Séminaire Problèmes spectraux en physique mathématique IHP, 11/4/22

An Eyring-Kramers law for slowly oscillating bistable diffusions

[Ref: NB, Probability & Mathematical Physics, 2-4: 685-743 (2021)]

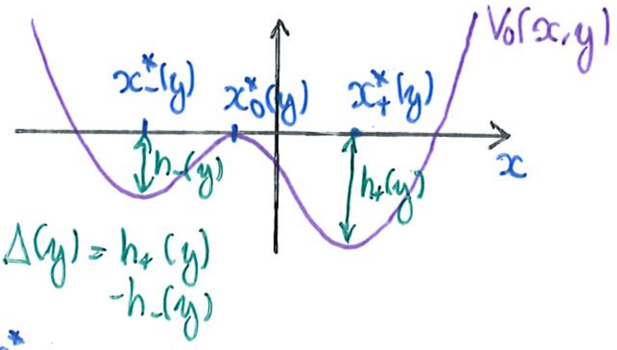
SDE

$$\begin{cases} dx_t = -\partial_x V_0(x_t, y_t)\,dt + \sigma\, dW_t^x \\ dy_t = \varepsilon\, dt + \sigma\sqrt{\varepsilon}\,\rho\, dW_t^y \end{cases}$$

PDE

$$\mathcal{L} = \frac{\sigma^2}{2}\left(\partial_{xx} + \rho^2\varepsilon\,\partial_{yy}\right) - \partial_x V_0\,\partial_x + \varepsilon\,\partial_y$$

$V_0(x,y)$:
- $*$ class $\mathcal{C}^5$
- $*$ $V_0(x, y+1) = V_0(x,y)$
- $*$ growth at infinity
- $*$ double-well in x



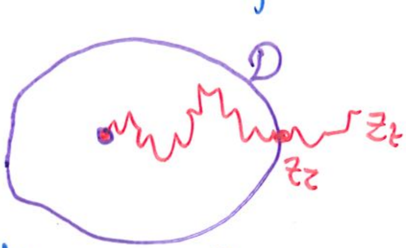
Questions:
- invariant measure
- law of transition time $x_-^* \to x_+^*$
- spectral gap

Links between SDEs and PDEs

$$dz_t = f(z_t)\,dt + g(z_t)\,dW_t \qquad \mathcal{L} = \sum_{i=1}^n f_i(z)\frac{\partial}{\partial z_i} + \frac{1}{2}\sum_{i,j=1}^n (gg^T)_{ij}(z)\frac{\partial^2}{\partial z_i \partial z_j}$$

Dynkin-Feynman-Kac formula:

$\mathcal{D} \subset \mathbb{R}^n$, $\tau = \inf\{t > 0 : z_t \notin \mathcal{D}\}$



$q : \mathcal{D} \to \mathbb{R}$, $\theta : \mathcal{D} \to \mathbb{R}$, $\varphi : \partial\mathcal{D} \to \mathbb{R}$ (smooth)

$$u(z) = \mathbb{E}_z\left[e^{-\int_0^\tau q(z_s)ds}\varphi(z_\tau) - \int_0^\tau e^{-\int_0^s q(z_v)dv}\,\theta(z_s)\,ds\right]$$

$$\Leftrightarrow \begin{cases} \mathcal{L}u = qu + \theta & z \in \mathcal{D} \\ u = \varphi & z \in \partial\mathcal{D} \end{cases}$$

Particular cases:

1) $q = 0$, $\varphi = 0$, $\theta = -1$: $\quad u(z) = \mathbb{E}_z[\tau] \Leftrightarrow \begin{cases} \mathcal{L}u = -1 & \mathcal{D} \\ u = 0 & \partial\mathcal{D} \end{cases}$

2) $q = 0$, $\varphi = 1_A$, $A \subset \partial\mathcal{D}$, $\theta = 0$: $\quad u(z) = \mathbb{P}_z\{z_\tau \in A\} \Leftrightarrow \begin{cases} \mathcal{L}u = 0 \\ u = 1_A \end{cases}$

