Dynamics of disordered systems

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Plan of Lectures

1. Introduction
2. Coarsening processes
3. **Formalism**
4. Dynamics of disordered spin models

Plan of 3rd Lecture

1. Langevin equation

   (derivation, time-scales)

2. Stochastic calculus

   (discretisation, chain-rule, Fokker-Planck, drift-force)

3. Generating functional formalism

   (Onsager-Machlup, Martin-Siggia-Rose)

4. Time-reversal symmetry

   (fluctuation-dissipation theorem, fluctuation theorems)

Formalism

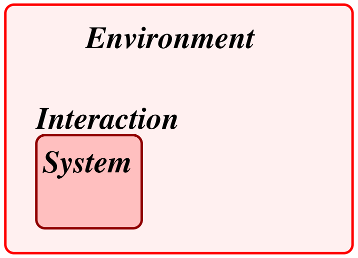
Dissipative systems

Aim

Interest in describing the **statics** and **dynamics** of a **classical or quantum physical system** coupled to a **classical or quantum environment**.

The Hamiltonian of the ensemble is

$$\boxed{H = H_{syst} + H_{env} + H_{int}}$$



The dynamics of all variables are given by Newton or Heisenberg rules, depending on the variables being classical or quantum.

The total energy is conserved, $E =$ ct, but each contribution is not, in particular, $E_{syst} \neq$ ct, and we'll take $E_{syst} \ll E_{env}$.

Reduced system

Model the environment and the interaction

E.g., an ensemble of harmonic oscillators and a linear in q_a and non-linear in x, via the function $\mathcal{V}(x)$, coupling :

$$H_{env} + H_{int} = \sum_{\alpha=1}^{\mathcal{N}} \left[\frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2} q_\alpha^2 \right] + \sum_{\alpha=1}^{\mathcal{N}} c_\alpha q_\alpha \mathcal{V}(x)$$

Equilibrium. Imagine the whole system in contact with a bath at inverse temperature β. Compute the reduced classical partition function or quantum density matrix by tracing away the bath degrees of freedom.

Dynamics. Classically (coupled Newton equations) and quantum (easier in a path-integral formalism) to get rid of the bath variables.

In all cases one can integrate out the oscillator variables as they appear only quadratically.

Reduced system

Statistics of a classical system

Imagine the coupled system in canonical equilibrium with a megabath

$$\mathcal{Z}_{syst\,+\,env} = \sum_{env,\,syst} e^{-\beta H}$$

Integrating out the environmental (oscillator) variables

$$\mathcal{Z}^{red}_{syst} = \sum_{syst} e^{-\beta\left(H_{syst} - \frac{1}{2}\sum_a \frac{c_a^2}{m_a \omega_a^2}\,[\mathcal{V}(x)]^2\right)} \neq \mathcal{Z}_{syst} = \sum_{syst} e^{-\beta H_{syst}}$$

One possibility : assume weak interactions and drop the new term.

Trick : add $H_{counter}$ to the initial coupled Hamiltonian, and choose it in such a way to cancel the quadratic term in $\mathcal{V}(x)$ to recover

$$\boxed{\mathcal{Z}^{red}_{syst} = \mathcal{Z}_{syst}}$$

i.e., the partition function of the system of interest.

Reduced system

Dynamics of a classical system : general Langevin equations

The system, p, x, coupled to an **equilibrium environment** evolves according to the multiplicative noise non-Markov **Langevin equation**

$$\overbrace{m\ddot{x}(t)}^{\text{Inertia}} + \mathcal{V}'(x(t)) \overbrace{\int_{t_0}^{\infty} dt'\, \gamma(t-t')\dot{x}(t')}^{\text{friction}}\, \mathcal{V}'(x(t')) = \underbrace{-\frac{\delta V(x)}{\delta x(t)}}_{\text{deterministic force}} + \mathcal{V}'(x(t))\, \underbrace{\xi(t)}_{\text{noise}}$$

The friction kernel is $\gamma(t-t') = \Gamma(t-t')\theta(t-t')$

The **noise** has zero mean and correlation $\langle\, \xi(t)\xi(t')\, \rangle = k_B T\, \Gamma(t-t')$ with T the temperature of the bath and k_B the Boltzmann constant.

Reduced system

Dynamics of a classical system : general Langevin equations

The system, p, x, coupled to an **equilibrium environment** evolves according to the multiplicative noise non-Markov **Langevin equation**

$$\overbrace{m\ddot{x}(t)}^{\text{Inertia}} + \mathcal{V}'(x(t)) \overbrace{\int_{t_0}^{\infty} dt' \, \gamma(t-t')\dot{x}(t') \, \mathcal{V}'(x(t'))}^{\textbf{friction}} = \underbrace{-\frac{\delta V(x)}{\delta x(t)}}_{\textbf{deterministic force}} + \mathcal{V}'(x(t)) \underbrace{\xi(t)}_{\textbf{noise}}$$

> **Important** Noise arises from lack of knowledge on bath ; noise can be multiplicative ; memory kernel generated ; equilibrium assumption on bath variables implies detailed balance between friction and noise

Separation of time-scales

Additive white noise

In classical systems one usually takes a bath kernel with the smallest relaxation time, $t_{env} \ll t_{all}$ other time scales.

