Field Theory Approach to Diffusion-Limited Reactions:

1. Models and Mappings

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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**

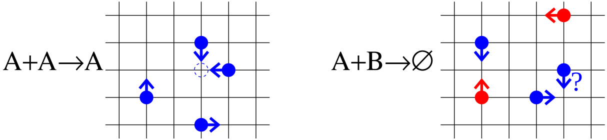
   Higher order reactions, disorder, Lévy flights, two-species reactions, coupled reactions.

4. **Active to Absorbing State Transitions**

   Directed percolation, branching and annihilating random walks, and all that.

Diffusion-Limited Reactions

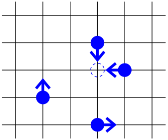
One or more species of particles undergoing random walks on a lattice, with a reactions occurring for particles on the same lattice site



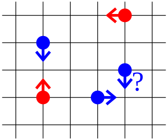
Diffusion-Limited Reactions

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

A+A→A



A+B→∅



Example: for $A + A \to 0$ the density of particles decays as

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

where A_d and $\tilde{A}$ are universal numbers!

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

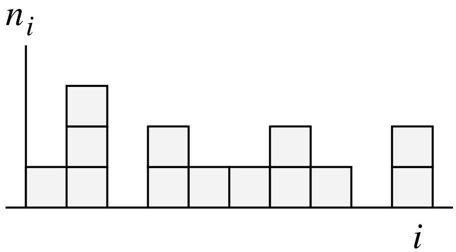
Master Equation for Lattice Models

Doi Representation

Mapping to Field Theory

Stochastic Classical Particles on a Lattice

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



Define

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

Probability Master Equation

Dynamical processes processes (hops, reactions, decays) will cause a change of state from α to β.

$$\boxed{w_{\alpha\to\beta} = \text{rate of transition from } \alpha \text{ to } \beta\text{, defines dynamics}}$$

Master Equation

$$\frac{d}{dt}P(\alpha,t) = \sum_\beta \Big[\underbrace{w_{\beta\to\alpha}P(\beta,t)}_{\text{flow into }\alpha} - \underbrace{w_{\alpha\to\beta}P(\alpha,t)}_{\text{flow out of }\alpha}\Big]$$

- $\sum_\alpha P(\alpha,t) = 1$ preserved by the master equation
- Initial conditions $P(\alpha,0)$ need to be specified

Master Equation for $A \to 0$ Decay

Consider a single lattice site that contains some number of identical particles. These particles decay at rate λ.

The rate for a transition from n to m particles is

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

and the master equation is

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

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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

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

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

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

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

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

$$= -\lambda \rho$$

$A + A \to 0$ Reaction

Again, consider a single lattice site, with the rule that a pair of particles may annihilate each other. The rates are

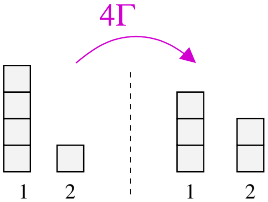
$$w_{n\to m} = \begin{cases} 0 & \text{for } m \neq n-2 \\ n(n-1)\lambda & \text{for } m = n-2 \end{cases}$$

and the master equation is

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

Hop

Now consider two sites, $i = 1$ and 2, with a rate Γ of hopping from site 1 to site 2.



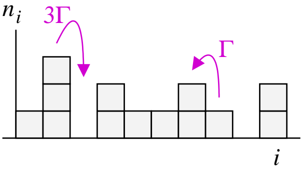
$$w_{(n_1,n_2)\to(m_1,m_2)} = \begin{cases} 0 & \text{for } m_1 \neq n_1 - 1 \;\text{ or }\; m_2 \neq n_2 + 1 \\ n_1\Gamma & \text{for } m_1 = n_1 - 1 \text{ and } m_2 = n_2 + 1 \end{cases}$$

and the master equation is

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

Diffusion

Consider a one-dimensional chain of lattice sites $i = 1, 2, \ldots$ and let all particles hop left or right with rate Γ. The master equation is



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

$$(n_j+1)P(n_i-1, n_j+1, \ldots, t) - n_j P(\alpha,t) \Big]$$

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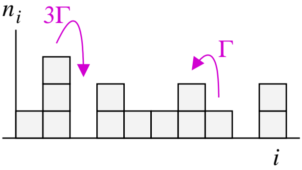

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Define $\rho(x,t) = \sum_\alpha n_i P(\alpha,t)$ where $x = i\Delta x$.

