Reaction models in stochastic field theory

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Outline

- Stochastic differential equation (SDE)
- White-noise limit
- From Langevin equation to field theory
- The Jacobian and the SDE ambiguity
- Dynamic action in Stratonovich form and in Ito form
- Second quantization of classical variables
- The Doi dynamic action for reaction $A + A \to A$
- Sources and sinks in the master equation
- The Doi action with random sources and sinks
- Lanchester's stochastic combat model

Stochastic differential equation

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Paradigmatic example: model A

$$\frac{\partial \varphi}{\partial t} = -\Gamma\left(-\nabla^2\varphi + a\varphi + \frac{\lambda}{6}\varphi^3\right) + f\,,$$

with the (white) noise statistics

$$\langle f(t,\mathbf{x}) f(t',\mathbf{x}')\rangle = 2\Gamma\delta(t-t')\delta(\mathbf{x}-\mathbf{x}')\,,\qquad \langle f\rangle = 0\,.$$

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The proper understanding of the SDE is integral equation

$$\varphi(t) = \varphi(0) + \int_0^t [-K\varphi + U(\varphi)]\,d\tau + \int_0^t B(\varphi)dW(t)\,,$$

which leads to stochastic integrals of Ito and Stratonovich.

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Consider a temporal δ sequence of correlation functions

$$\langle f(t,\mathbf{x})f(t',\mathbf{x}')\rangle = \overline{D}(t,\mathbf{x};t',\mathbf{x}') \underset{t'\to t}{\longrightarrow} \delta(t-t')D(\mathbf{x},\mathbf{x}')\,.$$

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This procedure gives rise to the solution of the SDE in the Stratonovich interpretation.

From Langevin equation to field theory

Functional integral for the generating function(al)

$$
\begin{aligned}
G(J) = \langle e^{\varphi[f]J} \rangle &= \int \mathcal{D}\varphi \, \langle \delta\left(\varphi - \varphi[f]\right) \rangle \, e^{\varphi J} \\
&= \int \mathcal{D}\varphi \, \langle \delta\left(-\partial_t \varphi + V(\varphi) + f B(\varphi)\right) |\det M| \rangle \, e^{\varphi J} \\
&= \int \mathcal{D}\varphi \int \mathcal{D}\tilde{\varphi} \, \left\langle |\det M| \, e^{\tilde{\varphi}(-\partial_t \varphi + V(\varphi) + f B(\varphi))} \right\rangle e^{\varphi J} \, .
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$$

This gives rise to the De Dominicis-Janssen dynamic action

$$
S[\varphi, \tilde{\varphi}, f] = \ln P\,[f] + \ln |\det M| + \tilde{\varphi}\left(-\partial_t \varphi + V(\varphi) + f B(\varphi)\right) \, .
$$

In case of multiplicative noise, $\ln |\det M|$ depends on f.

Functional Jacobi determinant

Loop expansion of $e^{\mathrm{Tr}\ln M}$ yields the representation

$$\det M = \det\left(\partial_t + K - U' - f B'\right) = \det\left(\partial_t + K\right) e^{-\Delta(0)(U' + f B')} \, .$$

Here, the shorthand notation stands for

$$\Delta(0)\left(U' + f B'\right) = \int dt \int d\mathbf{x} \int d\mathbf{x}' \Delta(t, \mathbf{x}; t, \mathbf{x}') \times \int du \left[\frac{\delta U(\mathbf{x}', \varphi(t))}{\delta\varphi(u, \mathbf{x})} + f(t, \mathbf{x}') \frac{\delta B(\mathbf{x}', \varphi(t))}{\delta\varphi(u, \mathbf{x})}\right] \, .$$

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Diagonal value of the propagator (response function of φ) $\Delta(0) := \Delta(t,\mathrm{x};t,\mathrm{x}')$ remains a free parameter.

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Note that all this does not require even random f. This ambiguity has nothing to do with the white-noise problem.

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Two popular choices for the parameter $\Delta(0)$

- $\Delta(0, \mathbf{x} - \mathbf{x}') = \frac{1}{2}\delta(\mathbf{x} - \mathbf{x}')$,
- $\Delta(0, \mathbf{x} - \mathbf{x}') = 0$.

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This looks like the choice between interpretations of SDE, but randomness is completely irrelevant here.