The bath is approximated by the white form $\boxed{\Gamma(t-t') = 2\gamma\delta(t-t')}$

Moreover, one assumes the coupling is bi-linear, $H_{int} = \sum_a c_a q_a x$.

The Langevin equation becomes

$$\boxed{m\ddot{x}(t) \ + \ \gamma\dot{x}(t) \ = \ -\frac{\delta V(x)}{\delta x(t)} \ + \ \xi(t)}$$

with $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = 2k_B T\gamma \, \delta(t-t')$.

Separation of time-scales

Velocities and coordinates

For $t \gg \tau_v = m/\gamma$ one expects the velocities to equilibrate to the

Maxwell distribution $$P(\{\vec{v}\}) = \prod_i P(\vec{v}_i) \propto \prod_i e^{-\beta m v_i^2/2}$$

In this limit, one can drop $m\dot{v}_i^a$ and work with the

overdamped equation $$\gamma \dot{r}_i^a = -\frac{V(\{\vec{r}_i\})}{\delta r_i^a} + \xi_i^a .$$

The positions can have highly **non-trivial dynamics**, see examples.

Message : be very careful when trying to prove equilibration.

Different variables could behave very differently.

Stochastic calculus

Two ways of writing the multiplicative noise equation

The physical eq. that comes from integrating away the bath (oscillators)

$$(\mathcal{V}'[x(t)])^2 \mathrm{d}_t x(t) = F[x(t)] + \mathcal{V}'[x(t)]\xi(t)$$

and the equation usually found in the mathematics literature

$$\mathrm{d}_t x(t) = f[x(t)] + g[x(t)]\xi(t)$$

are equivalent after identification

$$g[x(t)] = \frac{1}{\mathcal{V}'[x(t)]}$$

$$f[x(t)] = \frac{1}{(\mathcal{V}'[x(t)])^2} \, F(x(t)) = (g[x(t)])^2 \, F[x(t)]$$

Stochastic calculus

Discretization prescriptions

$$\mathrm{d}_t x(t) = f[x(t)] + g[x(t)]\,\xi(t)$$

with $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = 2D\,\delta(t-t')$ means

$$\boxed{x(t+\mathrm{d}t) = x(t) + f[\overline{x}(t)]\,\mathrm{d}t + g[\overline{x}(t)]\,\xi(t)\mathrm{d}t}$$

with

$$\boxed{\overline{x}(t) = \alpha x(t+\mathrm{d}t) + (1-\alpha)x(t)}$$

and $0 \leq \alpha \leq 1$. Particular cases are $\alpha = 0$ Itō ; $\alpha = 1/2$ Stratonovich.

Stratonovich 67, Gardiner 96, Øksendal 00, van Kampen 07

Stochastic calculus

Orders of magnitude & different stochastic processes

$\xi_k \equiv \xi(t_k) = \mathcal{O}(\mathrm{d}t^{-1/2})$ because of the Dirac-delta correlations

$\mathrm{d}x \equiv x(t_{k+1}) - x(t_k) = \mathcal{O}(\mathrm{d}t^{1/2})$ Variable increment

What is the difference between the two terms in the right-hand-side when they are evaluated using different discretisation schemes ?

$f[\overline{x}_\alpha(t_k)] - f[\overline{x}_{\overline{\alpha}}(t_k)] = \mathcal{O}(\mathrm{d}t^{1/2})$ vanishes for $\mathrm{d}t \to 0$

$g[\overline{x}_\alpha(t_k)]\xi(t_k) - g[\overline{x}_{\overline{\alpha}}(t_k)]\xi(t_k) = \mathcal{O}(\mathrm{d}t^{0})$ remains finite for $\mathrm{d}t \to 0$

For multiplicative noise processes the discretisation matters:
different α yields different stochastic processes.

Stochastic calculus

Discretization prescriptions

$$\mathrm{d}_t x(t) = f[x(t)] + g[x(t)]\,\xi(t)$$

with $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = 2D\,\delta(t-t')$ means

$$\boxed{x(t_{k+1}) = x(t_k) + f[\overline{x}(t_k)]\,\mathrm{d}t + g[\overline{x}(t_k)]\,\xi(t_k)\mathrm{d}t}$$

with

$$\boxed{\overline{x}(t_k) = \alpha x(t_{k+1}) + (1-\alpha)x(t_k)}$$

The **chain rule** for the time-derivative is (just from Taylor expansion)

$$\boxed{\mathrm{d}_t Y(x) = \mathrm{d}_t x\,\mathrm{d}_x Y(x) + D(1-2\alpha)\,g^2(x)\,\mathrm{d}_x^2 Y(x)}$$

Only for $\alpha = 1/2$ (Stratonovich) one recovers the usual expression.