For small Δx this becomes the diffusion equation:

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} \qquad D = \Gamma \Delta x^2 = \text{diffusion constant.}$$

Master Equation for $A + A \to 0$ Diffusion-Limited Reaction

$$
\begin{aligned}
\frac{d}{dt} P(\{n\}, t) = \\
& \frac{D}{\Delta x^2} \sum_{\langle ij \rangle} \Big[(n_i + 1) P(\ldots, n_i{+}1, n_j{-}1, \ldots, t) - n_i P(\{n\}, t) \\
& \qquad + (n_j + 1) P(\ldots, n_i{-}1, n_j{+}1, \ldots, t) - n_j P(\{n\}, t) \Big] \\
& + \lambda \sum_i \Big[(n_i + 2)(n_i + 1) P(\ldots, n_i + 2, \ldots, t) \\
& \qquad - n_i (n_i - 1) P(\{n\}, t) \Big]
\end{aligned}
$$

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

Master Equation for $A + A \to 0$ Diffusion-Limited Reaction

$$\frac{d}{dt}P(\{n\},t) =$$

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

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

$$+ \lambda\sum_i\Big[(n_i+2)(n_i+1)P(\ldots,n_i+2,\ldots,t)$$

$$- n_i(n_i-1)P(\{n\},t)\Big]$$

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

Yuck!

Doi Occupation Number Representation (Fock Space)

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

$$\hat{a}^\dagger \, |n\rangle = |n+1\rangle \qquad \hat{a} \, |n\rangle = n \, |n-1\rangle \qquad \hat{a}^\dagger \hat{a} \, |n\rangle = n \, |n\rangle$$

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

$$\{n\} = (n_1, n_2, \dots) \quad \Leftrightarrow \quad |\{n\}\rangle = \prod_i \hat{a}_i^{\dagger n_i}|0\rangle$$

Doi Representation, part II

We can pack the probability P into a Fock space state:

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

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

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

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

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

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

and formal solution $|\phi(t)\rangle = \exp(-\hat{H}t)|\phi(0)\rangle$.

$A + A \to 0$ on a Single Site

Master equation:

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

Multiply by $|n\rangle$ and sum over n:

$$\frac{d}{dt}|\phi(t)\rangle = \lambda\sum_n P(n{+}2,t)\,(n+2)(n+1)|n\rangle - \lambda\sum_n P(n,t)\,n(n-1)|n\rangle$$

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$$= \lambda\sum_n P(n+2,t)\,\hat{a}^2|n+2\rangle - \lambda\sum_n P(n,t)\,\hat{a}^{\dagger 2}\hat{a}^2|n\rangle$$

$$= \lambda(\hat{a}^2 - \hat{a}^{\dagger 2}a^2)\sum_n P(n,t)\,|n\rangle$$

$$= \lambda(1 - \hat{a}^{\dagger 2})\hat{a}^2|\phi(t)\rangle = -\hat{H}|\phi(t)\rangle$$

Hop from Site 1 to Site 2

Master Equation

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

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

$$\begin{aligned}
\frac{d}{dt}|\phi(t)\rangle &= \Gamma \sum_{n_1,n_2} P(n_1{+}1, n_2{-}1, t)\,(n_1{+}1)|n_1, n_2\rangle \\
&\qquad - \Gamma \sum_{n_1,n_2} P(n_1, n_2, t)\, n_1 |n_1, n_2\rangle \\
&= \Gamma \sum_{n_1,n_2} P(n_1{+}1, n_2{-}1, t)\, \hat{a}_2^\dagger \hat{a}_1\, |n_1{+}1, n_2{-}1\rangle \\
&\qquad - \Gamma \sum_{n_1,n_2} P(n_1, n_2, t)\, \hat{a}_1^\dagger \hat{a}_1\, |n_1, n_2\rangle \\
&= \Gamma(\hat{a}_2^\dagger - \hat{a}_1^\dagger)\hat{a}_1\, |\phi(t)\rangle
\end{aligned}$$

Diffusion

- Hop from site 1 to site 2:

$$\hat{H}_{1\to 2} = \Gamma(\hat{a}_1^\dagger - \hat{a}_2^\dagger)a_1$$

- Allow for the reverse hop with the same rate:

$$\hat{H}_{1\leftrightarrow 2} = \Gamma(\hat{a}_1^\dagger - \hat{a}_2^\dagger)(\hat{a}_1 - \hat{a}_2)$$

- For hops between all neighboring lattice sites:

$$\boxed{\hat{H}_D = \frac{D}{(\Delta x)^2}\sum_{\langle ij\rangle}(\hat{a}_i^\dagger - \hat{a}_j^\dagger)(\hat{a}_i - \hat{a}_j)}$$

Multiple Species

With two species reactions, such as $A + B \to 0$ 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: $\hat{a}_i$, $\hat{a}_i^\dagger$, $\hat{b}_i$, and $\hat{b}_i^\dagger$, and define state

