Building a path integral calculus

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Setting

Multiplicative Gaussian white noise Langevin equations

$d = 1$ stochastic equation for one $\mathbb{R}$ variable x

$$\dot{x}(t) = f(x(t)) + g(x(t))\eta(t)$$

Zero average Gaussian white noise $\langle \eta(t) \rangle = 0$ & $\langle \eta(t)\eta(t') \rangle = 2D\delta(t-t')$

$\mu = 1, \ldots, d \geq 1$ stochastic equations for $\mathbf{x} = (x^1, \ldots, x^d)$

$$\dot{x}^\mu(t) = f^\mu(\mathbf{x}(t)) + g^{\mu i}(\mathbf{x}(t))\eta_i(t)$$

Gaussian white noise $\langle \eta_i(t) \rangle = 0$ & $\langle \eta_i(t)\eta_j(t') \rangle = 2D\delta_{ij}\delta(t-t')$

Einstein's summation rule, $x(t)$ continuous time notation, x_t discrete time notation

The problem

Lack of covariance ($d=1$ notation)

– For any of the so-far used linear discretization schemes, x_t, one can make non-linear changes of variables $u(t) = U(x(t))$ at the level of the Langevin equations using the corresponding chain rules, and go back and forth.

– One next constructs the generating functional (path integral) for original $\mathbb{P}_X(\{x_t\})$ and transformed $\mathbb{P}_U(\{u_t\})$ stochastic processes.

– Surprisingly, one cannot transform one into the other one via the same non-linear transformation,

$$\prod_t \mathrm{d}x_t \, \mathbb{P}_X(\{x_t\}) \neq \prod_t \mathrm{d}u_t \, \mathbb{P}_U(\{u_t\})$$

U^{-1} exists, e.g. Cartesian & spherical coordinates, measure transf. taken into account

We found this problem in

Magnetization dynamics : path-integral formalism for the stochastic Landau-Lifshitz-Gilbert equation

C. Aron, D. G. Barci, L. F. Cugliandolo, Z. González-Arenas, G. S. Lozano

J. Stat. Mech. P09008 (2014)

but well-known in the literature

A problem already noticed in, *e.g.*

gravitation & quantum field theory, e.g. **de Witt Cécile & Bryce** 50s (quantization on curved spaces), **Gervais & Jevicki** 76, **Langouche, Roekaerts & Tirapegui** 80s,

statistical physics **Gulyaev & Edwards** 64, **Graham et al.** 80s, and

mathematics **Stratonovich** 60s, etc.

Solutions proposed but hard to find, read, understand...

Our first attempt to solve this problem

Rules of calculus in the path integral representation of white noise Langevin equations: the Onsager-Machlup approach

L. F. Cugliandolo & V. Lecomte, J. Phys. A 50, 345001 (2017)

Our solution in $d = 1$

Building a path-integral calculus : a covariant discretization approach

L. F. Cugliandolo, V. Lecomte & F. van Wijland, J. Phys. A 52, 50LT01 (2019)

and in $d > 1$

Path integrals and stochastic calculus

T. Arnoux de Pirey, L. F. Cugliandolo, V. Lecomte & F. van Wijland, Adv. Phys. (2023)

The solution

Our proposal : a higher order discretization prescription

The continuous time notation $\dot{x}(t) \stackrel{(\beta_g)}{=} f(x(t)) + g(x(t))\,\eta(t)$

with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = 2D\,\delta(t-t')$ is a short-hand notation for

$$x_{t+\Delta t} = x_t + f(\overline{x}_t)\,\Delta t + g(\overline{x}_t)\,\eta_t\,\Delta t$$ with **higher order**

$$\overline{x}_t = x_t + \tfrac{1}{2}\Delta x + \beta_g(x_t)(\Delta x)^2 \quad \text{where} \quad \Delta x = x_{t+\Delta t} - x_t$$

and $\beta_g = \frac{1}{12}\,[g_t''/(2g_t') - g_t'/g_t]$ with $g_t = g(x_t)$

While the finer discretization $\mathcal{O}((\Delta x)^2)$ is negligible to ensure covariance of the Langevin equation in the $\Delta t \to 0$ limit and $(\beta_g) = (S)$, it is needed to construct a covariant generating fct. Different form of the path probability ensuring the latter property. (Inspiration from non-Gaussian stochastic processes **Di Paola & Falsone 90s**.)

LFC, Lecomte & van Wijland 19

The solution

A higher order discretization prescription : the key properties

$\overline{x}_t = x_t + \frac{1}{2}\Delta x + \beta_g(x_t)(\Delta x)^2$

where $\Delta x = x_{t+\Delta t} - x_t$ and $\beta_g = \frac{1}{12}\,[g''_t/(2g'_t) - g'_t/g_t]$

with $g_t = g(x_t)$

— With the $\mathcal{O}((\Delta x)^2)$ discretization the usual chain rule is valid up to Δt corrections, while with the Stratonovich $\mathcal{O}(\Delta x)$ one it is only valid up to $\Delta t^{1/2}$ corrections.

— We solve the covariance problem of the generating functional.

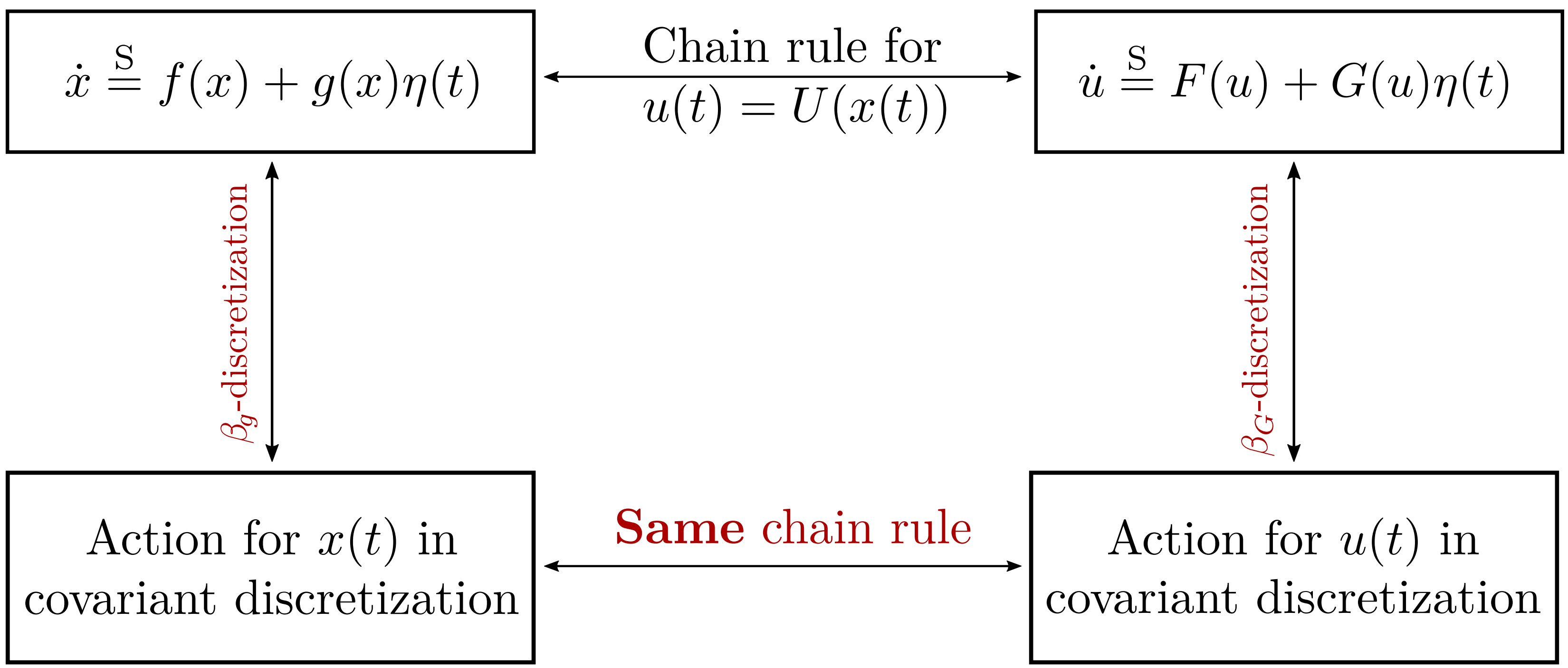
— We can generalize to $d > 1$.