Not even for additive noise the chain rule is the usual one if $\alpha \neq 1/2$

Stochastic calculus

Fokker-Planck equations for different α

The Fokker-Planck equation

$$\begin{aligned}\partial_t P(x,t) &= -\partial_x[(f(x) + 2D\alpha g(x)\mathrm{d}_x g(x))P(x,t)] \\ &\quad + D\,\partial_x^2[g^2(x)P(x,t)]\end{aligned}$$

depends on α and g

Two processes will be statistically the same if

$$f + 2D\,\alpha\,g\mathrm{d}_x g = f_{\mathrm{drifted}} + 2D\,\overline{\alpha}\,g\mathrm{d}_x g$$

Stochastic calculus

Fokker-Planck & stationary measure

The Fokker-Planck equation

$$\partial_t P(x,t) \;=\; -\partial_x[(f(x) + 2D\alpha g(x)\mathrm{d}_x g(x))P(x,t)] \\ +D\,\partial_x^2[g^2(x)P(x,t)]$$

has the stationary measure

$$P_{\rm st}(x) = Z^{-1}\,[g(x)]^{2(\alpha-1)}\,e^{\frac{1}{D}\int^x \frac{f(x')}{g^2(x')}} = Z^{-1}e^{-\frac{1}{D}U_{\rm eff}(x)}$$

with $U_{\rm eff}(x) = -\int^x \frac{f(x')}{g^2(x')} + 2D(1-\alpha)\ln g(x)$

Remark : the potential $U_{\rm eff}(x)$ depends upon α and $g(x)$ Non-equilibrium

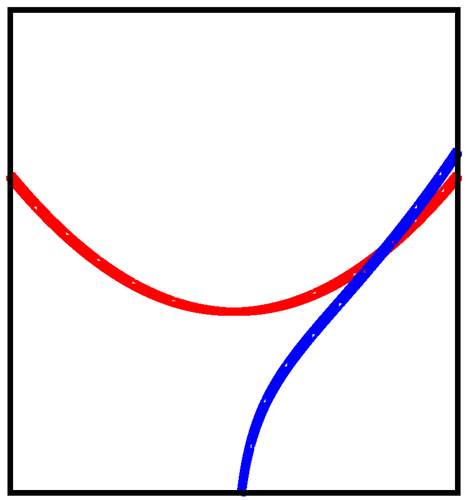
Noise induced phase transitions

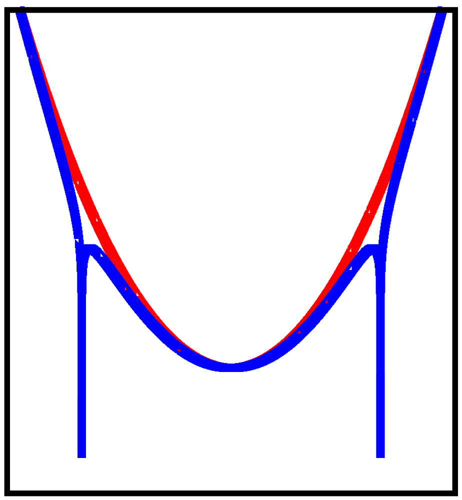
Stratonovich 67, Sagués, Sancho & García-Ojalvo 07

Stochastic calculus

Fokker-Planck & stationary measure

e.g. $f = -g^2 U$ and $U_{\rm eff} = U + 2D(1-\alpha)\ln g$





x^2 + $2D(1-\alpha)\ln x$

$g(x) = x$

$U(x) = x^2$

x^2 + $2D(1-\alpha)\ln(1-x^2)$

$g(x) = (1-x^2)$

$U(x) = x^2$

Stochastic calculus

Drift

The **Gibbs-Boltzmann equilibrium**

$$P_{\mathrm{GB}}(x) = Z^{-1}\, e^{-\beta U(x)}$$

is approached if (recall the physical writing of the equation)

$$\boxed{f(x) \mapsto \underbrace{-g^2(x)\mathrm{d}_x U(x)}_{\text{Potential}} + \underbrace{2D(1-\alpha)g(x)\mathrm{d}_x g(x)}_{\text{drift}}}$$

Remark: the drift is also needed for the Stratonovich mid-point scheme.

Important choice: if one wants the dynamics to approach thermal equilibrium independently of α and g the drift term has to be added.

Stochastic calculus

Fokker-Planck & stationary measure

The Fokker-Planck equation

$$\partial_t P(x,t) = -\partial_x[(f(x) + 2D\alpha g(x)\mathrm{d}_x g(x))P(x,t)] \\ +D\,\partial_x^2[g^2(x)P(x,t)]$$

for the drifted force $f(x) \mapsto -g^2(x)\mathrm{d}_x U(x) + 2D(1-\alpha)g(x)\mathrm{d}_x g(x)$

becomes

$$\partial_t P(x,t) = -\partial_x[(-g^2(x)\mathrm{d}_x U(x) + 2Dg(x)\mathrm{d}_x g(x))P(x,t)] \\ +D\,\partial_x^2[g^2(x)P(x,t)]$$

with the expected Gibbs-Boltzmann measure stationary measure

$$P_{\mathrm{st}}(x) = Z^{-1} e^{-\frac{1}{D}U(x)}$$

independently of $g(x)$ and α

Why care about multiplicative noise ?