Perturbation expansion vs. iterative solution

Consider the simplest SDE with multiplicative noise (fixed f)

$$\partial_t \varphi = -K\varphi + f\varphi \quad \rightarrow \quad S = -\Delta(0) f + \tilde{\varphi}\left(-\partial_t \varphi - K\varphi + f\varphi\right) \,,$$

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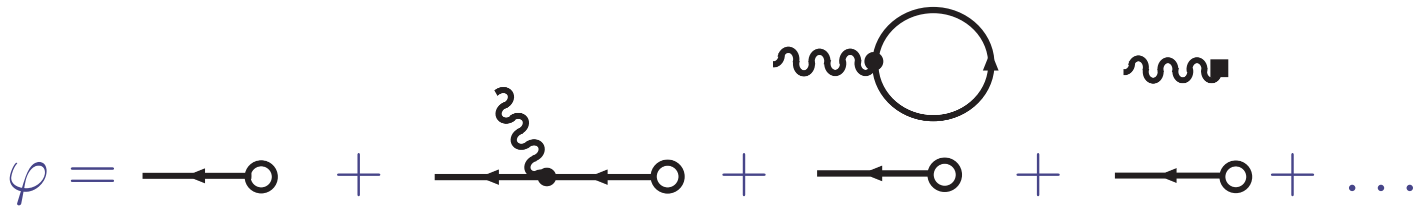
whose dynamic action yields the perturbation expansion



Wavy line – f,

black square – vertex factor due to Jacobian [here, $\Delta(0)$],

circle – initial condition for φ.

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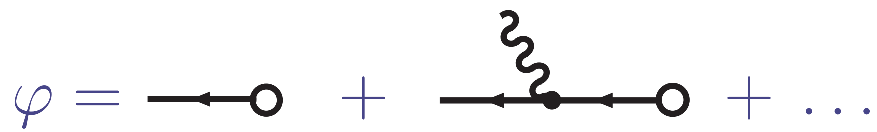
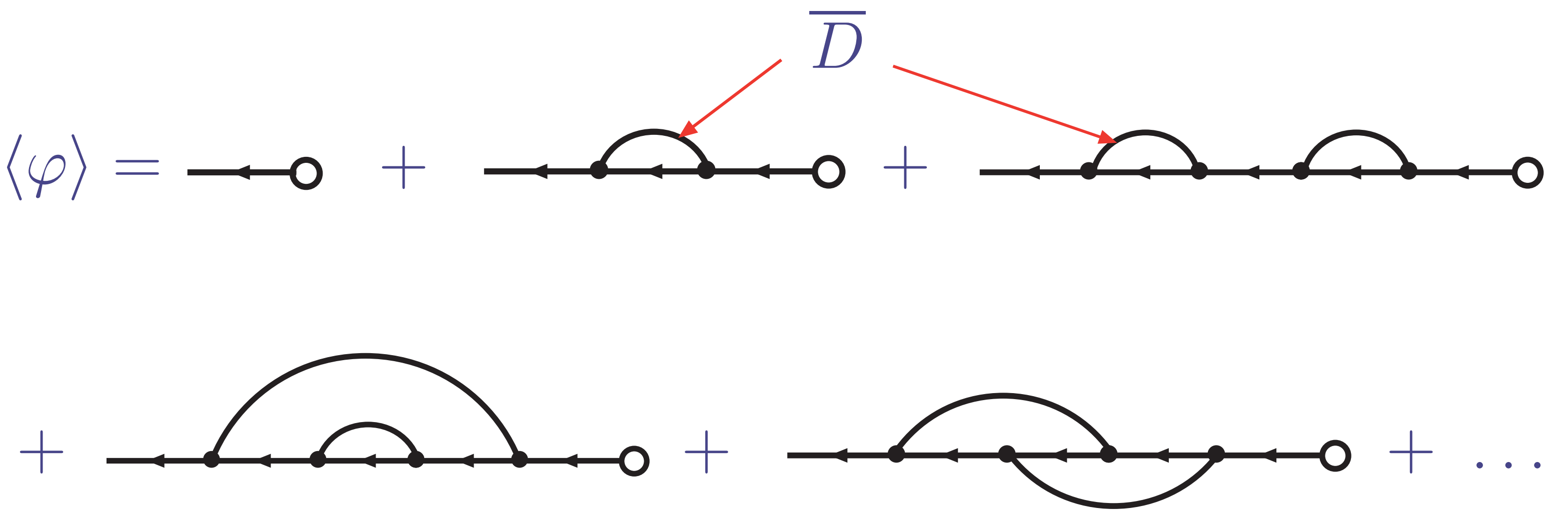
With the proper choice of $\Delta(0)$ the determinant contribution restores the tree expansion of the iterative solution



Perturbation expansion independent of the parameter $\Delta(0)$!