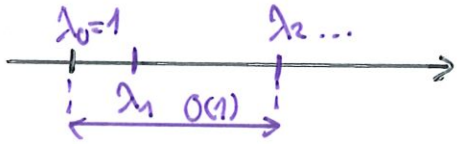
3) $q = \lambda$, $\varphi = 1$, $\theta = 0$: $\quad u(z) = \mathbb{E}_z[e^{-\lambda\tau}]$

1. Static case

$$dx_t = -\partial_x V_0(x)\,dt + \sigma\, dW_t$$

$$\mathcal{L}_x = \frac{\sigma^2}{2}\partial_{xx} - \partial_x V_0\, \partial_x = \frac{\sigma^2}{2} e^{2V_0/\sigma^2}\partial_x\left(e^{-2V_0/\sigma^2}\partial_x \cdot\right)$$

$$\pi_0(x) = \frac{1}{Z_0} e^{-2V_0(x)/\sigma^2} \Rightarrow \mathcal{L}_x^\dagger \pi_0 = 0$$



Spectrum of $-\mathcal{L}_x$: $0 = \lambda_0 < \lambda_1 < \lambda_2 \leq \dots$

$$\lambda_1 = [r_+ + r_-][1 + O(\sigma^2)] \qquad r_\pm = \frac{\omega_\pm \omega_0}{2\pi} e^{-2h_\pm/\sigma^2} \qquad \begin{cases} \omega_\pm = \sqrt{V_0''(x_\pm^*)} \\ \omega_0 = \sqrt{-V_0''(x_0^*)} \end{cases}$$

Eigenfunction: $\begin{cases} \phi_1(x) \cong e^{\Delta/\sigma^2} h_0(x) + e^{-\Delta/\sigma^2}(1 - h_0(x)) \\ h_0(x) = \mathbb{P}^x\{\tau_{x_-^*} < \tau_{x_+^*}\} = \frac{1}{N}\int_x^{x_+^*} e^{2V_0(\bar{x})/\sigma^2}\,d\bar{x} \end{cases}$

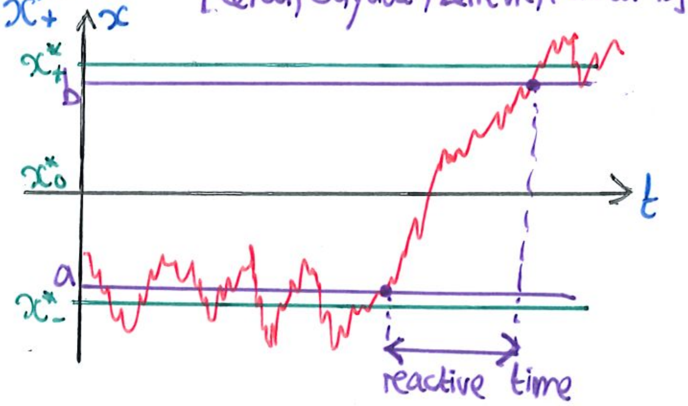
* First-hitting time of x_+^* (starting in $x < x_+^*$)

$$\mathbb{E}^x[\tau_+] = \frac{2}{\sigma^2}\int_x^{x_+^*}\int_{-\infty}^{x_2} e^{2[V_0(x_2) - V_0(x_1)]/\sigma^2}\,dx_1\,dx_2$$

$$\overset{x < x_0^*}{=} \frac{2\pi}{\omega_0\omega_-} e^{2h_-/\sigma^2}[1 + O(\sigma^2)] \cong \frac{1}{\lambda_1} \qquad \text{[Eyring-Kramers]}$$

* Law of τ_+: $\forall s \geq 0, \quad \lim_{\sigma\to 0} \mathbb{P}^{x_-^*}\{\tau_+ > s\,\mathbb{E}^{x_-^*}[\tau_+]\} = e^{-s}$ [Day '83]

