| = \sum_{m,n} \frac{1}{n!}|n\rangle\langle m|\delta_{mn} = \int \frac{d^2\phi}{\pi} |\phi\rangle\langle \phi|$$

by use of

$$\delta_{mn} = \frac{1}{m!\pi} \int \phi^m\phi^* n e^{-|\phi|^2} d^2\phi$$
Given $\hat{H}(\hat{a}_i^\dagger, \hat{a}_i)$, take formal solution $|\phi(t)\rangle = e^{-\hat{H}t}|\phi(0)\rangle$ and divide time $t$ into a number of small increments $\Delta t$ via

$$e^{-\hat{H}t} = \exp(-\hat{H}\Delta t)^{t/\Delta t}$$

Insert $\hat{1} = \int \frac{d^2\phi}{\pi} |\phi\rangle\langle\phi|$ between each successive time step:

$$\int \cdots |\phi_{t+\Delta t}\rangle\langle\phi_{t+\Delta t}|e^{-\hat{H}\Delta t}|\phi_{t}\rangle\langle\phi_{t}|e^{-\hat{H}\Delta t}|\phi_{t-\Delta t}\rangle\langle\phi_{t-\Delta t}| \cdots$$
Coherent State Representation

Given $\hat{H}(\hat{a}^\dagger_i, \hat{a}_i)$, take formal solution $|\phi(t)\rangle = e^{-\hat{H}t}|\phi(0)\rangle$ and divide time $t$ into a number of small increments $\Delta t$ via

$$e^{-\hat{H}t} = \exp(-\hat{H} \Delta t)^{t/\Delta t}$$

Insert $\hat{1} = \int \frac{d^2\phi}{\pi} |\phi\rangle \langle \phi|$ between each successive time step:

$$\int \cdots |\phi_{t+\Delta t}\rangle \langle \phi_{t+\Delta t}| e^{-\hat{H} \Delta t} |\phi_t\rangle \langle \phi_t| e^{-\hat{H} \Delta t} |\phi_{t-\Delta t}\rangle \langle \phi_{t-\Delta t}| \cdots$$

Now focus on a single matrix element:

$$\langle \phi_t| e^{-\hat{H} \Delta t} |\phi_{t-\Delta t}\rangle = e^{-H(\phi^*_t,\phi_{t-\Delta t})\Delta t} \langle \phi_t| \phi_{t-\Delta t}\rangle$$

$$\simeq e^{-H(\phi^*_t,\phi_t)\Delta t} e^{\phi^*_t \phi_{t-\Delta t} - \frac{1}{2}|\phi_t|^2 - \frac{1}{2}|\phi_{t-\Delta t}|^2}$$

$$\simeq e^{-H(\phi^*_t,\phi_t)\Delta t} e^{-\phi^*_t \partial_t \phi_t \Delta t}$$
Path Integral

String together many time slices in the limit $\Delta t \to 0$ and we get

$$e^{-\hat{H}t} \to \int \mathcal{D}\phi^* \mathcal{D}\phi \exp \left( - \int_0^t dt' [\phi^* \partial_{t'} \phi + H(\phi^*, \phi)] \right)$$

where $\prod_j \left( \frac{d^2 \phi_j}{\pi} \right) \to \mathcal{D}\phi^* \mathcal{D}\phi$
String together many time slices in the limit $\Delta t \to 0$ and we get

$$e^{-\hat{H}t} \to \int \mathcal{D}\phi^* \mathcal{D}\phi \exp \left( -\int_0^t dt' [\phi^* \partial_{t'} \phi + H(\phi^*, \phi)] \right)$$

where $\prod_j \left( \frac{d^2 \phi_j}{\pi} \right) \to \mathcal{D}\phi^* \mathcal{D}\phi$

Generalize to multiple lattice sites:

$$e^{-\hat{H}t} \to \int \prod_j (\mathcal{D}\phi_j^* \mathcal{D}\phi_j) e^{-S[\{\phi_j^*\}, \{\phi_j\}]}$$

with

$$S = \int_0^t \sum_j dt' \left[ \phi_j^* \partial_{t'} \phi_j + H(\{\phi_j^*\}, \{\phi_j\}) \right]$$
\[ \langle A(t) \rangle = \langle \mathcal{P} | \hat{A} e^{-\hat{H}t} | \phi(0) \rangle = \mathcal{N}^{-1} \int \prod_j (\mathcal{D}\phi_j^* \mathcal{D}\phi_j) A(\phi(t)) e^{-S[\phi^*, \phi]} \]

with action \( S \) given by

\[ S = \sum_i \left\{ -\phi_i(t) + \int_0^t dt' \left[ \phi_i^* \partial_{t'} \phi_i + H(\{\phi_i^*\}, \{\phi_i\}) \right] - n_0 \phi_i^*(0) \right\} \]

Can eliminate projection state term by field shift \( \phi^* \rightarrow 1 + \tilde{\phi} \):

\[ \int_0^t (1 + \tilde{\phi}) \partial_{t'} \phi \, dt' = \phi(t) - \phi(0) + \int_0^t \tilde{\phi} \partial_t \phi \, dt' \]

which takes \( H \rightarrow H(\{1 + \tilde{\phi}_j\}, \{\phi_j\}) \)
Diffusion

\[ S_D = \int dt \left[ \sum_i \tilde{\phi}_i \partial_t \phi_i + \frac{D}{\Delta x^2} \sum_{\langle ij \rangle} (\tilde{\phi}_i - \tilde{\phi}_j)(\phi_i - \phi_j) \right] - \sum_{i} n_0 \tilde{\phi}_i(0) \]

\[ = \int dt \; d^d x \left[ \tilde{\phi} \, \partial_t \phi + D \nabla \tilde{\phi} \cdot \nabla \phi - n_0 \tilde{\phi} \, \delta(t) \right] \]