Step-function ambiguity of SDE

Average over the Gaussian random field by Wick's theorem



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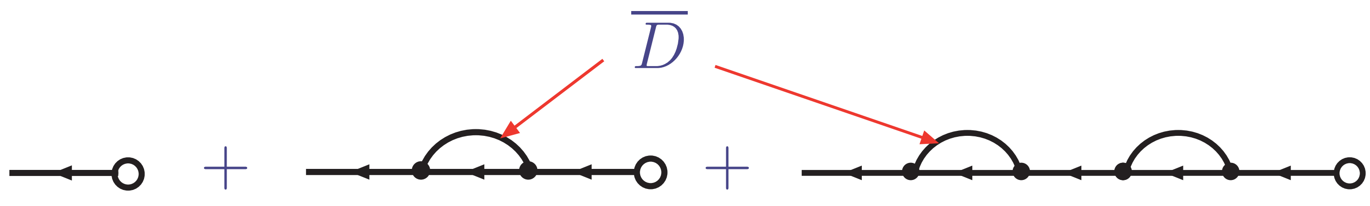

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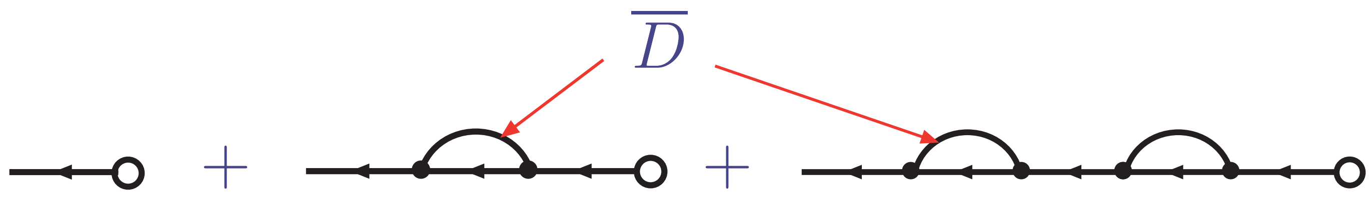
$\langle\varphi\rangle =$ 

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The remaining subgraph reduces to a point:

$$= \frac{1}{2}\int dt_1 \int d\mathbf{x}_1 \int d\mathbf{x}_3\, \Delta(t-t_1, \mathbf{x}-\mathbf{x}_1) D(\mathbf{x}_1, \mathbf{x}_1) \Delta(t_1, \mathbf{x}_1-\mathbf{x}_3) \chi(\mathbf{x}_3)\,.$$

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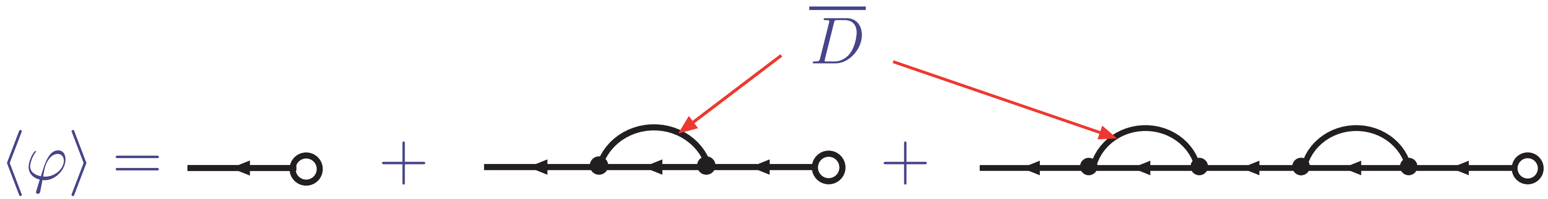

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No ambiguity in the coefficient here, $\frac{1}{2}$ it is!

Stratonovich form of the dynamic action

Shrinking one-loop subgraph to a point effected by the rule

- $\Delta(0,\mathbf{x}-\mathbf{x}') = \frac{1}{2}\delta(\mathbf{x}-\mathbf{x}')$.