* Reactive time: $x_-^* < a < x_0 < x_0^* < b < x_+^*$ [Cérou, Guyader, Lelièvre, Malrieu '13]



$$\text{Law}\left(\omega_0^2 \tau_b - 2\log(\sigma^{-1}) \,\middle|\, \tau_b < \tau_a\right) \xrightarrow[\sigma\to 0]{} \text{Law}\left(\mathcal{G} + T(x_0, b)\right)$$

deterministic

Gumbel: $\mathbb{P}\{\mathcal{G} < t\} = e^{-e^{-t}}$

$$\Rightarrow \text{Reactive time} \cong \frac{1}{\omega_0^2}\left[T(x_0,b) + 2\log(\sigma^{-1}) + \mathcal{G}\right]$$

2. Law of transition time, non-static case

$$\begin{cases} dx_t = -\frac{1}{\varepsilon} \partial_x V_0(x_t, y_t)\,dt + \frac{\sigma}{\sqrt{\varepsilon}}\, dW_t^x \\ dy_t = dt + \sigma\rho\, dW_t^y \end{cases}$$

τ_0: 1st-hitting time of periodic orbit (det.) tracking $x_0^*(y_t)$

Thm: [B & Gentz 2014]

$$\theta(y_{\tau_0}) \underset{\sigma\to 0}{\cong} \log(\sigma^{-1}) + \frac{\lambda_+}{\varepsilon} Y^\sigma + \frac{G}{2} + \frac{\log 2}{2}$$

1-periodic parametrization

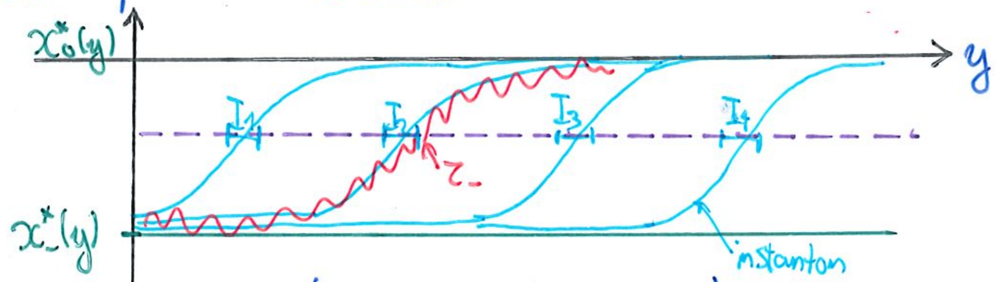
G: Gumbel

Y^σ: asympt. geometric

$$\lim_{n\to\infty} \mathbb{P}\{Y^\sigma = n+1 \mid Y^\sigma > n\} = p(\sigma) \simeq e^{-I/\sigma^2}$$

Rem: $\mathbb{E}[\tau_0] \cong p(\sigma)^{-1} \simeq \mathbb{E}[\tau_+]$

Main idea:



$$\mathbb{P}\{Y^\sigma = n\} \cong \mathbb{P}\{y_{\tau_-} \in I_n\}$$

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3. Eyring-Kramers law for $\mathbb{E}[\tau_+]$

Recall:
$$\begin{cases} \omega_\pm(y) = \sqrt{\partial_{xx} V_0(x_\pm^*(y), y)} \\ \omega_0(y) = \sqrt{-\partial_{xx} V_0(x_0^*(y), y)} \end{cases}$$

$$r_\pm(y) = \frac{\omega_\pm(y)\,\omega_0(y)}{2\pi} e^{-2h_\pm(y)/\sigma^2}$$

$$\lambda_1(y) = [r_+(y) + r_-(y)][1 + O(\sigma^2)]$$

Thm: [B 2021]

$$\mathbb{E}^{(x_-^*(y_0), y_0)}[\tau_+] = \frac{2\pi\varepsilon\,[1 + R(\varepsilon,\sigma)]}{\int_0^1 \omega_0(y)\,\omega_-(y)\, e^{-2h_-(y)/\sigma^2}\,dy}$$

with $R(\varepsilon,\sigma) \ll 1$ if $\langle\lambda_1\rangle := \int_0^1 \lambda_1(y)\,dy \ll \varepsilon \ll \langle\lambda_1\rangle^{1/4}$

