On the time scales in stochastic systems

Partial Noise–Averaging Method

in analysis of an escape over a fluctuating barrier



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Dynamics of physical systems

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phenomena separated in time – different time-scales

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the larger number of time-scales, the more complex behaviour

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equilibrium systems (complex) \longleftrightarrow many degrees of freedom

nonequilibrium systems (driven by external signals) \longleftrightarrow independent time-scales

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Partial noise-averaging method (PNAM) applies for the whole range of time variability of the stochastic perturbation

activation of an overdamped Brownian particle over a potential barrier



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Langevin equation



 $\frac{dx}{dt} = -U'(x) + \xi(t), \ \langle \xi(t) \rangle = 0, \ \langle \xi(t)\xi(t') \rangle = 2q\delta(t-t'), \ q = kT$

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Fokker-Planck equation

$$\frac{\partial}{\partial t}P(x,t) = \left[\frac{\partial}{\partial x}U'(x) + q\frac{\partial^2}{\partial x^2}\right]P(x,t) \equiv \mathbf{L}_0(x)P(x,t) \equiv -\frac{\partial}{\partial x}J(x,t)$$

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probability current
$$J(x,t) = -U'(x)P(x,t) - q\frac{\partial P(x,t)}{\partial x}$$

Kramers problem – escape time



probability of remaining in the well up to time t:

$$\mathbf{P}(t) = \int_{-\infty}^{x_{max}} dx \ P(x,t)$$

Kramers problem – escape time



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probability for escape times:

$$\mathbf{Q}(t) = -\frac{d\mathbf{P}(t)}{dt} = J(x_{max}, t)$$

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mean escape time:

$$\mathcal{T} = \int_0^\infty dt \ t \ \mathbf{Q}(t) = \int_0^\infty dt \ \int_{-\infty}^{x_{max}} dx \ P(x,t)$$

relaxation inside the well $t_r \sim \mathcal{O}(1) \{+\mathcal{O}(\ln q)\}$

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escape over the barrier



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weak noise approx. $q \ll \Delta U$ $t_r \ll T$

escape over the barrier $T \sim \exp\left(\frac{\Delta U}{q}\right)$



weak noise approx. $q \ll \Delta U$ $t_r \ll T$ thermalization inside the well

escape over the barrier $T \sim \exp\left(\frac{\Delta U}{q}\right)$



For weak noise approx. $t_r/T = \epsilon \ll 1$. Let $t_0 = t$, $t_1 = \epsilon t$, so $t = t(t_0, t_1)$ and

$$\frac{d}{dt} = \frac{\partial t_0}{\partial t} \frac{\partial}{\partial t_0} + \frac{\partial t_1}{\partial t} \frac{\partial}{\partial t_1} = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1}$$

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$$\frac{\partial P(x,t_0,t_1)}{\partial t_0} + \epsilon \frac{\partial P(x,t_0,t_1)}{\partial t_1} = L_0(x)P(x,t_0,t_1) = -\frac{\partial}{\partial x}J(x,t) \quad (*)$$

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stationary solution: $\lim_{t_0 \to \infty} P(x, t_0; t_1) = \rho(t_1) \cdot N^{-1} \exp\left[-U(x)/q\right] \equiv \rho(t_1) P_{st}(x)$ quasiequilibrium

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O u

$$\epsilon rac{d
ho(t_1)}{dt_1} = -J(x_{thr},t_1) pprox -k
ho(t_1)$$
 flux-over-population method

kinetic approx. – the escape process is described by a single kinetic coefficient k and $T = k^{-1} = \int_0^\infty dt \ \rho(t)$

$$\frac{\partial P(x, y, t)}{\partial t} = \left[L_0(x; y) + \epsilon L_1(y)\right] P(x, y, t)$$



parametric dependence

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parametric dependence slow variation along y

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parametric dependence slow variation along y

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$$\epsilon \frac{\partial \rho(y, t_1)}{\partial t_1} = -J(x_{thr}, y, t_1) + \epsilon L_1(y)\rho(y, t_1) \approx -k(y)\rho(y, t_1) + \epsilon L_1(y)\rho(y, t_1)$$

mean escape time:
$$T = \int_0^\infty dt \int dy \ \rho(y,t) \qquad k(y) = \{T(y)\}^{-1} \sim \epsilon$$