Magnetisation precession

Bloch equation

Evolution of the time-dependent $3d$ magnetisation density per unit volume, $\mathbf{M} = (M_x, M_y, M_z)$, with constant modulus $M_s = |\mathbf{M}|$

$$\boxed{\mathrm{d}_t\mathbf{M} = -\overline{\mu}\,\mathbf{M} \wedge \mathbf{H}_{\mathrm{eff}}}$$

$\overline{\mu} \equiv \gamma\mu_0$ is the product of $\gamma = \mu_B g/\hbar$, the gyromagnetic ratio, and μ_0, the vacuum permeability constant (μ_B Bohr's magneton and g Lande's g-factor)

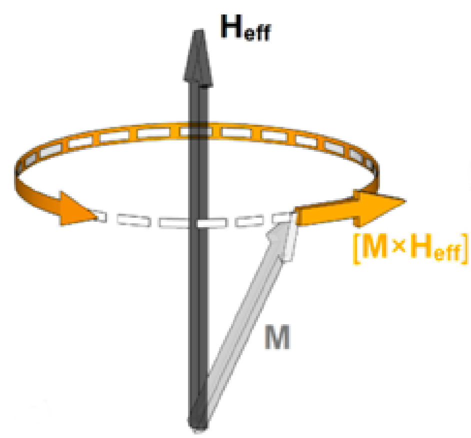
For the initial condition $\mathbf{M}(t_{\mathrm{i}}) = \mathbf{M}_{\mathrm{i}}$

the magnetisation precesses around $\mathbf{H}_{\mathrm{eff}}$

with $2\mathbf{M}\cdot\mathrm{d}_t\mathbf{M} = \mathrm{d}_t|\mathbf{M}|^2 = 0$

and $\mathrm{d}_t(\mathbf{M}\cdot\mathbf{H}_{\mathrm{eff}}) = 0$ (if $\mathbf{H}_{\mathrm{eff}} =$ ct)

Bloch 32



Dissipative effects

Landau-Lifshitz & Gilbert equations

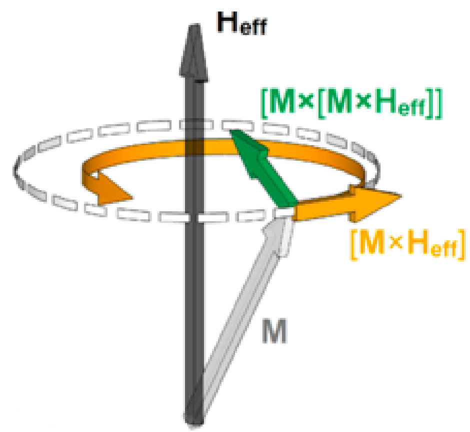
$$\mathrm{d}_t\mathbf{M} = -\frac{\overline{\mu}}{1+\gamma_0^2\overline{\mu}^2}\,\mathbf{M}\wedge\left[\mathbf{H}_{\text{eff}} + \frac{\gamma_0\overline{\mu}}{M_s}\,(\mathbf{M}\wedge\mathbf{H}_{\text{eff}})\right]$$

Landau & Lifshitz 35

$$\mathrm{d}_t\mathbf{M} = -\overline{\mu}\,\mathbf{M}\wedge\left(\mathbf{H}_{\text{eff}} - \frac{\gamma_0}{M_s}\mathrm{d}_t\mathbf{M}\right)$$

Gilbert 55

2nd terms in RHS: dissipative mechanisms slow down the precession and push $\mathbf{M}$ towards $\mathbf{H}_{\text{eff}}$ with $2\mathbf{M}\cdot\mathrm{d}_t\mathbf{M} = \mathrm{d}_t|\mathbf{M}|^2 = 0$ and $\mathrm{d}_t(\mathbf{M}\cdot\mathbf{H}_{\text{eff}}) > 0$



Thermal fluctuations

À la Langevin in Gilbert's formulation

$$\boxed{\mathrm{d}_t\mathbf{M} = -\overline{\mu}\mathbf{M} \wedge \left(\mathbf{H}_{\mathrm{eff}} + \mathbf{H} - \frac{\gamma_0}{M_s}\mathrm{d}_t\mathbf{M}\right)}$$

$\mathbf{H}$ is a white random noise, with zero mean $\langle H_i(t) \rangle = 0$ and correlations

$$\langle H_i(t) H_j(t') \rangle = 2D\delta_{ij}\delta(t - t')$$

The (diffusion) parameter D is proportional to $k_B T$ **Brown 63**

The noise $\mathbf{H}$ **multiplies** the magnetic moment $\mathbf{M}$ and one cannot always write $2\mathbf{M} \cdot \mathrm{d}_t\mathbf{M} = \mathrm{d}_t M^2$ (only if the Stratonovich calculus is used)

This is the **Markov stochastic Landau-Lifshitz-Gilbert-Brown (sLLGB)** multiplicative white noise stochastic differential equation.