The action has one more term.

LFC, Lecomte & van Wijland 19 (d=1) Arnoulx de Pirey ***et al*** **22 (d>1)**

The sketch

Langevin equation & path integral representation



Measure defined so that $\mathcal{D}x \leftrightarrow \mathcal{D}u$

Plan of the talk

Like a lecture

1. Multiplicative noise Langevin equation

   (derivation, over-damped limit)

2. Stochastic calculus

   (discretization, chain-rule, Fokker-Planck, drift-force, change of variables)

3. Generating functional formalisms

   (Onsager-Machlup, Martin-Siggia-Rose)

4. Problems with non-linear transformations in the path-integral

5. The solution : a higher order discretization scheme

1. Langevin equations

Langevin equation

Focus on $d = 1$, generalization at the end

Multiplicative white noise stochastic equation

$$\dot{x}(t) = f(x(t)) + g(x(t))\eta(t)$$

Restriction : g^{-1} exists, that is, $g^{-1}(g(x)) = g(g^{-1}(x)) = x$

Zero average Gaussian white noise $\langle \eta(t) \rangle = 0$ & $\langle \eta(t)\eta(t') \rangle = 2D\delta(t-t')$

$x(t)$ continuous time notation, later x_t discrete time notation

One can derive this equation by coupling the selected variable x to an ensemble of harmonic oscillators $\sum_\alpha c_\alpha q_\alpha h(x)$ and taking an over-damped limit

2. Stochastic calculus

Stochastic calculus

Linear (usual) discretization prescriptions

The continuous time notation $\dot{x}(t) \stackrel{(\alpha)}{=} f(x(t)) + g(x(t))\,\eta(t)$

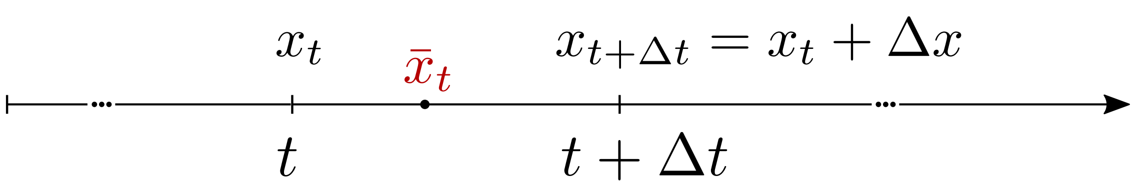
with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = 2D\,\delta(t-t')$ needs a time-discretization

$$\boxed{x_{t+\Delta t} \stackrel{(\alpha)}{=} x_t + f(\overline{x}_t)\,\Delta t + g(\overline{x}_t)\,\eta_t\,\Delta t}$$

with, **usually**,

$$\boxed{\overline{x}_t \equiv \alpha x_{t+\Delta t} + (1-\alpha) x_t = x_t + \alpha \Delta x \text{ where } \Delta x = x_{t+\Delta t} - x_t}$$

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



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

Stochastic calculus

Noise correlation

The continuous time notation $\dot{x}(t) \stackrel{(\alpha)}{=} f(x(t)) + g(x(t))\,\eta(t)$

with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = 2D\,\delta(t-t')$ is a short-hand notation for

$x(t) \mapsto x_t$ where $t = k\Delta t$ and $k = 0, \dots, N$, Δt infinitesimal, and

$$x_{t+\Delta t} \stackrel{(\alpha)}{=} x_t + f(\overline{x}_t)\,\Delta t + g(\overline{x}_t)\,\eta_t\,\Delta t$$

with

$$\overline{x}_t = \alpha x_{t+\Delta t} + (1-\alpha)x_t = x_t + \alpha \Delta x$$

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

The **noise-noise $\boldsymbol{\delta}$-corr.** becomes $\langle \eta_t \eta_{t'} \rangle = \dfrac{2D}{\Delta t}\,\delta_{tt'} \Rightarrow \boxed{\langle \eta_t^2 \rangle = \frac{2D}{\Delta t}}$

Stochastic calculus

Orders of magnitude & different stochastic processes

$$\boxed{\eta_t = \mathcal{O}(\Delta t^{-1/2})}$$ because of the Dirac-delta correlations of a **white bath**

Scaling of the variable increment $$\boxed{\Delta x \equiv x_{t+\Delta t} - x_t = \mathcal{O}(\Delta t^{1/2})}$$

What is the difference between the two terms in the right-hand-side of the Langevin eq. when they are evaluated using different α discretization schemes ?

$f(\overline{x}_t^{(\alpha)}) - f(\overline{x}_t^{(\overline{\alpha})}) = \mathcal{O}(\Delta t^{1/2})$ vanishes for $\Delta t \to 0$

$g(\overline{x}_t^{(\alpha)})\eta_t - g(\overline{x}_t^{(\overline{\alpha})})\eta_t = \mathcal{O}(\Delta t^0)$ **remains finite** for $\Delta t \to 0$

For multiplicative noise processes **the discretization matters**:
different α yield different stochastic processes, unless f modified to f_α

Stochastic calculus

The chain rule: time derivative of a function $U(x)$

$$\dot{x}(t) \stackrel{(\alpha)}{=} f(x(t)) + g(x(t))\,\eta(t)$$

means $$\boxed{x_{t+\Delta t} \stackrel{(\alpha)}{=} x_t + f(\overline{x}_t)\,\Delta t + g(\overline{x}_t)\,\eta_t\,\Delta t}$$

with $$\boxed{\overline{x}_t = \alpha x_{t+\Delta t} + (1-\alpha)x_t}$$ and $$\boxed{\langle \eta_t \eta_{t'} \rangle = \frac{2D}{\Delta t}\,\delta_{tt'}}$$

