§3 Langevin equation and Fokker-Planck equation

Langevin equation

$$\dot{x} = \underbrace{f(x)}_{\text{det. drift}} + \underbrace{\sqrt{2D}\,\xi(t)}_{\text{random noise}}$$

$\xi(t) \equiv$ gaussian white noise with $\langle \xi(t) \rangle = 0$, $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$

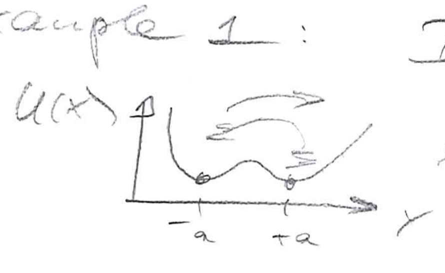
$\Rightarrow$ diffusion in effective potential $U(x) = -\int_0^x dx'\, f(x')$.

∘ Generalization

$$\dot{x}_i = f_i(\underline{x}, t) + g_{ij}(\underline{x})\,\xi_j(t), \quad i = 1, \dots, n$$

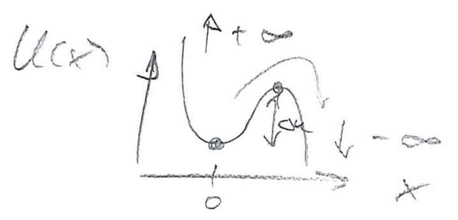
$\xi_j(t)$, $j = 1, \dots, k$ $\equiv$ indep. gaussian white noise with $\langle \xi_j(t)\xi_e(t') \rangle = \delta_{je}\,\delta(t-t')$

Example 1: Double-well potential



$x(t=0) = +a$.

Example 2: Escape over a barrier.



$x(t=0) = 0$.

∘ escape rate?

Numerics

Example: $\dot{x} = \xi(t)$.

$x_n = x(t_n)$, $t_n = n\,dt$.

Euler scheme:

$$x_{n+1} = x_n + \sqrt{2D\,dt}\, W_n.$$

with W_n normal distributed random variable with mean zero and variance 1.

N.B. $x_{n+1} - x_n = \sqrt{2D}\, dW$.

$$\langle dW^2 \rangle = 2D\,dt.$$

General case:

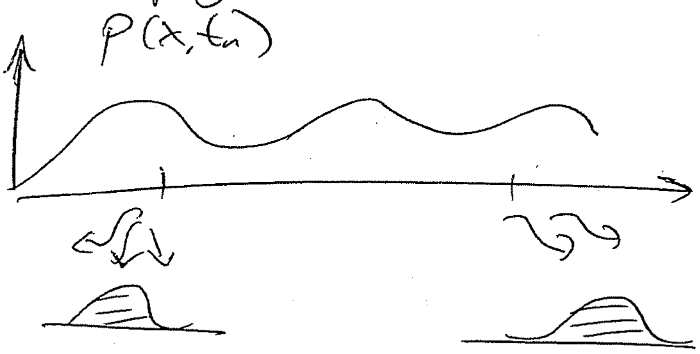
$$\dot{x} = f(x) + \xi(t).$$

$$x_{n+1} = x_n + f(x_n)\,dt + \sqrt{2D\,dt}\, W_n.$$

Caution: Take care if $D = D(x)$.

Q: How to find L?

A: Propagate $P(x, t_n)$ to $P(x, t_{n+1})$.



$$N\left(\frac{x - x_n - f(x_n)\,dt}{\sqrt{2D\,dt}}\right)$$

$\equiv$ normal distribution

$$x_{n+1} = x_n + f(x_n)\,dt + \sqrt{2Dt}\,\mathcal{N}.$$

Markov property $\Rightarrow$

Chapman-Kolmogorov equation

$$P(x, t_{n+1}) = \int dx_n\, P(x_n, t_n) \cdot N\left(\frac{x - x_n - f(x_n)\,dt}{\sqrt{2D\,dt}}\right). \quad (1)$$

probability to have been at x_n at $t = t_n$

probability to have moved from x_n to x_{n+1}.

We restrict ourselves to case

$D(x) = D_0$.

(1) $P(x, t_{n+1} | x_0, t_0) = \int dx_n\, P(x, t_{n+1}; x_n, t_n | x_0, t_0)$

$= \int dx_n\, P(x, t_{n+1} | x_n, t_n, x_0, t_0) \cdot P(x_n, t_n | x_0, t_0)$

- We have

$$P(x, t_{n+1}) = \int dx_n \; I(x_n, y)\big|_{y = x - x_n}$$

$x_n = x - y$

with

$$I(x_n, y) = p(x_n) \cdot n(x_n, y)$$

$$p(x_n) = P(x_n, t_n)$$

$$n(x_n, y) = \mathcal{N}\left(\frac{y - f(x_n)\,dt}{\sqrt{2D\,dt}} \right)$$

- Integrand $I(x_n, y)$ will contribute only for small $y = O(dt)$. and thus $x_n \approx x$.
- Taylor expand $I(x_n, y)$ in $x_n - x$.

$$I(x_n, y) = I(x, y) + \frac{\partial}{\partial x_n} I(x_n)\Big|_{x_n = x} \cdot \underbrace{(x_n - x)}_{-y}$$

$$+ \frac{\partial^2}{\partial x_n^2} I(x_n)\Big|_{x_n = x} \frac{(x_n - x)^2}{2} + \ldots$$