Escape over a fluctuating barrier


1. Large systems, many degrees of freedom





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 - chemical reaction with large molecules, e.g. CO binding to myoglobine
 - transport in membranes (stochastic changes of channel shape)
 - relaxation in compose materials, e.g. in glasses



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- chemical reaction with large molecules, e.g. CO binding to myoglobine
- transport in membranes (stochastic changes of channel shape)
- relaxation in compose materials, e.g. in glasses

2. Fluctuations of external parameters

- dye laser pumped by an another laser
 - Supeconducting QUantum Interference Device acting under the external magnetic field
- dynamics of populations of species in the presence of external random factors, e.g. climatic

Langevin equation

 $\dot{x} = -U'(x) - z(t) V'(x) + \sqrt{2q} \,\xi(t)$

Langevin equation

 $\dot{x} = -U'(x) - z(t) V'(x) + \sqrt{2q} \xi(t)$ COLOURED noise z(t):

- 1. dichotomic DN
- 2. Ornstein-Uhlenbeck OUN

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COLOURED noise z(t):
1. dichotomic – DN
2. Ornstein-Uhlenbeck – OUN

 $\langle z(t)z(t')\rangle = D\exp(-|t-t'|/\tau)$

au - correlation time D(au) - variance Q(au) = au D(au) - intensity

Langevin equation

 $\dot{x} = -U'(x) - z(t) \, V'(x) + \sqrt{2q} \, \xi(t)$

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$$\frac{\partial}{\partial t}P(x,z,t) = \left[\mathsf{L}_{0}(x) + z\mathsf{L}_{b}(x) + \frac{1}{\tau}\mathsf{L}_{z}(z)\right]P(x,z,t) \equiv \mathsf{L}(x,z)P(x,z,t)$$
$$(x) = \frac{\partial}{\partial x}V'(x)$$

Langevin equation

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values	$\{-\sqrt{D}, +\sqrt{D}\}$	$(-\infty,\infty)$
differential equation	$\frac{dz_{\pm}}{dt} = -\gamma z_{\pm} + \gamma z_{\mp}$ $\gamma = 1/(2\tau)$	$\frac{dz}{dt} = -\frac{1}{\tau}z + \frac{\sqrt{2D}}{\tau}\eta(t)$ $\langle \eta(t)\rangle = 0, \ \langle \eta(t)\eta(t')\rangle = \delta(t-t')$

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 $\{-\sqrt{D}, +\sqrt{D}\}$

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 $\frac{dz_{\pm}}{dt} = -\gamma z_{\pm} + \gamma z_{\mp}$ $\gamma = 1/(2\tau)$

evolution operator

$$\mathbf{L}_z = \frac{1}{2} \begin{pmatrix} -1 & 1\\ 1 & -1 \end{pmatrix}$$

OUN

 $(-\infty,\infty)$

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$$\mathsf{L}_z = \frac{\partial}{\partial z} z + D \frac{\partial^2}{\partial z^2}$$

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$$\mathsf{L}_z = \frac{\partial}{\partial z} z + D \frac{\partial^2}{\partial z^2}$$

operator stationary

distribution

evolution

$$W_0(z) = \begin{cases} \frac{1}{2} & \text{for } z = +\sqrt{D} \\ \frac{1}{2} & \text{for } z = -\sqrt{D} \end{cases}$$