The **chain rule** for the time-derivative is (just from Langevin-eq. & Taylor)

$$\frac{U(x_{t+\Delta t}) - U(x_t)}{\Delta t} = \frac{x_{t+\Delta t} - x_t}{\Delta t}\,U'(\overline{x}_t) + D(1-2\alpha)\,g^2(\overline{x}_t)\,U''(\overline{x}_t) + U''(\overline{x}_t)\,\boldsymbol{\mathcal{O}(\Delta t^{1/2})}$$

Note the $\boldsymbol{\mathcal{O}(\Delta t^{1/2})}$ correction (that vanishes for $\Delta t \to 0$)

Make it $\boldsymbol{\mathcal{O}(\Delta t)}$ (or exact) with a higher order discretization scheme

Stochastic calculus

The chain rule: time derivative of a function $U(x)$

$$\dot{x}(t) \stackrel{(\alpha)}{=} f(x(t)) + g(x(t))\,\eta(t)$$

means $$x_{t+\Delta t} \stackrel{(\alpha)}{=} x_t + f(\overline{x}_t)\,\Delta t + g(\overline{x}_t)\,\eta_t\,\Delta t$$

with $$\overline{x}_t = \alpha x_{t+\Delta t} + (1-\alpha)x_t$$ and $$\langle \eta_t \eta_{t'} \rangle = \frac{2D}{\Delta t}\,\delta_{tt'}$$

The **chain rule** for the time-derivative is (just from Langevin-eq. & Taylor) in continuous time notation

$$\dot{U}(x) = \dot{x}\,U'(x) + D(1-2\alpha)\,g^2(x)\,U''(x)$$

Only for $\alpha = 1/2$ (Stratonovich) or $U(x) = ax$ one recovers the usual form. Even for additive noise $g = ct$ the chain rule is unusual if $\alpha \neq 1/2$

Stochastic calculus

The chain rule: time derivative of a function $U(x)$

$$\dot{x}(t) \stackrel{(\alpha)}{=} f(x(t)) + g(x(t))\,\eta(t)$$

means $$x_{t+\Delta t} \stackrel{(\alpha)}{=} x_t + f(\overline{x}_t)\,\Delta t + g(\overline{x}_t)\,\eta_t\,\Delta t$$

with $$\overline{x}_t = \alpha x_{t+\Delta t} + (1-\alpha)x_t$$ and $$\langle \eta_t \eta_{t'} \rangle = \frac{2D}{\Delta t}\,\delta_{tt'}$$

The **chain rule** for the time-derivative is (just from Langevin-eq. & Taylor) in continuous time notation

$$\dot{U}(x) = \dot{x}\,U'(x) + D(1-2\alpha)\,g^2(x)\,U''(x)$$

Note that the **continuous time limit** of the **chain rule** will not be modified if we use a higher order discretization scheme

Stochastic calculus

Apply a non-linear transformation of variables to the Langevin-eq.

Take a generic function $U(x)$ with an inverse.

Calculate the infinitesimal increment $u_{t+\Delta t} - u_t \equiv U(x_{t+\Delta t}) - U(x_t)$ to derive the stochastic equation satisfied by u_t.

Replace $x_{t+\Delta t} = x_t + f(\overline{x}_t)\Delta t + g(\overline{x}_t)\eta_t \Delta t$, with $\overline{x}_t = x_t + \alpha \Delta x$ in the 1st term in the rhs, replace $\overline{x}_t$ in terms of $\overline{u}_t$, and Taylor expand for small Δt

$$\boxed{\frac{u_{t+\Delta t} - u_t}{\Delta t} \stackrel{(\alpha)}{=} F(\overline{u}_t) + G(\overline{u}_t)\eta_t + \mathcal{O}(\boldsymbol{\Delta t^{1/2}})}$$

with $F(\overline{u}_t) = (U' \circ U^{-1})(\overline{u}_t)(f \circ U^{-1})(\overline{u}_t) + D(1 - 2\alpha)(g \circ U^{-1})(\overline{u}_t))^2$ and $G(\overline{u}_t) = (U' \circ U^{-1})(\overline{u}_t)(g \circ U^{-1})(\overline{u}_t)$.

The right-hand-side takes the Langevin form up to corrections $\mathcal{O}(\boldsymbol{\Delta t^{1/2}})$

3. Generating functionals with linear discretizations

Generating functionals

From noise to trajectories: Onsager-Machlup

From the noise joint pdf $\mathbb{P}_\eta[\{\eta_t\}] = \prod_{0\leq t<t_f} P_{\rm n}(\eta_t)$

(independently drawn at each time step)

with $P_{\rm n}(\eta_t) = \left(\frac{\Delta t}{4\pi D}\right)^{1/2} e^{-\frac{\Delta t}{4D}\eta_t^2}$ (Gaussian white statistics)

Use the recursion at each time step (i.e., the Langevin equation in discretization d)

$$\frac{x_{t+\Delta t} - x_t}{\Delta t} \stackrel{(d)}{=} f(\overline{x}_t) + g(\overline{x}_t)\,\eta_t \quad \Rightarrow \quad x_{t+\Delta t} = R_d(x_{t+\Delta t}, x_t, \eta_t)$$

to derive the trajectory (joint) probability

$$\mathbb{P}_X[\{x_t\}] \stackrel{(d)}{=} \prod_{0\leq t<t_f} \underbrace{T_d(x_{t+\Delta t}, t+\Delta t | x_t, t)}_{\rm trans.prob.} \; \underbrace{P^{\rm i}_X(x_0)}_{\rm initial\,cond.}$$

$$\equiv \underbrace{\mathcal{N}^{(d)}_X[\{x_t\}]}_{\rm pre-factor} \; \exp\{-\underbrace{S^{(d)}_X[\{x_t\}]}_{\rm action}\}$$

Three slides with details of the derivation

for the linear discretization (α)

– skip them –

Generating functionals

Infinitesimal transition probability from t to $t+\Delta t$

Langevin eq. in generic discretization scheme $x_{t+\Delta t} = R_\alpha(x_{t+\Delta t}, x_t, \eta_t)$

Definition of the infinitesimal transition probability

$$T_\alpha(x_{t+\Delta t}, t+\Delta t | x_t, t) = \int \mathrm{d}\eta_t \, P_\mathrm{n}(\eta_t) \, \delta(x_{t+\Delta t} - R_\alpha(x_{t+\Delta t}, x_t, \eta_t))$$

In order to integrate over $\mathrm{d}\eta_t$ we have to transform the δ into one with the form $\delta(\eta_t - \tilde{R}_\alpha(x_{t+\Delta t}, x_t))$, but we need a Jacobian

Use of $\delta(f(\eta)) = 1/|\mathrm{d}_\eta f(\eta)| \; \delta(\eta - \eta^*) = |J(\eta)|^{-1} \; \delta(\eta - \eta^*)$ with $f(\eta^*) = 0$