Subtleties of Markov multiplicative noise processes are now posed.

Thermal fluctuations

À la Langevin in Gilbert's formulation

$$\mathrm{d}_t\mathbf{M} = -\overline{\mu}\mathbf{M} \wedge \left(\mathbf{H}_{\text{eff}} + \mathbf{H} - \frac{\gamma_0}{M_s}\mathrm{d}_t\mathbf{M}\right) - \frac{2D(1-2\alpha)\overline{\mu}^2}{1+\overline{\mu}^2\gamma_0^2}\mathbf{M}$$

$\mathbf{H}$ is a white random noise, with correlations $\langle H_i(t)H_j(t')\rangle = 2D\delta_{ij}\delta(t-t')$

The (diffusion) parameter D is proportional to k_BT **Brown 63**

The modulus of the magnetic moment is now conserved $\mathrm{d}_t\mathbf{M}^2 = 0$ for all α

One also proves that the dynamics approaches the asymptotic Gibbs-Boltzmann distribution

$$P_{\text{GB}}(\mathbf{M}) \propto e^{-\frac{1}{D}\mathbf{M}\cdot\mathbf{H}_{\text{eff}}}$$

Methods

Dynamic generating functional

- Glassy models with and without disorder:

  The "order parameter" is a composite object depending on two-times.

  It's handy to use functional methods to write a dynamic generating functional as a path-integral

  Onsager-Machlup & Martin-Siggia-Rose-Janssen-deDominicis formalisms

  Similar to Feynman path-integral

The construction will follow **LFC & Lecomte,** "Rules of calculus in the path integral representation of white noise Langevin equations : the Onsager-Machlup approach", **arXiv :1704.03501, J. Phys. A (to appear)** where special care of discretisation effects was taken.

Generating functional

Onsager-Machlup representation

Definition of the transition probability

$$P(x_k, t_k | x_{k-1}, t_{k-1}) = \int d\xi_{k-1} P_{\text{noise}}(\xi_{k-1}) \delta(x_k - \mathsf{R}(x_k, x_{k-1}, \xi_{k-1}))$$

A Jacobian is needed to transform the δ in which ξ_{k-1} appears within a function to $J^{-1}\delta(\xi_{k-1} - \ldots)$:

Generalisation of $|f'(f^{-1}(a))|\delta(f(z) - a) = \delta(z - f^{-1}(a))$

$$J = \det_{kk'} \left[\frac{\delta x_k - \mathsf{R}[x_k, x_{k-1}, \xi_{k-1}; \alpha]}{\delta \xi_{k'}} \right]$$

$$P(x_k, t_k | x_{k-1}, t_{k-1}) = \int d\xi_{k-1} P_{\text{noise}}(\xi_{k-1}) J^{-1} \delta(\xi_k - \mathsf{H}(x_k, x_{k-1}))$$

Generating functional

Onsager-Machlup representation

The transition probability now reads

$$P(x_k, t_k | x_{k-1}, t_{k-1}) = \sqrt{\frac{1}{4\pi k_B T \mathrm{d}t}} \, \frac{1}{|g(\overline{x}_{k-1})|} \, e^{S_{\mathrm{OM}}[x_k, x_{k-1}; \alpha]}$$

For $\mathrm{d}_t x(t) = f(x(t)) + g(x(t))\xi(t)$, the **Onsager-Machlup** action is

$$S_{\mathrm{OM}}[x_k, x_{k-1}; \alpha] \equiv \ln P_{\mathrm{i}}(x_{-\mathcal{T}}) - \frac{\mathrm{d}t}{4k_B T} \left[\frac{1}{g^2(\overline{x}_{k-1})} \left(\frac{(x_k - x_{k-1})}{\mathrm{d}t} - f(\overline{x}_{k-1}) + \underbrace{2D\alpha g(\overline{x}_{k-1}) g'(\overline{x}_{k-1})} \right)^2 \underbrace{-\alpha f'(x_{k-1})} \right]$$

From the integration over the noise

Jacobian

Generating functional

Onsager-Machlup representation, continuous time notation

The transition probability now reads

$$P(x_k, t_k | x_{k-1}, t_{k-1}) = \sqrt{\frac{1}{4\pi k_B T \mathrm{d}t}} \, \frac{1}{|g(\overline{x}_{k-1})|} \, e^{S_{\mathrm{OM}}[\{x\};\alpha]}$$

For $\mathrm{d}_t x(t) = f(x(t)) + g(x(t))\xi(t)$, the **Onsager-Machlup** action is

$$S_{\mathrm{OM}}[\{x\};\alpha] \equiv \ln P_{\mathrm{i}}(x_{-\mathcal{T}}) - \frac{\mathrm{d}t}{4k_B T} \left[\frac{1}{g_t^2} \underbrace{(\mathrm{d}_t x_t - f_t + 2D\alpha g_t \mathrm{d}_x g_t)^2}_{\text{From the integration over the noise}} \underbrace{-\alpha \mathrm{d}_x f_t}_{\text{Jacobian}} \right]$$

From the integration over the noise   Jacobian

Generating functional

MSR path-integral representation

The initial state at time $-\mathcal{T}$ is drawn from a probability distribution $P_{\rm i}(x_{-\mathcal{T}})$.