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

Doi Hamiltonians

Each process contributes two terms to $\hat{H}$, of the form

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

(reactants) = creation and annihilation operator for each reactant, normal ordered

(reaction) = annihilation operator for each reactant, creation operator for each product, normal ordered

Examples:

$A + A \to 0 \quad \lambda[\hat{a}^{\dagger 2}\hat{a}^2 - \hat{a}^2]$

$A + A \to A \quad \lambda[\hat{a}^{\dagger 2}\hat{a}^2 - \hat{a}^{\dagger}\hat{a}^2]$

$A \to A + A \quad \lambda[\hat{a}^{\dagger}\hat{a} - \hat{a}^{\dagger 2}\hat{a}]$

$A + B \to C \quad \lambda[\hat{a}^{\dagger}\hat{b}^{\dagger}\hat{a}\hat{b} - \hat{c}^{\dagger}\hat{a}\hat{b}]$

Hop $1 \to 2 \quad \Gamma[\hat{a}_1^{\dagger}a_1 - \hat{a}_2^{\dagger}a_1]$

Observables

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

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

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

$$1 = \langle\mathcal{P}|\hat{1}e^{-\hat{H}t}|\phi(0)\rangle = \langle\mathcal{P}|(1-\hat{H}t+\tfrac{1}{2}t^2\hat{H}^2-\dots)|\phi(0)\rangle$$

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!

Coherent States

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

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

and the overlap relation

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

Can construct a resolution of the identity operator

$$\hat{1} = \sum_n \frac{1}{n!}|n\rangle\langle n|$$

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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

$$\delta_{mn} = \frac{1}{m!\pi}\int \phi^{*m}\phi^n e^{-|\phi|^2}\, d^2\phi$$

Coherent State Representation

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 Δt 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:

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

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Now focus on a single matrix element:

$$\begin{aligned}\langle\phi_t|e^{-\hat{H}\Delta t}|\phi_{t-\Delta t}\rangle &= e^{-H(\phi_t^*,\phi_{t-\Delta t})\Delta t}\langle\phi_t|\phi_{t-\Delta t}\rangle \\ &\simeq e^{-H(\phi_t^*,\phi_t)\Delta t}\ e^{\phi_t^*\phi_{t-\Delta t}-\frac{1}{2}|\phi_t|^2-\frac{1}{2}|\phi_{t-\Delta t}|^2} \\ &\simeq e^{-H(\phi_t^*,\phi_t)\Delta t}\ e^{-\phi_t^*\partial_t\phi_t\Delta t}\end{aligned}$$

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

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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

$$S = \int_0^t \sum_j dt' \Big[\phi_j^* \partial_{t'} \phi_j + H(\{\phi_j^*\}, \{\phi_j\})\Big]$$

Path Integral Observables

$$\langle A(t) \rangle = \langle \mathcal{P} | \hat{A} e^{-\hat{H}t} | \phi(0) \rangle = \mathcal{N}^{-1} \int \prod_j (\mathcal{D}\phi_j^* \mathcal{D}\phi_j) A\big(\phi(t)\big) e^{-S[\phi^*, \phi]}$$

with action S given by

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

Can eliminate projection state term by field shift $\phi^* \to 1 + \tilde{\phi}$:

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

which takes $H \to H(\{1 + \tilde{\phi}_j\}, \{\phi_j\})$

Diffusion

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

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

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

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: $\partial_t \phi = D \nabla^2 \phi + n_0\, \delta(t)$

Diffusion-Limited $A + A \to 0$ Reaction

The reaction part of the hamiltonian is

$$H_{\text{reac}} = -\lambda \sum_i (1 - \phi_i^{*2})\phi_i^2 \to \int d^d x (2\lambda_0 \tilde{\phi}\phi^2 + \lambda_0 \tilde{\phi}^2 \phi^2)$$

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

Thus the complete $A + A \to 0$ action is

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

Now we're ready to do some calculations!

The $A + A \to 0$ Stochastic PDE

Can make the action linear in $\tilde{\phi}$ via an auxiliary field η:

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

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 δ-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

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The $\tilde{\phi}$ integration creates a δ-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!?

Summary and Observations

- 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!

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Exercises

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 $\partial_t \rho = D \partial_x^2 \rho$ 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

   $$\partial_t \phi = -\lambda \phi + n_0\, \delta(t)$$

Exercises

3. Write down the Doi hamiltonian for the reversible reaction $\ell A + mB \rightleftharpoons nC$, with rates λ for the forward reaction and μ for the reverse reaction. Here ℓA, for example, means ℓ 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 $d^2\phi = d(\text{Re}\phi)\, d(\text{Im}\phi)$.