$\mathrm{d}_\eta f(\eta) \mapsto$

$$J \equiv \frac{\mathrm{d}[x_{t+\Delta t} - \mathsf{R}_\alpha(x_{t+\Delta t}, x_t, \eta_t)]}{\mathrm{d}\eta_t}$$

$$T_\alpha(x_{t+\Delta t}, t+\Delta t | x_t, t) = \int \mathrm{d}\eta_t \, P_\mathrm{n}(\eta_t) \, |J|^{-1} \, \delta(\eta_t - \tilde{R}_\alpha(x_{t+\Delta t}, x_t))$$

One can forget the modulus if there is a single solution

Generating functionals

Infinitesimal transition probability from t to $t + \Delta t$

The $\delta(\eta_t - \tilde{R}_\alpha(x_{t+\Delta t}, x_t))$ forces the Gaussian noise weight to be

$$e^{-\frac{\Delta t}{4D}\left[\tilde{R}_\alpha(x_{t+\Delta t}, x_t)\right]^2} = e^{-\frac{\Delta t}{4D}\left[\frac{x_{t+\Delta t} - x_t - \Delta t f(\overline{x}_t)}{\Delta t\, g(\overline{x}_t)}\right]^2}$$

What about the Jacobian ?

$\mathrm{d}_\eta f(\eta) \mapsto$
$$J = \frac{\mathrm{d}[x_{t+\Delta t} - R_\alpha(x_{t+\Delta t}, x_t, \eta_t)]}{\mathrm{d}\eta_t}$$

Since $R_\alpha(x_{t+\Delta t}, x_t, \eta_t) = x_t + \Delta t\, f(\overline{x}_t) + \Delta t\, g(\overline{x}_t)\, \eta_t$, the noise is also in $\overline{x}_t$ via the Langevin equation itself. One has to expand, to the relevant $\mathcal{O}(\Delta t^n)$ and only later take the d_η. This is a long calculation.

Three ways of doing it in **LFC & Lecomte 17**

Generating functionals

Infinitesimal transition probability from t to $t+\Delta t$

The $\delta(\eta_t - \tilde{R}_\alpha(x_{t+\Delta t}, x_t))$ forces the Gaussian noise weight to be

$$e^{-\frac{\Delta t}{4D}\left[\tilde{R}_\alpha(x_{t+\Delta t},x_t)\right]^2} = e^{-\frac{\Delta t}{4D}\left[\frac{x_{t+\Delta t}-x_t-\Delta t f(\overline{x}_t)}{\Delta t\, g(\overline{x}_t)}\right]^2}$$

After the lengthy calculation, one can write the Jacobian as

$$J^{-1} \propto \frac{1}{|g(x_t)|}\exp\Big\{ -2\alpha\Delta t\eta_t g'(\overline{x}_t) - \alpha\Delta t f'(\overline{x}_t) - \alpha\Delta t f(\overline{x}_t)\frac{g'(\overline{x}_t)}{g(\overline{x}_t)} - D\alpha^2\Delta t\left[2(g'(\overline{x}_t))^2 - g(\overline{x}_t)g''(\overline{x}_t))\right]\Big\}$$

Note that J^{-1} depends on the functions f and g, the pre and post points & the noise: $J^{-1} = J^{-1}(x_t, x_{t+\Delta t}, \eta_t)$. **We kept up to $\mathcal{O}(\Delta t)$ terms in the exp.**

For additive noise $g'(x) = 0$, the familiar form $J^{-1} \propto \exp[-\alpha f'(\overline{x}_t)\Delta t]$ is found and $J^{-1} \propto ct$ for Itō.

Important

one has to keep $\mathcal{O}(\Delta t)$ terms in the exponential

because there is a sum over all time steps

The final expressions for the $(S) = (\alpha = 1/2)$ discretization is

Generating functionals

Onsager-Machlup representation

After some rearrangements (e.g. the prefactor re-expressed in $x_{t+\Delta t}$, etc.) and cancellations, the Stratonovich ($S, \alpha = 1/2$) transition probability reads

$$T_{(S)}(x_{t+\Delta t}, t + \Delta t | x_t, t) = \sqrt{\frac{\Delta t^{-1}}{2\pi 2D}} \; \frac{1}{|g(x_{t+\Delta t})|} \; e^{-\Delta S_X^{(S)}(x_{t+\Delta t}, x_t, \Delta t)}$$

with the prefactor in $\mathcal{N}_X^{(S)}$ and the **Onsager-Machlup** infinitesimal action

$$\Delta S_X^{(S)}(x_{t+\Delta t}, x_t, \Delta t) \equiv \underbrace{\frac{1}{2}\frac{\Delta t}{2D}\;\frac{1}{g^2(\overline{x}_t)}\left[\frac{(x_{t+\Delta t} - x_t)}{\Delta t} - f(\overline{x}_t)\right]^2}_{\text{Gaussian noise weight}}$$

$$\underbrace{+\frac{\Delta t}{2}\left[f'(\overline{x}_t) - \frac{f(\overline{x}_t)g'(\overline{x}_t)}{g(\overline{x}_t)}\right] + \frac{D\,\Delta t}{4}\left[2(g'(\overline{x}_t))^2 - g(\overline{x}_t)g''(\overline{x}_t)\right]}_{\text{Jacobian, originates in the change of variables from } \eta_t \text{ to } x_t}$$

Generating functionals

From Onsager-Machlup to Martin-Siggia-Rose

Use the Hubbard-Stratonovich (Gaussian integral) trick to go from the exponential of a square (from the Gaussian noise) to the one of a linear term

$$\sqrt{\frac{2\pi}{a}}\; e^{-\frac{1}{2}\frac{y^2}{a}} = \int_{\mathrm{i}\mathbb{R}} \mathrm{d}\hat{x}\; e^{\pm \hat{x} y + \frac{a}{2}\hat{x}^2}$$

that with the parameters in the action $y_t = \left[\frac{x_{t+\Delta t} - x_t}{\Delta t} - f(\overline{x}_t)\right]\Delta t$ and $a_t = 2D(g(\overline{x}_t))^2\Delta t$, and a convenient choice of sign, yields

$$\sqrt{\frac{2D(g(\overline{x}_t))^2\Delta t}{2\pi}} \int_{\mathrm{i}\mathbb{R}} \mathrm{d}\hat{x}_t\; e^{-\hat{x}_t \left[\frac{x_{t+\Delta t} - x_t}{\Delta t} - f(\overline{x}_t)\right]\Delta t + D(g(\overline{x}_t))^2 \hat{x}^2}$$

Note that the normalization prefactor is proportional to $\frac{g(\overline{x}_t)}{g(x_{t+\Delta t})}$ **Important !**

4. Problems w/non-linear transformations

Linear discretization

Failure of the non-linear transformation

Why does it fail at the level of the action ? Because

$$\Delta S_U^{(\alpha)}(u_{t+\Delta t}, u_t, \Delta t) \mapsto \Delta S_X^{(\alpha)}(x_{t+\Delta t}, x_t, \Delta t) + \underbrace{\boldsymbol{\mathcal{O}}(\Delta t)}_{\textbf{change}}$$

Indeed, the guilty term in the Onsager-Machlup action is

$$\left(\frac{1}{G(\overline{u}_t)}\frac{\Delta u}{\Delta t}\right)^2 \Delta t \quad \xrightarrow{\text{(S)}} \quad \left[\frac{1}{g(\overline{x}_t)}\frac{\Delta x}{\Delta t} + \boldsymbol{\mathcal{O}}(\boldsymbol{\Delta t^{1/2}})\right]^2 \Delta t$$

transformed using the discrete time chain rule.

