Field Theoretic Description of reacting Random-Walks

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A Simple Example

reaction-diffusion model:

one species A

- random walk on a lattice
- annihilation: $A + A \to \emptyset$ at a rate λ

$\leadsto$ rate-equation for the particle density n

$$\frac{\partial n}{\partial t} = D\nabla^2 n - 2\lambda n^{(2)}$$

where $n^{(2)}$ is the probability of finding two particles at one site.

mean-field:

$$n^{(2)} \approx n^2$$

$\leadsto$

$$\frac{\partial n}{\partial t} = D\nabla^2 n - 2\lambda n^2$$

solution for the homogenious case:

$$n(t) = \frac{n_0}{1 + 2\lambda n_0 t}$$

for $t \to \infty$:

$$n(t) \sim (\lambda t)^{-1}$$

Field Theoretic description:

master equation

$$\frac{dP(\alpha)}{dt} = \sum_\beta R_{\beta\to\alpha} P(\beta) - \sum_\beta R_{\alpha\to\beta} P(\alpha)$$

lattice: $\alpha \; \leftrightarrow$ occuptation numbers

compare with Schrödinger equation:

- linear in $P(\alpha)$

- first order in $\frac{\partial}{\partial t}$

second-quantized formalism:

- $p(n_1, n_2, ..., t) \sim P(\{n\}, t)$
- annihilation and creation operators $a_i, a_i^\dagger$, $[a_i, a_i^\dagger] = 1$ ($i \in$lattice)
- $|0>$ defined by $a_i|0>= 0\,\forall i$
- $|\psi(t)>= \sum_{\{n\}} p(\{n\}, t) a_1^{\dagger n_1} a_2^{\dagger n_2} \cdots |0>$

$\leadsto$ master equation can be written as

$$\frac{d}{dt}|\psi(t)>= -H|\psi(t)>$$

where H depends on the $a_i, a_i^\dagger$.

example:
2 sites, hopping $1 \to 2$ at rate D

$$\frac{dP(n_1,n_2)}{dt} = D(n_1+1)P(n_1+1,n_2-1) - Dn_1P(n_1,n_2)$$

wave function:

$$|\psi(t)> := \sum_{n_1,n_2} a_1^{\dagger n_1} a_2^{\dagger n_2} P(n_1,n_2)|0>$$

this yields

$$\begin{aligned}
\frac{d|\psi(t)>}{dt} &= D\sum_{n_1,n_2}\Big(P(n_1+1,n_2-1)(n_1+1) \\
&\quad -P(n_1,n_2)n_1\Big)a_1^{\dagger n_1}a_2^{\dagger n_2}|0> \\
&= D\sum_{n_1,n_2} P(n_1+1,n_2-1)a_2^\dagger a_1 \cdot \\
&\quad \cdot a_1^{\dagger(n_1+1)}a_2^{\dagger(n_2-1)}|0> \\
&\quad -D\sum_{n_1,n_2} P(n_1,n_2)a_1^\dagger a_1 a_1^{\dagger n_1}a_2^{\dagger n_2}|0> \\
&= D(a_2^\dagger a_1 - a_1^\dagger a_1)|\psi(t)>
\end{aligned}$$

$\rightsquigarrow$

$$H = -D(a_2^\dagger a_1 - a_1^\dagger a_1)$$

<u>2nd example:</u>

simple annihilation at a single site

$$\begin{aligned}\frac{dP(n)}{dt} &= \lambda(n+2)(n+1)P(n+2) \\ &\quad -\lambda n(n-1)P(n)\end{aligned}$$

$$|\psi> = \sum_n P(n) a^{\dagger n}|0>$$

$$\begin{aligned}\frac{d|\psi>}{dt} &= \lambda\sum_n (n+2)(n+1)P(n+2)a^{\dagger n}|0> \\ &\quad -\lambda\sum_n n(n-1)P(n)a^{\dagger n}|0> \\ &= \lambda\sum_n P(n+2)a^2 a^{\dagger(n+2)}|0> \\ &\quad -\lambda\sum_n P(n)a^{\dagger 2}a^2 a^{\dagger n}|0>\end{aligned}$$

time-evolution-operator: e^{-tH}, where

$$H = -\lambda(a^2 - a^{\dagger 2}a^2)$$

hopping and annihilation on a lattice:

$$\begin{aligned} H &= D \sum_{<ij>} (a_i^\dagger - a_j^\dagger)(a_i - a_j) \\ &\quad -\lambda \sum_i (a_i^2 - a_i^{\dagger 2} a_i^2) \end{aligned}$$

differences from many-particle quantum mechanics:

- no i

- H not necessarily hermitian

- expecation value of observable A is not $\bar{A} =< \psi(t)|A|\psi(t) >$, since this would be bilinear in the $p(\{n_i\})$.