Heuristics: two-state jump process

$$\begin{tikzcd} \ominus \arrow[r, bend left, "\Gamma_-(y)/\varepsilon"] & \oplus \arrow[l, bend left, "\Gamma_+(y)/\varepsilon"] \end{tikzcd}$$

$$\frac{d}{dy} \mathbb{P}^{-,y_0}\{\tau_+ > y\} = -\frac{1}{\varepsilon}\Gamma_-(y)\,\mathbb{P}^{-,y_0}\{\tau_+ > y\}$$

$$\Rightarrow \mathbb{P}^{-,y_0}\{\tau_+ > y\} = e^{-R_-(y,y_0)/\varepsilon} \qquad R_-(y_1,y_0) = \int_{y_0}^{y_1}\Gamma_-(y)\,dy$$

$$\Rightarrow \mathbb{E}^{-,y_0}[\tau_+] = \int_{y_0}^{\infty} e^{-R_-(y,y_0)/\varepsilon}\,dy \cong \frac{\varepsilon}{R_-(1,0)} \quad \text{for } \varepsilon \gg \max_{y\in[0,1]}\Gamma_-(y)$$

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4. Idea of proof ← [Landim, Mariani & Seo '19]

$$\mathcal{L} = \frac{1}{\varepsilon}\mathcal{L}_x + \mathcal{L}_y \qquad \mathcal{L}_y = \frac{\rho^2\sigma^2}{2}\partial_{yy} + \partial_y$$

Invariant measure: $d\pi = e^{-2V(x,y;\sigma)/\sigma^2}\,dx\,dy$ $\quad V$ solves Hamilton-Jacobi eq.

$$\Rightarrow \mathcal{L} = \mathcal{L}_s + \mathcal{L}_a \qquad \begin{cases} \mathcal{L}_s = \frac{\sigma^2}{2\varepsilon} e^{2V/\sigma^2}\nabla\cdot D e^{-2V/\sigma^2}\nabla = \mathcal{L}_s^\dagger \\ \mathcal{L}_a = C\cdot\nabla = -\mathcal{L}_a^\dagger \end{cases} \qquad D = \begin{pmatrix}1 & 0\\ 0 & \varepsilon\rho^2\end{pmatrix}$$

Adjoint system: $\mathcal{L}^* = \mathcal{L}_s - \mathcal{L}_a$

Thm: [LMS] $A\cap B = \emptyset$

$$\int_{\partial A} \mathbb{E}^{(x,y)}[\tau_B]\,d\nu_{AB} = \frac{1}{\operatorname{cap}(A,B)}\int_{B^c} h^*_{AB}(x,y)\,d\pi$$

prdoa measure on ∂A

Capacity, satisfies variational principles

$= \mathbb{P}^{*,(x,y)}\{\tau_A < \tau_B\}$

Apply to A, B nbh of $x^*_-(y)$, $x^*_+(y)$

Main difficulty: estimate $\pi(x,y)$

Prop: [B'21]

$$\pi(x,y) = \underbrace{\frac{e^{-2V_0(x,y)/\sigma^2}}{Z_0(y)}}_{\text{static inv. meas.}}\Big[1 + \alpha_1(y)\phi_1(x|y) + \underbrace{\Phi_1(x,y)}_{\perp\ \operatorname{span}\{\phi_0,\phi_1\}}\Big]$$

satisfies 2nd order ODE, close to 2-state process

Proof based on expansion $\pi = \pi_0\big[1 + \sum_{n\geq 1}\alpha_n\phi_n\big]$ $\qquad \alpha_n'' = \dots$