The double product is $\boxed{\propto \frac{\boldsymbol{\Delta x}}{\boldsymbol{\Delta t}} \boldsymbol{\mathcal{O}(\Delta t^{1/2}) = \mathcal{O}(\Delta t^{0})}}$ and cannot be neglected

Increase the order of the extra terms improving the accuracy of the chain rule

Quadratic discretization

Orders of magnitude, chain rule & transformations

Take a generic function $U(x)$ with an inverse.

Calculate the infinitesimal increment $u_{t+\Delta t} - u_t \equiv U(x_{t+\Delta t}) - U(x_t)$

Replace $x_{t+\Delta t} = x_t + f(\overline{x}_t)\Delta t + g(\overline{x}_t)\eta_t \Delta t$

with $\overline{x}_t = x_t + \frac{1}{2}\Delta x + \beta_g \Delta x^2$ and $\beta_g = \frac{1}{12}[g''/(2g') - g'/g]$

in the 1st term in the rhs, transform to $\overline{u}_t$ and Taylor expand for small Δt

$$\frac{u_{t+\Delta t} - u_t}{\Delta t} \overset{(\beta_g)}{=} F(\overline{u}_t) + G(\overline{u}_t)\eta_t + \boldsymbol{\mathcal{O}(\Delta t)}$$

with $F(\overline{u}_t) = U'(U^{-1}(\overline{u}_t))f(U^{-1}(\overline{u}_t))$ and similarly for G.

The right-hand-side takes the Langevin form up to corrections $\boldsymbol{\mathcal{O}(\Delta t)}$

In the $\Delta t \to 0$ limit the improvement is irrelevant at the level of the Langevin equation ; but it is not to build the path integral !

Quadratic discretization

Orders of magnitude, chain rule & transformations

Why does the transformation fail at the level of the action for the linear Stratonovich rule ?

$$\Delta S_U^{(S)}(u_{t+\Delta t}, u_t, \Delta t) \mapsto \Delta S_X^{(S)}(x_{t+\Delta t}, x_t, \Delta t) + \mathcal{O}(\Delta t)$$

$$\left(\frac{1}{G(\overline{u}_t)}\frac{\Delta u}{\Delta t}\right)^2 \xrightarrow{\text{(S)}} \left[\frac{1}{g(\overline{x}_t)}\frac{\Delta x}{\Delta t} + \mathcal{O}(\Delta t^{1/2})\right]^2$$

the double product is $\propto \dfrac{\Delta x}{\Delta t}\,\mathcal{O}(\Delta t^{1/2}) = \mathcal{O}(\Delta t^0)$ and cannot be neglected

Why does the transformation work fine for the β_g discretization ?

$$\Delta S_U^{(\beta_g)}(u_{t+\Delta t}, u_t, \Delta t) \mapsto \Delta S_X^{(\beta_g)}(x_{t+\Delta t}, x_t, \Delta t) + \boldsymbol{\mathcal{O}(\Delta t^{3/2})}$$

$$\left(\frac{\Delta u}{\Delta t}\right)^2 \Delta t \xrightarrow{(\beta_g)} \left[U'(\overline{x}_t)\frac{\Delta x}{\Delta t} + \boldsymbol{\mathcal{O}(\Delta t)}\right]^2 \Delta t$$

the double product is $\boxed{\propto \boldsymbol{\dfrac{\Delta x}{\Delta t}\,\mathcal{O}(\Delta t) = \mathcal{O}(\Delta t^{1/2})}}$ and drop it

Generating functional

Onsager-Machlup path integral representation

Using standard procedures (careful calculation of the Jacobian)

$$T_{(\beta_g)}(x_{t+\Delta t}, t+\Delta t | x_t, t) = \frac{1}{\sqrt{4\pi D \Delta t}\, |g(x_{t+\Delta t})|}\, e^{-\Delta S_X^{(\beta_g)}(x_{t+\Delta t}, x_t)}$$

$$\Delta S_X^{(\beta_g)}(x_{t+\Delta t}, x_t) = \frac{1}{2}\frac{\Delta t}{2D}\left[\frac{\frac{\Delta x}{\Delta t} - f(\overline{x}_t)}{g(\overline{x}_t)}\right]^2 + \frac{\Delta t}{2}\left[f'(\overline{x}_t) - \frac{f(\overline{x}_t)g'(\overline{x}_t)}{g(\overline{x}_t)}\right]$$

which in the continuous-time writing reads

$$S_X^{(\beta_g)}[\{x\}] = \int_0^{t_f} \mathrm{d}t \, \left\{ \frac{1}{4D}\left[\frac{\dot{x} - f(x)}{g(x)}\right]^2 + \frac{1}{2}\, f'(x) - \frac{1}{2}\frac{f(x)g'(x)}{g(x)} \right\}$$

New term

Remarks:

- The action is more sensitive to discretization details than the Langevin equation
- The pre-factor in $T_{(\beta_g)}$ takes care of the transformation of the measure
- A trivial example: the kinetic energy $\frac{1}{2}mv^2$ of a Brownian particle $m\dot{v} + \gamma v = \eta$

Generating functional

Onsager-Machlup path integral representation

Using standard procedures (careful calculation of the Jacobian)

$$T_{(\beta_g)}(x_{t+\Delta t}, t+\Delta t | x_t, t) = \frac{1}{\sqrt{4\pi D \Delta t}\, |g(x_{t+\Delta t})|} \, e^{-\Delta S_X^{(\beta_g)}(x_{t+\Delta t}, x_t)}$$

$$\Delta S_X^{(\beta_g)}(x_{t+\Delta t}, x_t) = \frac{1}{2}\frac{\Delta t}{2D}\Big[\frac{\frac{\Delta x}{\Delta t} - f(\overline{x}_t)}{g(\overline{x}_t)}\Big]^2 + \frac{\Delta t}{2}\Big[f'(\overline{x}_t) - \frac{f(\overline{x}_t) g'(\overline{x}_t)}{g(\overline{x}_t)}\Big]$$

which encodes the continuous-time writing

$$S_X^{(\beta_g)}[\{x\}] = \int_0^{t_f} \mathrm{d}t \, \left\{ \frac{1}{4D}\Big[\frac{\dot{x} - f(x)}{g(x)}\Big]^2 + \frac{1}{2} f'(x) - \frac{1}{2}\frac{f(x) g'(x)}{g(x)} \right\}$$