Instead we have

$$\begin{aligned}
\bar{A} &= \sum_{\{n_i\}} p(\{n_i\}) A(n_1, n_2, ...) \\
&= < 0|e^{\sum_i a_i} \sum_{\{n_i\}} A(n_1, n_2, ...) \\
&\quad \cdot p(\{n_i\}) a_1^{\dagger n_1} a_2^{\dagger n_2} ...|0 > \\
&= < \psi_0|A|\psi(t) > \\
&= < \psi_0|A e^{-Ht}|\psi(0) >
\end{aligned}$$

where $< \psi_0| \sim < 0|e^{\sum_i a_i}$.

Note:

$< 0|e^{\sum_i a_i}$ is a left-eigenstate of $a_i^\dagger$ with eigenvalue 1, i.e. $[e^a, a_i^\dagger] = e^a$, $< 0|a_i^\dagger = 0$.

Path-integral representation

for simplicity one single site

$$e^{-Ht} = ?$$

Consider:

$$\begin{aligned} e^{-Ht} &= \lim_{\Delta t \to 0} (1 - H\Delta t)^{t/\Delta t} \\ &= \lim_{\Delta t \to 0} \underbrace{(1 - H\Delta t)(1 - H\Delta t)...(1 - H\Delta t)}_{t/\Delta t \text{ factors}} \end{aligned}$$

into each slice insert a complete set of coherent states

$$1 = \int \frac{d\phi^\star \phi}{\pi} e^{-\phi^\star \phi} e^{\phi a^\dagger} |0 >< 0| e^{\phi^\star a}$$

This leads to

$$\prod e^{\phi^\star(t+\Delta t)\phi(t) - \phi^\star(t+\Delta t)\phi(t+\Delta t) - \Delta t H(\phi^\star, \phi)}$$

$$\approx \quad e^{-\int dt \{\phi^\star \partial_t \phi + H(\phi^\star, \phi)\}}$$

in $d \neq 0$ spacial dimensions this generalizes to a path-integral

$$\int D\phi^\star D\phi e^{-\int dt d^d x \mathcal{L}[\phi^\star, \phi]}$$

in the hopping-annihilation model:

$$\begin{aligned} \mathcal{L} &= \phi^\star \partial_t \phi + D(\nabla \phi^\star)(\nabla \phi) \\ &\quad -\lambda(\phi^2 - \phi^{\star 2}\phi^2) \end{aligned}$$

or before taking the continuum limit

$$\begin{aligned} \mathcal{L} &= \sum_j \phi_j^\star \partial_t \phi_j \\ &\quad + D \sum_{<ij>} (\phi_i^\star - \phi_j^\star)(\phi_i - \phi_j) \\ &\quad -\lambda \sum_i (\phi_i^2 - \phi_i^{\star 2}\phi_i^2) \end{aligned}$$

Interpretation as a Langevin equation

shift: $\phi_j^\star = 1 + \tilde{\phi}_j$
$\leadsto$

$$\exp\left\{ \int dt d^d x [\tilde{\phi}\partial_t \phi + D(\nabla\tilde{\phi})(\nabla\phi) + 2\lambda\tilde{\phi}\phi^2 + \lambda\tilde{\phi}^2\phi^2 \right\}$$

now write

$$\exp\left\{ -\lambda \int dt d^d x\, \tilde{\phi}^2 \phi^2 \right\} = \int D\xi \exp\left\{ dt d^d x\, \tilde{\phi}\zeta \right\} P[\xi]$$

P probability density for the noise ξ

equation of motion:

$$\partial_t \phi = D\nabla^2\phi - 2\lambda\phi^2 + \xi$$

a Langevin equation

Reaction-controlled diffusion

2 species A,B

- A hops $i \to j$ only if j already occupied by a B
- B diffusion
- $nB \to \emptyset$
- $B \to (m+1)B$

<u>case a)</u> $\rho_B(\vec{x}, t \to \infty) = \rho_B^\infty > 0$

$\rightsquigarrow D_A \sim \rho_B^\infty$ normal diffusion of A particle

<u>case b)</u> $\rho_B(\vec{x}, t \to \infty) \sim e^{-\lambda t}$

<u>case c)</u> $\rho_B(\vec{x}, t \to \infty) \sim t^{-\alpha}$

$\rightsquigarrow < \vec{x}_A^2 > \sim t^{1-\alpha}$ or $< \vec{x}_A^2 > \sim \ln(t)$ for $\alpha = 1$