 $W_0(z) = \frac{1}{\sqrt{2\pi D}} \exp(-z^2/2D)$

alues	$\{-\sqrt{D},+\sqrt{D}\}$	$(-\infty,\infty)$
differential equation	$\frac{dz_{\pm}}{dt} = -\gamma z_{\pm} + \gamma z_{\mp}$ $\gamma = 1/(2\tau)$	$\frac{dz}{dt} = -\frac{1}{\tau}z + \frac{\sqrt{2D}}{\tau}\eta(t)$ $\langle \eta(t) \rangle = 0, \ \langle \eta(t)\eta(t') \rangle = \delta(t-t')$
evolution operator	$L_z = \frac{1}{2} \left(\begin{array}{cc} -1 & 1\\ 1 & -1 \end{array} \right)$	$L_z = \frac{\partial}{\partial z} z + D \frac{\partial^2}{\partial z^2}$
stationary distribution	$W_0(z) = \begin{cases} \frac{1}{2} & \text{for } z = +\sqrt{D} \\ \frac{1}{2} & \text{for } z = -\sqrt{D} \end{cases}$	$W_0(z) = \frac{1}{\sqrt{2\pi D}} \exp(-z^2/2D)$
imit	behaviour survival	

 $\tau \to 0 \qquad \quad C(t) \to Q\,\delta(t) \qquad \qquad Q(\tau) \to {\rm const} \neq 0$

 $\tau \to \infty$ $C(t) \to D$ $D(\tau) \to \text{const} \neq 0$

Single escape event





 $\frac{dx}{dt} = -U'(x) + \xi(t)$

$$U(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$$

 $\overline{\mathcal{T}} = \overline{t_w} + \overline{t_t}$

Single escape event







$$U(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$$

 $\mathcal{T} = t_w + t_t$

If the potential variations influence the escape process

this happens mostly during the time interval t_t .

Idea of Partial Noise–Averaging Method



 $z(t) = z_s(t) + z_f(t) \qquad \begin{cases} z_s(t) & \text{slow component} - \text{constant within } t_t \\ z_f(t) & \text{fast component} - \text{white noise within } t_t \end{cases}$

$$z_s(t_0) \equiv \left\langle \frac{1}{t_t} \int_{t_0}^{t_0+t_t} ds \, z(s) \right\rangle \qquad \langle \dots \rangle \text{- noise realisations}$$

$$z_s(t_0) = rac{1}{\Delta} \left(1 - e^{-\Delta}
ight) \, z_0 \,$$
 where $\Delta = t_t/ au$

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 where $\Delta = t_t / \tau$
random gaussian number

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$$D_s \equiv \langle z_s^2 \rangle = \frac{D}{\Delta^2} \left(1 - e^{-\Delta} \right)^2 \xrightarrow[\tau \to \infty]{} D_s$$

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$$\left\langle \left(\frac{1}{t_t} \int_{t_t}^{t+t_t} ds \ z(s)\right)^2 \right\rangle = \langle z_s^2 \rangle + \langle z_f^2 \rangle = D_s + 2\frac{D_f}{\Delta}$$

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limit

fast component slow component

 $\tau \to 0 \qquad Q_f = Q \qquad Q_s = \mathcal{O}(\tau^2)$

 $\tau \to \infty$ $D_f = \mathcal{O}(1/\tau^2)$ $D_s = D$

$$z_s(t_0) = rac{1}{\Delta} \left(1 - e^{-\Delta}\right) z_0$$
 where $\Delta = t_t/ au$ random gaussian number

$$D_s \equiv \langle z_s^2 \rangle = \frac{D}{\Delta^2} \left(1 - e^{-\Delta} \right)^2 \xrightarrow[\tau \to \infty]{} D_s$$

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limit

fast component

slow component

 $\tau \to 0 \qquad Q_f = Q$ $Q_s = \mathcal{O}(\tau^2)$

 $\tau \to \infty$ $D_f = \mathcal{O}(1/\tau^2)$ $D_s = D$

 $z(t) = z_s(t) + z_f(t)$ independent gaussian noises with correlation time τ

 $egin{array}{ccc} z_f & ext{exists for } au \lesssim t_t \ z_s & ext{exists for } au \gtrsim t_t \end{array}$

$z(t) = z_s(t) + z_f(t)$

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$z_s(t)$ and $z_f(t)$ are not independent dichotomic noises

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$z_s(t)$ and $z_f(t)$ are not independent dichotomic noises BUT...