Comments:

- **Once written this way one can operate with the usual chain rule.**
- Same continuous-time writing as **de Witt 57, Stratonovich 60, Graham 77** but different meaning, none of them identified the **discrete time origin**

Proof of covariance

Onsager-Machlup path integral representation

The measure with the normalization transforms as desired, e.g. $\dfrac{du_t}{G(u_t)} = \dfrac{dx_t}{g(x_t)}$

Using

$$\frac{\mathrm{d}u}{\mathrm{d}t} = U'(x)\,\frac{\mathrm{d}x}{\mathrm{d}t}$$

(note that we now work in the continuous time formulation)

$$\begin{aligned} F'(u) &= \frac{\mathrm{d}F(u)}{\mathrm{d}u} = \frac{1}{U'(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\left[U'(x)f(x)\right] \\ &= \frac{1}{U'(x)}\,\left[U''(x)f(x) + U'(x)f'(x)\right] \end{aligned}$$

& similarly for G, to transform the action $S_U[\{u\}]$

$$S_U[\{u\}] = \int_0^{t_f} \mathrm{d}t\,\left\{\frac{1}{4D}\left[\frac{\dot{u} - F(u)}{G(u)}\right]^2 + \frac{1}{2}F'(u) - \frac{1}{2}\,\frac{F(u)G'(u)}{G(u)}\right\}$$

$$\begin{aligned} = \int_0^{t_f} \mathrm{d}t\,\Bigg\{ &\frac{1}{4D}\left[\frac{U'(x)\dot{x} - U'(x)f(x)}{U'(x)g(x)}\right]^2 + \frac{1}{2}\,\frac{1}{U'(x)}\,\left[U''(x)f(x) + U'(x)f'(x)\right] \\ &- \frac{1}{2}\,\frac{U'(x)f(x)}{U'(x)g(x)}\,\frac{1}{U'(x)}\,\left[U''(x)g(x) + U'(x)g'(x)\right]\Bigg\} \end{aligned}$$

we identify many cancellations

Proof of covariance

Onsager-Machlup path integral representation

The measure with the normalization are transform as desired, e.g. $\dfrac{du_t}{G(u_t)} = \dfrac{dx_t}{g(x_t)}$

Using

$$\frac{\mathrm{d}u}{\mathrm{d}t} = U'(x)\,\frac{\mathrm{d}x}{\mathrm{d}t}$$

(note that we now work in the continuous time formulation)

$$F'(u) = \frac{\mathrm{d}F(u)}{\mathrm{d}u} = \frac{1}{U'(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\,[U'(x)f(x)]$$

$$= \frac{1}{U'(x)}\,\left[U''(x)f(x) + U'(x)f'(x)\right]$$

& similarly for G, to transform the action $S_U[\{u\}]$, we recover $S_X[\{x\}]$

$$S_U[\{u\}] = \int_0^{t_f} \mathrm{d}t\,\left\{\frac{1}{4D}\left[\frac{\dot{u} - F(u)}{G(u)}\right]^2 + \frac{1}{2}F'(u) - \frac{1}{2}\,\frac{F(u)G'(u)}{G(u)}\right\}$$

$$= \int_0^{t_f} \mathrm{d}t\,\left\{\frac{1}{4D}\left[\frac{\cancel{U'(x)}\,\dot{x} - \cancel{U'(x)}\,f(x)}{\cancel{U'(x)}\,g(x)}\right]^2 + \frac{1}{2}\,\frac{1}{U'(x)}\,\left[\cancel{U''(x)f(x)} + U'(x)f'(x)\right] - \frac{1}{2}\,\frac{\cancel{U'(x)}\,f(x)}{\cancel{U'(x)}\,g(x)}\,\frac{1}{U'(x)}\,\left[\cancel{U''(x)g(x)} + U'(x)g'(x)\right]\right\}$$

$$= \int_0^{t_f} \mathrm{d}t\,\left\{\frac{1}{4D}\left[\frac{\dot{x} - f(x)}{g(x)}\right]^2 + \frac{1}{2}f'(x) - \frac{1}{2}\,\frac{f(x)g'(x)}{g(x)}\right\} = S_X[\{x\}]$$

The solution

Martin-Siggia-Rose (Janssen) path integral representation

$$\mathbb{P}_U[\{u_t, \hat{u}_t\}] = \mathrm{d}u_0 P_U^{\mathrm{i}}(u_0) \frac{g(\overline{x}_0)}{g(x_1)} \prod_{0<t<t_f} \mathrm{d}u_t \mathrm{d}\hat{u}_t \; \frac{g(\overline{x}_t)}{g(x_{t+\Delta t})} e^{-S_U^{(\beta g)}[\{u_t, \hat{u}_t\}]}$$

One $\hat{u}_t$ per t. Using standard procedures, in the continuous-time writing

$$S_U^{(\beta g)}[\{u, \hat{u}\}] = \int_0^{t_f} \mathrm{d}t \left\{ \hat{u}[\dot{u} - F(u)] - D(G(u))^2 \hat{u}^2 + \frac{1}{2} F'(u) \underbrace{- \frac{1}{2} \frac{G'(u)}{G(u)} F(u)}_{\text{new}} \right\}$$

Remarks :

- The last term would be absent in the linear Stratonovich discretization.
- It is absent for additive white noise $G' = 0$.

Proof of covariance using $\hat{u} = \hat{x}/U'(x)$ and the same transformations of u and $\dot{u}$ as for Onsager-Machlup

$$S_U^{(\beta g)}[\{u, \hat{u}\}] = \int_0^{t_f} \mathrm{d}t \left\{ \frac{\cancel{U'(x)}}{\cancel{U'(x)}} \hat{x}[\dot{x} - f(x)] - D(g(x))^2 \hat{x}^2 \frac{\cancel{(U'(x))^2}}{\cancel{(U'(x))^2}} \right.$$

$$\left. + \frac{1}{2} \frac{1}{U'(x)} \left[\cancel{U''(x) f(x)} + U'(x) f'(x) \right] - \frac{1}{2} \frac{U'(x) f(x)}{(U'(x))^2 g(x)} \left[\cancel{U''(x) g(x)} + U'(x) g'(x) \right] \right\}$$

Stochastic calculus

In higher dimension $\mu = 1, \ldots, d > 1$

In continuous time notation the Langevin equation for the d dimensional time-dependent contra-variant vector $\mathbf{x}(t) = (x^1(t), \ldots, x^d(t))$ is

$$\dot{x}^\mu(t) = f^\mu(\mathbf{x}(t)) + g^{\mu i}(\mathbf{x}(t))\, \eta_i(t)$$

(sum over $i = 1, \ldots, \overline{d}$) and means

$$x^\mu_{t+\Delta t} = x^\mu_t + f^\mu(\overline{\mathbf{x}}_t)\, \Delta t + g^{\mu i}(\overline{\mathbf{x}}_t)\, \eta_i(t)\, \Delta t$$

After a non-linear change of variables $\mathbf{u}(t) = \mathbf{U}(\mathbf{x}(t))$, in the $\Delta t \to 0$ limit, the Langevin equation keeps the same form,

$$u^\mu_{t+\Delta t} = u^\mu_t + F^\mu(\overline{\mathbf{u}}_t)\, \Delta t + G^{\mu i}(\overline{\mathbf{u}}_t)\, \eta_i(t)\, \Delta t$$

with

$$F^\mu(\overline{\mathbf{u}}_t) = \frac{\partial U^\mu}{\partial x^\nu} f^\nu[\mathbf{U}^{-1}(\overline{\mathbf{u}}_t)]$$

if Stratonovich, otherwise extra term, etc.