Adopt this rule for the Jacobi determinant contribution as well, then the Stratonovich SDE

$$\partial_t\varphi = -K\varphi + U(\varphi) + f\,B(\varphi)$$

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$$S''[\varphi,\tilde\varphi,f] = -\frac{1}{2}\left[U'(\varphi)+B'(\varphi)f\right] - \frac{1}{2}fD^{-1}f + \tilde\varphi\left[-\partial_t\varphi - K\varphi + U(\varphi) + f\,B(\varphi)\right].$$

Ito form of the dynamic action

Reduced subgraphs effected by an additional term in action. Append perturbation expansion everywhere by the rule

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$$S'[\varphi,\tilde\varphi,f] = -\frac{1}{2} f D^{-1} f + \tilde\varphi\left[-\partial_t\varphi - K\varphi + U(\varphi) + \frac{1}{2}B'(\varphi)DB(\varphi) + fB(\varphi)\right]\,,$$

where the detailed form of the additional term in action is

$$B'(\varphi)DB(\varphi) = \int d\mathbf{x}'\int du\frac{\delta B(\mathbf{x},\varphi(u))}{\delta\varphi(t,\mathbf{x}')}D(\mathbf{x}-\mathbf{x}')B(\mathbf{x}',\varphi(t))\,.$$

Master equation of a one-step process

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For the DLR $A+A\to A$ the set of master equations is

$$
\begin{aligned}
&\partial_t P\left(t,\{n_i\}\right)\\
&=\frac{D}{b^2}\sum_{\mathbf{e}}\left[(n_{i+\mathbf{e}}+1)P\left(t,n_1,\ldots,n_i-1,n_{i+\mathbf{e}}+1,\ldots\right)-n_iP\left(t,\{n_i\}\right)\right]\\
&+\frac{k}{V}\left[(n_i+2)(n_i+1)P\left(t,n_1,\ldots,n_i+2,\ldots\right)-(n_i+1)n_iP\left(t,\{n_i\}\right)\right].
\end{aligned}
$$

Second quantization of classical variables

The set of master equations for $P(t, \{n_i\})$ is reduced to a single equation by ”second quantization” of Doi.

Fock space: operators $\hat{a}_i$, $\hat{a}_i^+$ and basis vectors $|\,\{n_i\}\,\rangle$:

$$\hat{a}_i|\,0\,\rangle = 0\,, \quad \hat{a}_j^+|\,\{n_i\}\,\rangle = |\,\{n_i + \delta_{ij}\}\,\rangle\,, \quad [\,\hat{a}_i, \hat{a}_j^+] = \delta_{ij}\,.$$

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Master equations yield kinetic equation for state vector $|\,\Phi\,\rangle$:

$$\frac{\mathrm{d}|\,\Phi\,\rangle}{\mathrm{d}t} = \hat{L}(\hat{a}^+,\,\hat{a})|\,\Phi\,\rangle\,, \quad |\,\Phi\,\rangle = \sum_{n_i=0}^{\infty} P(t,\{n_i\})|\,\{n_i\}\,\rangle\,.$$

The Liouville operator $\hat{L}$ is determined by the set of master equations ($n_i|\,\{n_i\}\,\rangle = \hat{a}_i^+\hat{a}_i|\,\{n_i\}\,\rangle$ etc.).

Functional integral for expectation values

From the kinetic equation, functional integral representation for expectation values is inferred in the form

$$\langle Q(\{n_i\})\rangle = \int\!\!\int \prod_i \mathcal{D}a_i^+ \mathcal{D}a_i \, Q_N \left[\{a_i^+(t)\}+1, \{a_i(t)\}\right]\Big|_{a_i^+(t)\to 0} \times e^{\left[S(a^+,a)+S_{\rm in}[a^+(0)]\right]} \,,$$

where the dynamic action $S(a^+,a) = \int dt \, L_N(a^+ + 1, a)$ and the second term expresses the initial condition

$$S_{\rm in}[a^+(0)] = \ln\left\{\sum_{n_i=0}^{\infty} P(0,\{n_i\}) \prod_i [a_i^+(0)+1]^{n_i}\right\} .$$

Continuum limit and the Doi action

Continuum limit: $a_i^+ \to \psi^+(\mathbf{x})$, $a_i/V \to \psi(\mathbf{x})$ and $\sum_i V \to \int d\mathbf{x}$.