Hamiltonians:

$$
\begin{aligned}
H_B &= D \sum_{<ij>} (b_i^\dagger - b_j^\dagger)(b_j - b_i) \\
H_A &= \tilde{D} \sum_{<ij>} (a_i^\dagger - a_j^\dagger)(a_j - a_i) b_i^\dagger b_i \\
H_R &= \lambda_n \sum_i (1 - b_i^{\dagger n}) b_i^n \\
H_P &= \sigma_m \sum_i (b_i^{\dagger m} - 1) b_i^\dagger b_i
\end{aligned}
$$

actions:

$$
\begin{aligned}
S_B &= \int d^d x dt \, \hat{b}(\partial_t b - D\nabla^2 b) \\
S_A &= \int d^d x dt \, \hat{a}(\partial_t a - \tilde{D}\hat{b} b D\nabla^2 a) \\
S_R &= -\lambda_n \int d^d x dt \, (1 - \hat{b}^n) b^n \\
S_P &= \sigma_m \int d^d x dt \, (1 - \hat{b}^m) \hat{b} b
\end{aligned}
$$

$\rightsquigarrow$ Langevin equations:

$$\begin{aligned}
\partial_t a &= D'\nabla^2 a + \tilde{D} b \nabla^2 a + \xi \\
\partial_t b &= D\nabla^2 b - 2\lambda b^2 + \eta
\end{aligned}$$

where we have added ordininary A-diffusion $\sim D'$

<u>expecation:</u> induced diffusion $\sim \tilde{D}b$ is suppressed, standard diffusion for $t \to \infty$

<u>power-counting</u>

$$\begin{aligned}
[x] &= \kappa^{-1} \\
[t] &= \kappa^{-2} \\
[D] = [D'] &= \kappa^{0} \\
[\hat{a}] = [\hat{b}] &= \kappa^{0} \\
[a] = [b] &= \kappa^{d} \\
[\sigma_m] &= \kappa^{2} \\
[\lambda_n] &= \kappa^{2-(n-1)d} \\
[\tilde{D}] &= \kappa^{-d}
\end{aligned}$$

positive scaling dimensions $\leadsto$ relevant in the RG-sense

annihilation rate λ_n
- relevant for $d < \frac{2}{n-1}$
- irrelevant for $d > \frac{2}{n-1}$

upper critical dimension $d_c(n) = \frac{2}{n-1}$

$\tilde{D}$ irrelevant
ρ_B either vanishes or approaches a constant $\leadsto$ normal diffusion where D' is possibly renormalized.

anomalous diffusion: crossover feature

field theoretically speaking

$$\begin{aligned} & \frac{\partial}{\partial q^2} \tilde{D}_R(\vec{q}, \omega)|_{q=0} \\ = \;& \tilde{D} \left[1 + \frac{\tilde{D}}{D} \left(\frac{\omega}{D} \right)^{d/2} \int \frac{d^4 k}{(2\pi)^d} \frac{k^2}{-i + k^2} \right]^{-1} \end{aligned}$$

for $\omega \to \infty$ $\tilde{D}_R \to \tilde{D}$.

the coupling of the B pair annihilation rate however gets renormalized

$d > d_c(2) = 2 \ \lambda_R(0,0) = \lambda$
$\Rightarrow < \rho_B(t) > \sim t^{-1}$

$d < d_c(2) = 2 \ \lambda_R(0,\omega) \sim \omega^{1-d/2}$
$\Rightarrow < \rho_B(t) > \sim t^{-d/2}$

B process not influenced by the A dynamics
($\tilde{D}$ irrelevant for the $t \to \infty$ behaviour

- solve B kinetics first
- determine influence on A dynamics

from now on $D' = 0$

$n = 1$

$\rho_B(t) \sim e^{-\lambda_1 t}$
ρ_A Gaussisch

Varianz $< \vec{x}^2(t) >\sim (1 - e^{-\lambda_1 t})$

$\lambda_1 t << 1$: normal diffusion

$\lambda_1 t >> 1$: $< x_A^2(t) >\to$ const.

$n = 2$

$d < 2$: $< x_A^2(t) >\sim t^{1-d/2}$

$d \geq 2$: $< x_A^2 >\sim (\ln t)^2$

$n = 3$ $d = 1$ also logarithmically

$n > 3$, $n = 3, d \geq 2$:

$< x_A^2(t) >\sim t^{2/(2+\theta)}$

$\theta \to 0$ for $n \to \infty$ normal diffusion