Under changes of coordinates (i.e. reparametrization of variables), $\mathbf{f}$ and $\mathbf{g}^i$ transform as contra-variant vectors in d-dimensional Riemann geometry.

Stochastic calculus

In higher dimension $\mu = 1, \ldots, d > 1$

A bit more on differential geometry

$$g^{\mu i}(\mathbf{x})g^{\nu j}(\mathbf{x})\delta_{ij} = \omega^{\mu\nu}(\mathbf{x}) \qquad (d = 1 \;\Rightarrow\; \omega^{\mu\nu} \mapsto g^2)$$

transforms as a contra-variant rank two tensor field, is symmetric with respect to $\mu \leftrightarrow \nu$ and positive definite for all $\mathbf{x}$. It defines a proper Riemann metric with inverse $\omega^{\mu\nu}\omega_{\nu\rho} = \delta^{\mu}_{\rho}$ $\qquad (d = 1 \;\Rightarrow\; \omega_{\mu\nu} \mapsto g^{-2})$

Using the notation $\partial_\mu \equiv \dfrac{\partial}{\partial x^\mu}$ and $\partial^\mu \equiv \omega^{\mu\nu}(\mathbf{x})\dfrac{\partial}{\partial x^\nu}$ the Christoffel symbol is

$$\Gamma^{\alpha}_{\mu\nu}(\mathbf{x}) = \tfrac{1}{2}\omega^{\alpha\rho}(\mathbf{x})\left(\partial_\mu\omega_{\rho\nu}(\mathbf{x}) + \partial_\nu\omega_{\rho\mu}(\mathbf{x}) - \partial_\rho\omega_{\mu\nu}(\mathbf{x})\right)$$

$(d = 1 \;\Rightarrow\; \Gamma \mapsto -g'/g)$ and the scalar curvature $\qquad (d = 1 \;\Rightarrow\; R \mapsto 0)$

$$R = \omega^{\mu\nu}\left(\partial_\alpha\Gamma^{\alpha}_{\mu\nu} - \partial_\mu\Gamma^{\alpha}_{\alpha\nu} + \Gamma^{\alpha}_{\alpha\beta}\Gamma^{\beta}_{\mu\nu} - \Gamma^{\alpha}_{\mu\beta}\Gamma^{\beta}_{\alpha\nu}\right)$$

The covariant derivative is $\nabla_\mu f^\nu = \frac{\mathrm{d}f^\nu}{\mathrm{d}x^\mu} + \Gamma^{\nu}_{\mu\rho}f^\rho$ $\qquad (d = 1 \;\Rightarrow\; f' - g'f/g)$

Stochastic calculus

In higher dimension $\mu = 1, \ldots, d > 1$

The trick is to find $B^{\mu}_{\alpha\beta}(\overline{\mathbf{x}})$, with $d^2(d+1)/2$ (1 in $d=1$) degrees of freedom, such that with the improved discretization

$$\overline{x}^{\mu} = x^{\mu} + \tfrac{1}{2}\Delta x^{\mu} + B^{\mu}_{\alpha\beta}(\overline{\mathbf{x}})\Delta x^{\alpha}\Delta x^{\beta}$$

the non-covariant terms in the action cancel (for $d=1$, $B^{\mu}_{\alpha\beta} \mapsto \beta_g$)

One finds an implicit scalar equation for the unknown $B^{\mu}_{\alpha\beta}$, involving the metric $\omega_{\mu\nu}$, the Christoffel's $\Gamma^{\mu}_{\alpha\beta}$, and the scalar curvature R. It has solution(s).

The infinitesimal action reads

$$\Delta S^{(B)}_{\mathbf{x}}(x_{t+\Delta t}, x_t) = \frac{1}{2}\omega_{\mu\nu}(\overline{\mathbf{x}})\left(\frac{\Delta x^{\mu}}{\Delta t} - h^{\mu}(\overline{\mathbf{x}})\right)\left(\frac{\Delta x^{\nu}}{\Delta t} - h^{\nu}(\overline{\mathbf{x}})\right)\Delta t + \frac{1}{2}\nabla_{\mu}h^{\mu}(\overline{\mathbf{x}})\Delta t + \boldsymbol{\lambda} R(\overline{\mathbf{x}})\Delta t$$

with $h^{\mu} = f^{\mu} - \tfrac{1}{2}g^{\mu i}\partial_{\nu}g^{\nu j}\delta_{ij} - \tfrac{1}{2}\omega^{\mu\nu}\Gamma^{\rho}_{\rho\nu}$

one recovers $B \mapsto \beta_g$, $h^{\mu} \mapsto f$, $\nabla_{\mu}h^{\mu} \mapsto f' - fg'/g$ and $S^{(\beta_g)}_X$ in $d=1$

Summary

Building path integral calculus

We are happy with our construction !

Discretization issues in stochastic classical ⇔ operator ordering in quantum

Revisit the (super) symmetry properties, cfr. **Barci & González Arenas 11, Marguet, Agoritsas, Canet & Lecomte 21**

Apply this to a physical problem, candidates are

interfaces with internal degrees of freedom

effect on pre-factor of Arrhenius law

Moreno, Barci, González Arenas 19

etc.

The initial measure

Non-linear transformation

Let us call x_0 the initial value of the time-dependent variable $x(t)$.

Its normalised probability density is $P_X(x_0)$, such that

$$\int_{x_0^{\min}}^{x_0^{\max}} \mathrm{d}x_0 \, P_X(x_0) = 1$$

We now perform a non-linear change of variables $u_0 = U(x_0)$, that implies $\mathrm{d}u_0 = U'(x_0)\mathrm{d}x_0$, and the measure transforms as

$$1 = \int_{u_0^{\min}}^{u_0^{\max}} \mathrm{d}u_0 \, P_U(u_0)$$

with

$$P_U(u_0) = \frac{P_X(U^{-1}(u_0))}{U'(u_0)}$$

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

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**

$$\overbrace{m\ddot{x}(t)}^{\text{Inertia}} + \mathcal{V}'(x(t)) \overbrace{\int_{t_0}^{\infty} dt' \, \gamma(t-t') \dot{x}(t')}^{\text{friction}} \mathcal{V}'(x(t')) =$$

$$\underbrace{F(x(t))}_{\text{deterministic force}} + \mathcal{V}'(x(t)) \underbrace{\eta(t)}_{\text{noise}}$$

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

The **noise** has zero mean and correlation $\langle \, \eta(t)\eta(t') \, \rangle = k_B T \, \Gamma(t-t')$ 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**

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

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

White noise

Assumption on the bath's time-scale

In classical systems one usually takes a bath kernel with the shortest relaxation time

$$t_{env} \ll t_{all}$$

with all representing all other time scales.