- $$P(x, t_{n+1}) = \int dy \; I(x_n, y)\big|_{x_n = x - y}$$

$$= \int dy \cdot \Big(p(x)\, n(x, y) - \frac{\partial}{\partial x}[p(x)\, n(x, y)]\, y$$

$$+ \frac{\partial^2}{\partial x^2}[p(x) \cdot n(x, y)]\, \frac{y^2}{2} \Big)$$

$$= p(x) \cdot \int dy \; n(x, y) - \frac{\partial}{\partial x}\Big(p(x) \cdot \Big[\int dy \; n(x, y)\, y\Big]\Big)$$

$$+ \frac{\partial^2}{\partial x^2}\Big(p(x) \Big[\int dy \; n(x, y) \cdot \frac{y^2}{2}\Big]\Big).$$

- Kramers Moyal coefficients.

$$\int dy \; n(x, y) = 1.$$

$$\int dy \; n(x, y)\, y = f(x)\, dt.$$

$$\int dy \; n(x, y)\, \frac{y^2}{2} = D \cdot dt + \tfrac{1}{2}[f(x)\, dt]^2 = D\, dt + O(dt^2)$$

- $$P(x, t_{n+1}) = P(x, t_n) - \frac{\partial}{\partial x}\left[P(x,t_n) f(x)\right] dt - \frac{\partial^2}{\partial x^2}\left[P(x,t_n)\, D\right] dt$$

$$\frac{P(x,t_{n+1}) - P(x,t_n)}{dt} = -\frac{\partial}{\partial x}\left[P(x,t_n) f(x)\right] + D_0 \frac{\partial^2}{\partial x^2} P(x,t_n)$$

$$\boxed{\frac{\partial}{\partial t} P(x,t) = -\frac{\partial}{\partial x}\left[P f\right] + D \frac{\partial^2}{\partial x^2} P}$$

Fokker-Planck equation for $D = D_0$

N.B.

N.B. recycle math tricks from Schrödinger equation (ladder operators, continued fractions, ... → Risken).

Fokker-Planck equation =

Conservation equation

$$\dot{P} = -\nabla J.$$

Different b.c. — different phys. meaning.

- Reflecting b.c.

$$J(x=0) = J(x=L) = 0.$$

$$\Rightarrow \frac{d}{dt}\int_0^L dx\, P = 0.$$

$$\dot{P} = LP, \quad \lambda p = Lp \Rightarrow \lambda_1 \geq \lambda_2 \geq \ldots$$

$$\Rightarrow \lambda_1 = 0, \; p_1 = p^*,$$
$$\lambda_i < 0 \text{ for } i > 1.$$

- Absorbing b.c.

$$P(x=L) = 0.$$

$$\frac{d}{dt}\int_0^L dx\, P(x,t) = -J_L(t)$$

$\equiv$ flux to absorber.

$\lambda_1 < 0 \equiv$ slowest time-scale

$$t \gg \frac{1}{\lambda_1}: \quad P(x,t) = a(t)\, p_1(x).$$
$$a(t) \sim \exp(-\lambda_1 t).$$

Diffusion in double well potential

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W[x_] := a x^4 - b x^2;
Plot[W[x] /. {a → 1, b → 2}, {x, -2, 2}];
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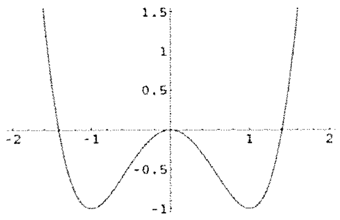


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P0[x_] := N0 Exp[-β W[x]];
Plot[P0[x] /. {a → 1, b → 2, β → 1}, {x, -2, 2}];
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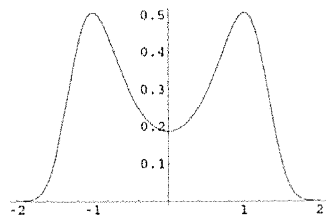
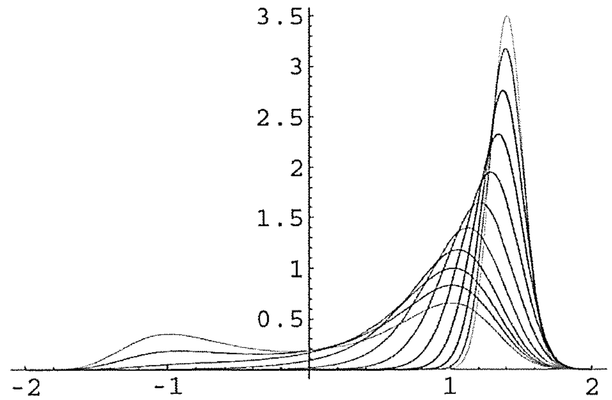
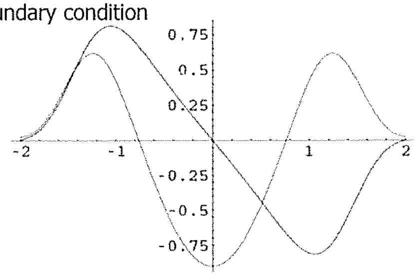


Relaxation of initial peak

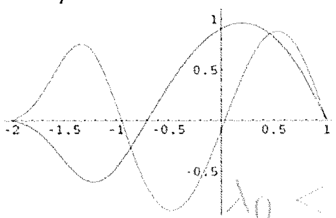


Eigenfunctions depend on boundary conditions

Reflecting boundary condition



Absorbing boundary condition



ϕ_0

ϕ_1

ϕ_2

$\lambda_0 < 0 \ldots$ escape rate