The noise generates random trajectories with probability density

$$P(\{x\};\alpha) = \langle \prod_{k=1}^{N} \delta(x_k - x_k^{\rm sol}) \rangle \, P_{\rm i}(x_{-\mathcal{T}})$$

where the angular brackets represent an average over the noise $\{\xi\}$ weighted with its probability distribution.

$x_k^{\rm sol}$ is the (possibly implicit) solution to the Langevin equation

$$0 = \text{Eqnt}[x_k, x_{k-1}, \xi_{k-1}; \alpha]$$

The integral over the noise can be computed if one inverts to write $\xi_{k-1} = \text{L}(x_k, x_{k-1}; \alpha)$ and imposes this constraint with a delta function.

Generating functional

MSR path-integral representation

A Jacobian is needed to transform the δ in which ξ_{k-1} appears within a function to $J^{-1}\delta(\xi_{k-1} - \dots)$:

Generalisation of $|f'(f^{-1}(a))|\delta(f(z) - a) = \delta(z - f^{-1}(a))$

$$J = \det_{kk'}\left[\frac{\delta \mathsf{Eqnt}[x_k, x_{k-1}, \xi_{k-1}; \alpha]}{\delta \xi_{k'}}\right]$$

The path-probability now reads

$$P(\{x\}; \alpha) = \langle \textstyle\prod_{k=1}^{N} J^{-1}\delta(\xi_{k-1} - \mathsf{L}(x_k, x_{k-1}; \alpha))\rangle \, P_{\mathrm{i}}(x_{-\mathcal{T}})$$

where the angular brackets still represent an average over the noise $\{\xi\}$ weighted with its probability distribution.

This Jacobian is simple for additive noise but not so simple to compute for multiplicative noise.

Generating functional

MSR path-integral representation

A Jacobian is needed to transform the δ in which ξ_{k-1} appears within a function to $J^{-1}\delta(\xi_{k-1} - \dots)$:

Generalisation of $|f'(f^{-1}(a))|\delta(f(z) - a) = \delta(z - f^{-1}(a))$

$$J = \det_{kk'} \left[\frac{\delta \text{Eqnt}[x_k, x_{k-1}, \xi_{k-1}; \alpha]}{\delta \xi_{k'}} \right]$$

The path-probability now reads

$$P(\{x\}; \alpha) = \langle \textstyle\prod_{k=1}^{N} J^{-1} \delta(\xi_{k-1} - \mathsf{L}(x_k, x_{k-1}; \alpha)) \rangle \, P_{\mathrm{i}}(x_{-\mathcal{T}})$$

where the angular brackets still represent an average over the noise $\{\xi\}$ weighted with its probability distribution.

This Jacobian is simple for additive noise but not so simple to compute for multiplicative noise.

Generating functional

MSR path-integral representation

Using now the exponential representation of the delta $\delta(y) \propto \int d\hat{y}\, e^{\pm i\hat{y}y}$, the integral over the noise is now a Gaussian that can be computed and

$$P_{\rm OM}(\{x\};\alpha) = \int \mathcal{D}\{\hat{x}\} \prod_{k=0}^{N-1} (4\pi k_B T \mathrm{d}t g^2(\overline{x}_k))^{-1/2} \; e^{S_{\rm MSR}[\{x\},\{i\hat{x}\};\alpha]}$$

and the **Martin-Siggia-Rose-Janssen 79** action is

$$S_{\rm MSR}[\{x\}, i\{\hat{x}\};\alpha] \equiv \ln P_{\rm i}(x_{-\mathcal{T}}) + \int \Big[\pm i\hat{x}_t(\underbrace{\mathrm{d}_t x_t} - f_t + \underbrace{2D\alpha g_t \mathrm{d}_x g_t) + D(i\hat{x}_t)^2 g_t^2} \underbrace{-\alpha \mathrm{d}_x f_t} \Big]$$

proportional to γ_0 (not written) Jacobian

where we have also transformed the auxiliary field $i\hat{x}_t \mapsto i\hat{x}_t g_t$

Generating functional

Path-integral representation

$$P_{\rm OM}(\{x\};\lambda,\alpha) \propto \int \mathcal{D}\{\hat{x}\}\, P_{\rm MSR}(\{x\},\{{\rm i}\hat{x}\};\lambda,\alpha)$$

$$= \int \mathcal{D}\{\hat{x}\} \prod_{k=0}^{N-1} (4\pi k_B T {\rm d}t g^2(\overline{x}_k))^{-1/2}\, e^{S_{\rm MSR}[\{x\},\{{\rm i}\hat{x}\};\lambda,\alpha]}$$

$$S_{\rm MSR}[\{x\},\{{\rm i}\hat{x}\};\lambda,\alpha] \equiv \ln P_{\rm i}(x_{-\mathcal{T}},\lambda_{-\mathcal{T}})$$

$$+ \int \left[\pm{\rm i}\hat{x}_t({\rm d}_t x_t - f_t + 2D\alpha g_t {\rm d}_x g_t) + D({\rm i}\hat{x}_t)^2 g_t^2 - \alpha {\rm d}_x f_t\right]$$

λ_t is a time-dependent parameter, for example, a parameter in the potential that one can tune in time. The action depends on α and g.