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$$S[\psi^+, \psi] = \psi^+ \left(-\partial_t \psi + D\nabla^2 \psi - k\psi^2 \right) - k(\psi^+)^2 \psi^2 \,.$$

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The (Stratonovich) SDE for this reaction is

$$\partial_t \varphi = D\nabla^2 \varphi - k\varphi^2 + f\varphi \,, \quad \langle f(t,\mathbf{x}) f(t',\mathbf{x}')\rangle = \delta(t-t') C(\mathbf{x}-\mathbf{x}') \,.$$

and gives rise to the dynamic action in Ito form

$$S[\varphi, \tilde{\varphi}] = \tilde{\varphi} \left(-\partial_t \varphi + D\nabla^2 \varphi + \frac{1}{2} C(0)\varphi - k\varphi^2\right) + \frac{1}{2}\tilde{\varphi}^2 C \tilde{\varphi}^2 \,,$$

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Superfluous ”mass” term and wrong sign of quartic term!

Sources and sinks in the master equation

Add random source to the master equation. The simplest: reactions $A \to X$ (sink) and $Y \to A$ (source).

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The source-sink part of the master equation at one lattice site i:

$$\frac{\mathrm{d}P(t,n_i)}{\mathrm{d}t} = \mu_{+i}V\left[P(t,n_i-1) - P(t,n_i)\right] \\ + \mu_{-i}\left[(n_i+1)P(t,n_i+1) - n_iP(t,n_i)\right]\ldots$$

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Contribution to the dynamic Doi action is

$$S[a^+,a] = \sum_i \int\limits_0^\infty dt\, \left[\mu_{+i}Va_i^+(t) - \mu_{-i}a_i^+(t)a_i(t)\right]\ldots$$

Random sources and sinks

Split the time interval $\int dt \to \sum_\alpha \Delta t$. Let the rate coefficients $\mu_{\pm\alpha i} \geq 0$ be random variables with given moments

$$\langle \mu^n_{\pm\alpha i} \rangle = E_{\pm\,,n}\,.$$

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Averaging over $\mu_{\pm\alpha i}$ gives rise to cumulant expansion, e.g.

$$\prod_{\alpha,i} \left\langle \exp\left(\mu_{+\alpha i} V a^+_{\alpha i} \Delta t \right) \right\rangle$$

$$= \exp\left\{ \sum_{\alpha i} \left[\Delta t E_{+1} V a^+_{\alpha i} + \frac{1}{2}\left(E_{+2} - E^2_{+1} \right) \left(V a^+_{\alpha i} \Delta t \right)^2 \right.\right.$$

$$\left.\left. + \frac{1}{6}\left(E_{+3} - 3E_{+1}E_{+2} + E^3_{+1} \right) \left(V a^+_{\alpha i} \Delta t \right)^3 + \cdots \right] \right\}.$$

$A + A \to A$ with random sources and sinks

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$$\sum_{\alpha i} \Delta t E_{+1} V a_{\alpha,i}^+ \xrightarrow[\substack{\Delta t \to 0 \\ V \to 0}]{} E_{+1} \int dt \int d\mathbf{x}\, \psi^+(t,\mathbf{x}) := E_{+1} \psi^+ \,.$$

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Take finite variances only, let higher cumulants vanish, e.g.

$$\left(E_{+2} - E_{+1}^2\right) V \Delta t \to \sigma_+ \,, \; \left(E_{+3} - 3E_{+1}E_{+2} + E_{+1}^3\right) (V \Delta t)^2 \to 0 \,.$$

$A + A \to A$ with random sources and sinks

Continuum limit $a_i^+ \to \psi^+(\mathbf{x})$, $a_i/V \to \psi(\mathbf{x})$, $\sum_i V \to \int d\mathbf{x}$ and $\sum_\alpha \Delta t \to \int dt$. Linear term straightforward

$$\sum_{\alpha i} \Delta t E_{+1} V a^+_{\alpha,i} \xrightarrow[\substack{\Delta t \to 0 \\ V \to 0}]{} E_{+1} \int dt \int d\mathbf{x}\, \psi^+(t,\mathbf{x}) := E_{+1}\psi^+ \,.$$

Take finite variances only, let higher cumulants vanish, e.g.

$$\left(E_{+2} - E_{+1}^2\right) V \Delta t \to \sigma_+ \,, \ \left(E_{+3} - 3E_{+1}E_{+2} + E_{+1}^3\right) (V\Delta t)^2 \to 0 \,.$$