The bath is approximated by the white form $\Gamma(t-t') = 2\gamma_0 \delta(t-t')$

The Langevin equation becomes

$$m\ddot{x}(t) \; + \; \gamma_0 \, (\mathcal{V}'(x(t)))^2 \, \dot{x}(t) \; = \; F(x(t)) \; + \; \mathcal{V}'(x(t)) \, \eta(t)$$

with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = 2\gamma_0 k_B T \, \delta(t-t')$.

Separation of time-scales

Velocity and position

For $\boxed{t \gg \tau_v}$ one expects the velocity to equilibrate to the

Maxwell distribution $\quad P(v) \propto e^{-\beta m v^2/2}$

In this limit, one can drop $m\dot{v} = m\ddot{x}$ and work with the

over-damped equation

$$\boxed{\gamma_0 \, (\mathcal{V}'(x(t)))^2 \, \dot{x}(t) \; = \; F(x(t)) \; + \; \mathcal{V}'(x(t)) \, \eta(t)}$$

Stochastic calculus

Fokker-Planck equation

The probability of y at time $t + \Delta t$

$$P(y, t + \Delta t) = \int dx_t \, T(y, t + \Delta t | x_t, t) \, P(x_t, t)$$

with the transition probability

$$\begin{aligned} T(y, t + \Delta t | x_t, t) &\equiv \langle \delta(y - x_t - \Delta x) \rangle_{\eta_t} \\ &= \delta(y - x_t) - \partial_y [\delta(y - x_t) \langle \Delta x \rangle_{\eta_t}] \\ &\qquad + \frac{1}{2} \partial_y^2 [\delta(y - x_t) \langle (\Delta x)^2 \rangle_{\eta_t}] + \mathcal{O}(\Delta x^3) \end{aligned}$$

From the Langevin equation,

$$\begin{aligned} \langle \Delta x \rangle_{\eta_t} &= f(x_t) \, \Delta t + 2D\alpha \, g(x_t) g'(x_t) \, \Delta t \\ \langle (\Delta x)^2 \rangle_{\eta_t} &= 2D \, g^2(x_t) \, \Delta t \end{aligned}$$

Stochastic calculus

Fokker-Planck equations for different α

Call $y \mapsto x$, perform the integral over x_t and rearrange terms.

The Fokker-Planck equation

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

depends on α and g

Two processes will be statistically the same if

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

Correspondence between (f, α) and $(f_{\mathrm{drifted}}, \overline{\alpha})$

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

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

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

Remark : the potential $V_{\rm eff}(x)$ depends upon α and $g(x)$

Noise induced phase transitions

Stratonovich 67, Sagués, Sancho & García-Ojalvo 07

Stochastic calculus

Drift

The **Gibbs-Boltzmann equilibrium**

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

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

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

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 $f(x) \mapsto -g^2(x)\mathrm{d}_x V(x) + 2D(1-\alpha)g(x)\mathrm{d}_x g(x)$

becomes

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

with the expected Gibbs-Boltzmann measure stationary measure

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

independently of $g(x)$ and α

Symmetry

Transformations in the MSR path-integral representation

Let us group the two terms in the action that are due to the coupling to the bath

$$S^{(\beta g)}_{\rm diss}[\{x,\hat{x}\}] = \int_{-t_f}^{t_f} {\rm d}t \; \hat{x}(t) \; [\dot{x}(t) - D(g(x(t)))^2 \hat{x}(t)]$$

This expression suggests to use the transformation

$$\mathrm{T} = \begin{cases} x(t) & \mapsto \quad x(-t) \; , \\ \hat{x}(t) & \mapsto \quad \hat{x}(-t) + \dfrac{D^{-1}}{[g(x(-t))]^2} \; \dfrac{{\rm d}x(-t)}{{\rm d}t} \; , \end{cases}$$

Proof

$$S^{(\beta g)}_{\rm diss}[\{\mathrm{T}x,\mathrm{T}\hat{x}\}] = \int_{-t_f}^{t_f} {\rm d}t \; \left[\hat{x}(-t) + \frac{D^{-1}}{[g(x(-t))]^2} \; \frac{{\rm d}x(-t)}{{\rm d}t}\right]$$

$$\times \left\{ \frac{{\rm d}x(-t)}{{\rm d}t} - D[g(x(-t))]^2 \left[\hat{x}(-t) + \frac{D^{-1}}{[g(x(-t))]^2} \; \frac{{\rm d}x(-t)}{{\rm d}t}\right]\right\}$$

$$= \int_{-t_f}^{t_f} {\rm d}t \; \left[-D[g(x(-t))]^2 \hat{x}(-t) - \frac{{\rm d}x(-t)}{{\rm d}t}\right] \hat{x}(-t) \;\; = \;\; S^{(\beta g)}_{\rm diss}[\{x,\hat{x}\}]$$

Symmetry

Transformations in the MSR path-integral representation

What about the other terms ?

$$S^{(\beta_g)}_{\rm det,jac}[\{x,\hat{x}\}] = \int_{-t_f}^{t_f} {\rm d}t \left[-\hat{x}(t) f(x(t)) + \frac{1}{2} f'(x(t)) - \frac{1}{2} \frac{g'(x(t)) f(x(t))}{g(x(t))} \right]$$

Under the transformations

$$x(t) \mapsto x(-t) \qquad \text{and} \qquad \hat{x}(t) \mapsto \hat{x}(-t) + \frac{D^{-1}}{[g(x(-t))]^2} \frac{{\rm d}x(-t)}{{\rm d}t}$$

the last two terms are invariant. The first one transforms as

$$- \int_{-t_f}^{t_f} {\rm d}t \left[\hat{x}(-t) + \frac{D^{-1}}{[g(x(-t))]^2} \frac{{\rm d}x(-t)}{{\rm d}t} \right] f(x(-t))$$

$$= - \int_{-t_f}^{t_f} {\rm d}t \; \hat{x}(t) f(x(t)) + \int_{-t_f}^{t_f} {\rm d}t \; \frac{D^{-1}}{[g(x(t))]^2} \; \dot{x}(t) \; f(x(t))$$

For the drifted force $f = -g^2 V' + D g g'$ the last term yields $D^{-1}[-V(x(t_f)) + V(x(-t_f))] + \frac{1}{2D} \ln[g(x(t_f))/g(x(-t_f))]$: **the first one allows to rebuild the initial pdf and the last one cancels with the transformation of the prefactor !**