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

Action is linear in \( \tilde{\phi} \). Extremum:

\[ \frac{\delta S_D}{\delta \tilde{\phi}} = \partial_t \phi - D \nabla^2 \phi - n_0 \delta(t) = 0 \]

is the plain old diffusion equation: \( \partial_t \phi = D \nabla^2 \phi + n_0 \delta(t) \)
The reaction part of the hamiltonian is

\[ H_{\text{reac}} = -\lambda \sum_i (1 - \phi_i^* \phi_i^2) \phi_i^2 \rightarrow \int d^d x (2 \lambda_0 \phi \phi^2 + \lambda_0 \phi^2 \phi^2) \]

with the field shift \( \phi^* \rightarrow 1 + \tilde{\phi} \) and \( \lambda_0 = \lambda/\Delta x^d \).

Thus the complete \( A + A \rightarrow 0 \) action is

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

Now we’re ready to do some calculations!
Can make the action linear in $\tilde{\phi}$ via an auxiliary field $\eta$:

$$e^{-\lambda_0 \tilde{\phi}^2 \phi} \propto \int d\eta \exp\left\{ -\frac{1}{2} \eta^2 + i\eta \sqrt{2\lambda_0} \tilde{\phi} \phi \right\}$$

resulting in averages

$$\int \mathcal{D}\eta e^{-\eta^2/2} \int \mathcal{D}\phi \int \mathcal{D}\tilde{\phi} e^{-\int \tilde{\phi}(\partial_t - D\nabla^2)\phi + 2\lambda_0 \tilde{\phi}^2 + i\eta \sqrt{2\lambda_0} \tilde{\phi} \phi}$$

The $\tilde{\phi}$ integration creates a $\delta$-function that enforces

$$\partial_t\phi = D\nabla^2\phi - 2\lambda_0 \phi^2 + i\sqrt{2\lambda_0} \phi \eta$$

A stochastic reaction-diffusion equation with multiplicative noise
Can make the action linear in $\tilde{\phi}$ via an auxiliary field $\eta$:

$$e^{-\lambda_0 \tilde{\phi}^2 \phi^2} \propto \int d\eta \exp \left\{ -\frac{1}{2} \eta^2 + i \eta \sqrt{2\lambda_0} \tilde{\phi} \phi \right\}$$

resulting in averages

$$\int \mathcal{D}\eta \, e^{-\eta^2/2} \int \mathcal{D}\phi \int \mathcal{D}\tilde{\phi} \, e^{-\int \tilde{\phi} (\partial_t - D \nabla^2) \phi + 2\lambda_0 \tilde{\phi} \phi^2 + i \eta \sqrt{2\lambda_0} \tilde{\phi} \phi}$$

The $\tilde{\phi}$ integration creates a $\delta$-function that enforces

$$\partial_t \phi = D \nabla^2 \phi - 2\lambda_0 \phi^2 + i \sqrt{2\lambda_0} \phi \eta$$

A stochastic reaction-diffusion equation with multiplicative noise that is complex!?
Mapping to Doi representation simplifies the master equation by getting rid of pesky factors involving $n$.

This Fock space description natural for identical particles acting independently, not restricted to quantum mechanics.

Fock space dynamics can be converted to a field theory without resorting to Langevin-type phenomenology.

Technique can easily include multiple species, long-range hops, birth/death processes, convected fields.

Mechanical forces not so easily included. $\hat{H}$ is not an energy but rather rates.

SPDE’s are fraught with peril!
Fock space representation:


Reaction diffusion field theory (Bargmann representation):

- L. Peliti, *J. Physique* 46, 1469 (1985)

General path integral techniques:


Reaction diffusion field theory (Coherent state representation):

1. **Diffusion equation:**
   (a) Show that the diffusion master equation is equivalent to
   
   \[
   \frac{d}{dt} \langle n_i \rangle = \frac{D}{\Delta x^2} \sum_j (\langle n_j \rangle - \langle n_i \rangle)
   \]
   
   where the sum on $j$ runs over nearest neighbors of site $i$.
   
   (b) Show that $\rho(x, t) = \langle n_i \rangle$ with $x = i \Delta x$ satisfies $\partial_t \rho = D \partial_{xx}^2 \rho$ as $\Delta x \to 0$.
   
   (c) Generalize the result to a $d$-dimensional hypercubic lattice.

2. **Consider the decay $A \to 0$ on a single lattice site.** Map the problem from the master equation to the Doi Hamiltonian to the shifted field theory. Show that the $\mathcal{D}\tilde{\phi}$ integration yields the expected result
   
   \[
   \partial_t \phi = -\lambda \phi + n_0 \delta(t)
   \]
3. Write down the Doi hamiltonian for the reversible reaction \( \ell A + mB \rightleftharpoons nC \), with rates \( \lambda \) for the forward reaction and \( \mu \) for the reverse reaction. Here \( \ell A \), for example, means \( \ell \) \( A \) particles are required for the reaction.

4. Coherent states:
   (a) Determine the coefficients \( C_n \) in the expansion of the coherent state \( |\phi\rangle = \sum_n C_n |n\rangle \)
   (b) Confirm the identity
   \[
   \delta_{mn} = \frac{1}{m!\pi} \int \phi^* m \phi^* n e^{-|\phi|^2} \, d^2\phi
   \]
   (c) Use the results from (a) and (b) confirm \( \hat{1} = \int \frac{d^2\phi}{\pi} |\phi\rangle \langle \phi| \). Note that \( d^2\phi = d(\text{Re}\phi) \, d(\text{Im}\phi) \).