With random sources and sinks Doi action for $A + A \to A$:

$$S[\psi^+, \psi] = \psi^+ \left(-\partial_t \psi + D\nabla^2\psi - k\psi^2\right) - k(\psi^+)^2\psi^2$$
$$+ E_{+1}\psi^+ + \frac{1}{2}\sigma_+ \left(\psi^+\right)^2 - E_{-1}\psi^+\psi + \frac{1}{2}\sigma_- \left(\psi^+\psi\right)^2 \,.$$

Stochastic combat equations

Two species: Lanchester's combat equations for force levels

$$\frac{\mathrm{d}n_r}{\mathrm{d}t} = -\alpha_r n_b\,, \qquad \frac{\mathrm{d}n_b}{\mathrm{d}t} = -\alpha_b n_r\,.$$

Attrition rate on each side independent of its own force level.

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Master equations for the stochastic combat model:

$$\begin{aligned}\frac{\mathrm{d}P(t,n_r,n_b)}{\mathrm{d}t} &= \alpha_r n_b\left[P(t,n_r+1,n_b) - P(t,n_r,n_b)\right] \\ &\quad + \alpha_b n_r\left[P(t,n_r,n_b+1) - P(t,n_r,n_b)\right], \quad n_r, n_b \geq 1\,, \\ \frac{\mathrm{d}P(t,0,n_b)}{\mathrm{d}t} &= \alpha_r n_b P(t,1,n_b)\,,\ n_r = 0, n_b \geq 1\,, \\ \frac{\mathrm{d}P(t,n_r,0)}{\mathrm{d}t} &= \alpha_b n_r P(t,n_r,1)\,,\ n_b = 0, n_r \geq 1\,.\end{aligned}$$

Doi action for Lanchester's combat model

Independent of n death rate requires a special operator

$$\hat{A} = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n!} (\hat{a}^{+})^{n-1} \hat{a}^{n}\,, \;\; \hat{A}|\,0\,\rangle = 0\,, \;\; \hat{A}|\,n\,\rangle = |\,n-1\,\rangle\,, \; n \geq 1\,,$$

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which leads to rather complicated Doi action for DLR

$$\begin{aligned} S(\psi_r^\dagger, \psi_r, \psi_b^\dagger, \psi_b) &= -\psi_r^\dagger \partial_t \psi_r + D_r \psi_r^\dagger \nabla^2 \psi_r - \psi_b^\dagger \partial_t \psi_b + D_b \psi_b^\dagger \nabla^2 \psi_b \\ &\quad - \alpha_r (1 + \psi_b^\dagger) \psi_b \psi_r^\dagger \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} (1 + \psi_r^\dagger)^n \psi_r^{n+1} \\ &\quad - \alpha_b (1 + \psi_r^\dagger) \psi_r \psi_b^\dagger \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} (1 + \psi_b^\dagger)^n \psi_b^{n+1}\,. \end{aligned}$$

Effective large-scale action

Analysis of scaling and one-loop renormalization yields

$$S_{\text{eff}} = -\psi_r^\dagger \partial_t \psi_r + D_r \psi_r^\dagger \nabla^2 \psi_r - \psi_b^\dagger \partial_t \psi_b + D_b \psi_b^\dagger \nabla^2 \psi_b$$
$$- \alpha_{rb} \psi_r^\dagger \psi_r \psi_b^\dagger \psi_b - \psi_b \psi_r^\dagger \sum_{n=0}^{\infty} \frac{\alpha_{rn} \psi_r^{n+1}}{(n+1)!} - \psi_r \psi_b^\dagger \sum_{n=0}^{\infty} \frac{\alpha_{bn} \psi_b^{n+1}}{(n+1)!} .$$

Multiplicatively renormalizable, IR-stable fixed point at $d < 2$.

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Multiplicatively renormalizable, IR-stable fixed point at $d < 2$.

In the "critical" case [$n_r(\tau) = n_b(\tau)$, $\alpha_{rn} = \alpha_{bn} = \alpha \; \forall \, n$] asymptotics for large and small force levels, respectively:

$$n_r(t) \sim n_r(\tau) e^{-\alpha\tau (t/\tau)^{d/2}} , \quad n_r(t) \sim \frac{1}{\alpha\tau (t/\tau)^{d/2}} .$$

However, severe problems with the scaling functions.

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- Asymptotic analysis of Lanchester's combat model.