Observable averages can now be calculated as

$$\langle A(x_t,{\rm i}\hat{x}_{t'})\rangle = \int \mathcal{D}\{x\}\mathcal{D}\{\hat{x}\}\, P_{\rm MSR}(\{x\},\{{\rm i}\hat{x}\};\lambda,\alpha)\, A(x_t,{\rm i}\hat{x}_{t'})$$

Generating functional

Path-integral representation

For the drifted force $f_t = -g^2 \mathrm{d}_x V_t + 2D(1-\alpha) g_t \mathrm{d}_x g_t$

$$
\begin{aligned}
S_{\mathrm{MSR}}(\{x\}, \{\mathrm{i}\hat{x}\}; \lambda, \alpha) \equiv \ln P_{\mathrm{i}}(x_{-\mathcal{T}}, \lambda_{-\mathcal{T}}) \\
+ \int \big[\pm \mathrm{i}\hat{x}_t (\mathrm{d}_t x_t + g_t^2 \mathrm{d}_x V_t - 2D(1-2\alpha) g_t \mathrm{d}_x g_t) \\
+ D(\mathrm{i}\hat{x}_t)^2 g_t^2 - \alpha \mathrm{d}_x f_t \big]
\end{aligned}
$$

Remark: The action depends on α and g.

Observable averages can now be calculated as

$$
\langle A(x_t, \mathrm{i}\hat{x}_{t'}) \rangle = \int \mathcal{D}\{x\} \mathcal{D}\{\hat{x}\} \, P_{\mathrm{MSR}}(\{x\}, \{\mathrm{i}\hat{x}\}; \alpha, \lambda) \, A(x_t, \mathrm{i}\hat{x}_{t'})
$$

and do not depend on α

Stochastic calculus

Path-integral representation for additive noise

For $g = 1$ and the force $f_t = -\mathrm{d}_x V_t$ the action is

$$S_{\mathrm{MSR}}[\{x\}, \{\mathrm{i}\hat{x}\}; \alpha] \equiv \ln P_{\mathrm{i}}(x_{-\mathcal{T}}) + \int \left[\pm \mathrm{i}\hat{x}_t(\mathrm{d}_t x_t + \mathrm{d}_x V_t) + D(\mathrm{i}\hat{x}_t)^2 + \alpha \mathrm{d}_x^2 V_t \right]$$

Observable averages can now be calculated as

$$\langle A(x_t, \mathrm{i}\hat{x}_{t'}) \rangle = \int \mathcal{D}\{x\}\mathcal{D}\{\hat{x}\}\, P_{\mathrm{MSR}}(\{x\}, \{\mathrm{i}\hat{x}\}; \lambda, \alpha)\, A(x_t, \mathrm{i}\hat{x}_{t'})$$

and do not depend on α

Methods

Dynamical symmetry & exact results

The functional path-integral formalism allows one to obtain exact identities (fluctuation-dissipation theorem, fluctuation theorems) as consequences of a dynamic symmetry and its symmetry breaking.

Details in :

"Symmetries of generating functionals of Langevin processes with colored multiplicative noise" **Aron, Biroli & LFC, J. Stat. Mech. P11018 (2010)** ; "Dynamical symmetries of Markov processes with multiplicative white noise", **Aron, Barci, LFC, González Arenas & Lozano, J. Stat. Mech. 053207 (2016)**

Possible (though not easy) to extend to quantum system.

"(Non) equilibrium dynamics : a (broken) symmetry of the Keldysh generating functional"

Aron, Biroli & LFC, arXiv:1705.10800

Symmetry

Transformations in the path-integral representation

Let us define

$$\mathrm{d}_t^{(\alpha)} x_t \equiv \mathrm{d}_t x_t - 2D(1-2\alpha) g_t \mathrm{d}_x g_t$$

and group two terms in the action due to the coupling to the bath

$$S_{\text{diss}}[x, \mathrm{i}\hat{x}] = \int -\mathrm{i}\hat{x}_t \left[\mathrm{d}_t^{(\alpha)} x_t - D \mathrm{i}\hat{x}_t g_t^2\right]$$