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similarities between OUN and DN

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$z(t) = z_s(t) + z_f(t)$

z_s(t) and z_f(t) are not independent dichotomic noises
 BUT...
 similarities between OUN and DN
 SO...

assume this is true



 $\overline{D}_s, D_f, Q_s, \overline{Q_f}$ the same as for OUN



 $\overline{D}_s, D_f, Q_s, \overline{Q_f}$ the same as for OUN

What is t_t ?



3D Fokker–Planck equation

$$\frac{\partial}{\partial t}P(x, y_f, y_s, t) = L(x, y_f, y_s)P(x, y_f, y_s, t) \quad \text{normalized noise: } z(t) = \sqrt{D(\tau)}y(t)$$

Quasiequilibrium

Ways of solution:

Quasiequilibrium

Ways of solution:

DN: (almost) exact solution – weak noise approximation

Quasiequilibrium

Ways of solution:

DN: (almost) exact solution – weak noise approximation

OUN: path integral method with Padé approximant
Quasiequilibrium

Ways of solution:

DN: (almost) exact solution – weak noise approximation
 OUN: path integral method with Padé approximant
 Result:

$$\dot{x}(t) = -\mathcal{U}'_{eff}(x(t)) + \sqrt{2G(x(t))}\vartheta(t)$$

Quasiequilibrium

Ways of solution:

DN: (almost) exact solution – weak noise approximation
 OUN: path integral method with Padé approximant
 Result:

$$\dot{x}(t) = -\mathcal{U}'_{eff}(x(t)) + \sqrt{2G(x(t))}\vartheta(t)$$

mean first passage time:

$$-1 = \mathcal{L}^+(x; y_s) \mathcal{T}(x; y_s)$$
$$\mathcal{T}(x; y_s) = \int_x^{x_{thr}} du \, \frac{1}{\sqrt{G(u; y_s)}} \frac{1}{\Psi(u; y_s)} \int_{-\infty}^u dv \, \frac{1}{\sqrt{G(v; y_s)}} \Psi(v; y_s)$$
$$\Psi(x; y_s) = \exp\left(-\int_x^x du \, \frac{\mathcal{U}'_{eff}(u; y_s)}{G(u; y_s)}\right)$$

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kinetic rate

 $\overline{k(y_s)} \sim \{\mathcal{T}(x_{in}; y_s)\}^{-1}$

Kinetic approach

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DN: exact (trivial) solution

$$\frac{\partial}{\partial t} \begin{pmatrix} \varrho_+ \\ \varrho_- \end{pmatrix} = \begin{pmatrix} -\gamma - k_+ & \gamma \\ \gamma & -\gamma - k_- \end{pmatrix} \begin{pmatrix} \varrho_+ \\ \varrho_- \end{pmatrix}, \quad \gamma = \frac{1}{2\tau}$$
$$\mathcal{T}(\tau) = \frac{2\mathcal{T}_+\mathcal{T}_- + \tau(\mathcal{T}_+ + \mathcal{T}_-)}{\mathcal{T}_+ + \mathcal{T}_- + 2\tau}$$

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OUN:

PROBLEMS!!!

$$\frac{\partial}{\partial t}\varrho(y_s,t) = \left[\frac{1}{\tau}L_{y_s}(y_s) - k(y_s)\right]\varrho(y_s,t)$$

Solutions known only for limiting cases $\tau \to 0$ and $\tau \to \infty$.

WANTEDsolution of the simplest case $\frac{\partial}{\partial t} \varrho(y,t) = \left[\frac{1}{\tau} \left(\frac{\partial}{\partial y}y + \frac{\partial^2}{\partial y^2}\right) - k_0 e^{-\Delta V y}\right] \varrho(y,t)$

diffusion in the parabolic potential with exponentially distributed sink

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diffusion in the parabolic potential with exponentially distributed sink

REWARD 100's citations

PNAM at work I

Doering–Gadoua problem — exact results for triangle barrier driven by DN



 $Q(\tau) = Q_0 \tau^{\alpha}, \ 0 \le \alpha \le 1$ $\alpha = 0, 0.25, 0.5, 0.75, 1.0$

PNAM at work II













PNAM at work III





PNAM at work IV











PNAM for different problems with coloured noise

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THE END