This expression suggests to use the generalized transformation on the time-dependent variables $\{x_t, \mathrm{i}\hat{x}_t\}$

$$\mathcal{T}_c = \begin{cases} x_t & \mapsto & x_{-t} \ , \\ \mathrm{i}\hat{x}_t & \mapsto & \mathrm{i}\hat{x}_{-t} + D^{-1} g_{-t}^{-2} \mathrm{d}_t^{(\alpha)} x_{-t} \ , \end{cases}$$

and $\alpha \mapsto 1 - \alpha$

Remember $D = \beta^{-1} = k_B T$

Symmetry

Transformations in the path-integral representation

For initial conditions drawn from $P_{\rm i}(x) = Z^{-1} e^{-\beta V(x)}$ and

$$\boxed{f(x) = -g^2(x) {\rm d}_x V(x) + 2D(1-\alpha) g(x) {\rm d}_x g(x)}$$ one proves

$$S_{\rm det+jac}[\mathcal{T}_c {\rm i}\hat{x}, \mathcal{T}_c x; \mathcal{T}_c \alpha] = S_{\rm det+jac}[{\rm i}\hat{x}, x; \alpha]$$

that implies

$$P[\mathcal{T}_c {\rm i}\hat{x}, \mathcal{T}_c x; \mathcal{T}_c \alpha] = P[{\rm i}\hat{x}, x; \alpha]$$

Note that we have to use the non-trivial chain rule.

Moreover, the transformation leaves the integral measure invariant (no Jacobian) and the interval of integration as well.

Symmetry

Consequences of the transformation : FDT

From this result we can prove exact equilibrium relations such as the **fluctuation-dissipation theorem** linking the (causal) linear response to a field that changes the force as $f_t \mapsto f_t + h_t$

$$R(t,t') = \left. \frac{\delta \langle x(t) \rangle}{\delta h(t')} \right|_{h=0} \propto \theta(t-t')$$

and the correlation function in a model independent way :

$$\boxed{R(t,t') - R(-t,-t') = \beta \, \partial_{t'} \langle x(-t) x(-t') \rangle}$$

that for a stationary problem (in equilibrium) becomes

$$\boxed{R(t-t') - R(t'-t) = \beta \, \partial_{t'} C(t'-t) = \beta \, \partial_{t'} C(t-t')}$$

Broken symmetry

Relation under "any" transformation

$$\frac{P(\mathcal{T}_c x, \mathcal{T}_c \hat{x}; \mathcal{T}_c \alpha, \overline{\lambda})}{P(x, \hat{x}; \alpha, \lambda)} = e^{\Delta S(x,\hat{x};\alpha,\lambda)}$$

with ΔS the variation of the full action (and measure)

$\mathcal{T}_c x$ and $\mathcal{T}_c \hat{x}$ are transformed trajectories,

$\overline{\lambda}$ the transformed parameter in the potential,

$\mathcal{T}_c \alpha$ a different discretisation parameter ;

and from here obtain relations between observables by averaging this relation : equilibrium fluctuation dissipation ($\Delta S = 0$), or out of equilibrium theorems ($\Delta S \neq 0$).

e.g., **Jarzinsky 97, Crooks 00 & many others**

Broken Symmetry

Consequences of the transformation: Fluctuation-theorems

For initial conditions drawn from $P_{\mathrm{i}}(x) = Z^{-1} e^{-\beta V(x)}$ and

$$\boxed{f(x, \lambda_t) = -g^2(x)\partial_x V(x, \lambda_t) + 2D(1-\alpha)g(x)\mathrm{d}_x g(x)}$$ one

proves

with $$\frac{P[\mathcal{T}_c \mathrm{i}\hat{x}, \mathcal{T}_c x; \mathcal{T}_c \alpha, \overline{\lambda}_t = \lambda_{-t}]}{P[\mathrm{i}\hat{x}, x; \alpha, \lambda_t]} = e^{\beta W - \beta \Delta F}$$

$$\begin{aligned} W &= \int \mathrm{d}t\, \mathrm{d}_t \lambda_t\, \partial_\lambda V(x, \lambda) \\ \Delta F &= \ln Z(\lambda_{\mathcal{T}}) - \ln Z(\lambda_{-\mathcal{T}}) \end{aligned}$$

the work, and free-energy difference between initial and fictitious final states.

Exact out of equilibrium relations such as the **Jarzinsky relation** follow

$$\boxed{\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}}$$

Coloured noise

Langevin equation & generating functional

The generic **Langevin equation** for a particle in $1d$ is

$$m\ddot{x}(t) + \mathcal{V}'[x(t)] \int_{-\mathcal{T}}^{t} dt' \, \Gamma(t-t')\mathcal{V}'[x(t')]\dot{x}(t') = F(t) + \xi(t)M'[x(t)]$$

with the coloured noise $\langle \xi(t)\xi(t') \rangle = k_B T \, \Gamma(t-t')$

The dynamic generating functional is a path-integral

$$\mathcal{Z}_{dyn}[\eta] = \int dx_{-\mathcal{T}} d\dot{x}_{-\mathcal{T}} \int \mathcal{D}x\mathcal{D}\hat{x} \; e^{-S[x,\mathrm{i}\hat{x};\eta]}$$

with $\mathrm{i}\hat{x}(t)$ the ‘response’ variable.

$x_{-\mathcal{T}}$ and $\dot{x}_{-\mathcal{T}}$ are the initial conditions at time $-\mathcal{T}$.

Martin-Siggia-Rose-Jenssen-deDominicis formalism