Metastability and transition times for a space-time white noise stochastic partial differential equation in dimension 1

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For $(x,t) \in [0,1] \times \mathbb{R}^+$, $u(x,t) \in \mathbb{R}$ satisfies

$$\begin{cases} \partial_t u(x,t) &= \gamma \partial_{xx}^2 u(x,t) - V'(u(x,t)) + \sqrt{2\varepsilon} W \\ u(x,0) &= u_0(x) \end{cases}$$

with

- u_0 continuous function on $[0,1]$
- $\varepsilon, \gamma > 0$
- W space-time white noise.

with boundary conditions (Dirichlet or Neumann). Existence and unicity of a mild solution (Walsh 1984, Gyöngy, Pardoux).
Example: Allen-Cahn $V(x) = \frac{x^4}{4} - \frac{x^2}{2}$ (Faris, Jona-Lasinio 1982)

$$\partial_t u(x,t) = \gamma \partial_{xx}^2 u(x,t) - u^3(x,t) + u(x,t) + \sqrt{2\varepsilon} W$$

$$\partial_t u(x,t) = \gamma \partial_{xx}^2 u(x,t) - V'(u(x,t)) + \sqrt{2\varepsilon} W$$

Interpretations:

- elastic string in a viscous random environment submitted to a potential (Funaki, 1983)
- quantum field theory (Faris, Jona-Lasinio 1982)
- statistical mechanics as a reaction diffusion equation modeling phase transitions and evolution of interfaces (Vanden-Eijnden, Westdickenberg).

Analogue in infinite dimension of a gradient system:

$$\partial_t u = -\frac{\delta S}{\delta u} + \sqrt{2\varepsilon} W$$

where S is a functional potential (free energy)

$$S(\phi) = \int_0^1 \frac{\gamma}{2} \left|\phi'\right|^2 (x) + V(\phi(x)) \mathrm{d}x.$$

Gradient flow in infinite dimension : for $\phi, k \in C^2_{bc}([0,1])$

$$S(\phi) = \int_0^1 \frac{\gamma}{2} \left|\phi'\right|^2 (x) + V(\phi(x))\mathrm{d}x$$

Taylor expansion at the 2nd order:

$$S(\phi + k) = S(\phi) + \int_0^1 \frac{\delta S}{\delta \phi}(x)k(x) + \frac{1}{2}\frac{\delta^2 S}{\delta \phi^2}(k)(x)k(x)\mathrm{d}x + o(\|k\|^2)$$

$$\frac{\delta S}{\delta \phi}(x) = -\gamma\phi''(x) + V'(\phi(x))$$

$$\frac{\delta^2 S}{\delta \phi^2}(k) = -\gamma k'' + V''(\phi)k =: \mathcal{H}_\phi S k$$

$\mathcal{H}_\phi S$: Strum-Liouville operator on $[0,1]$ with eigenvalues $(\lambda_k(\phi))_k$.

Analogous to finite dimensional gradient system

$$\mathrm{d}X_t = -\nabla F(X_t)\mathrm{d}t + \sqrt{2\varepsilon}\mathrm{d}B_t \in \mathbb{R}^N$$

Properties:

- Metastable states: minima of the free energy (F).
- Transitions occur between metastable states through the lowest saddle points.
- The law of the hitting time is asymptotically exponential.

Simplest case: m^-, m^+ minima of F s.t. $F(m^-) \geqslant F(m^+)$ separated by a unique saddle point $\widehat{s}$.
Let $\tau_\varepsilon(B_+)$ be the hitting time of a small ball $B_+ = B_\rho(m^+)$. The Eyring-Kramers Formula reads (Bovier, Eckhoff, Gayrard, Klein, 2004)

$$\mathbb{E}_{m_-}(\tau_\varepsilon(B_+)) = \frac{2\pi}{|\lambda^-(\widehat{s})|}\sqrt{\frac{|\det HF(\widehat{s})|}{\det HF(m^-)}}\, e^{\frac{F(\widehat{s})-F(m^-)}{\varepsilon}}(1+O(\sqrt{\varepsilon}\,|\ln \varepsilon|^{3/2})).$$

HF Hessian matrix of F, and $\lambda^-(\widehat{s})$ the unique negative eigenvalue of $HF(\widehat{s})$.
Very strong link with the first eigenvalues of the infinitesimal generator. Other method: semi-classical analysis (Helffer, Klein, Nier...).

We consider the simplest situation: S have three stationary points, solutions of

$$\begin{cases} \frac{\delta S}{\delta \phi} & = -\gamma \phi''(x) + V'(\phi(x)) = 0 \\ & + b.c. \end{cases}$$

1. ϕ^+, ϕ^- two minima
2. $\widehat{\sigma}$ a single saddle point between ϕ^+ and ϕ^-.

Example : $V(x) = \frac{x^4}{4} - \frac{x^2}{2}$, for $\gamma > \gamma_0 = \frac{1}{\pi^2}$ (Allen-Cahn + Neumann b.c.)

- two minima $\phi^+ = +\mathbb{1}$, $\phi^- = -\mathbb{1}$
- one saddle point $\widehat{s} = 0$.

Eyring-Kramers Formula

Assume $S(\phi^-) \geqslant S(\phi^+)$, we let $B^+ = B_\rho^{H^1}(\phi^+)$ for $\rho_0 > \rho > 0$

$$\mathbb{E}_{\phi^-}\left[\tau_\varepsilon\left(B^+\right)\right] = \frac{2\pi}{|\lambda^-(\widehat{\sigma})|}\sqrt{\left|\frac{\mathrm{Det}\mathcal{H}_{\widehat{\sigma}}S}{\mathrm{Det}\mathcal{H}_{\phi^-}S}\right|}e^{\widehat{S}(\phi^-,\phi^+)/\varepsilon}\left(1 + O(\sqrt{\varepsilon}\,|\ln\varepsilon|^{\frac{3}{2}})\right)$$

where $\widehat{S}(\phi^-, \phi^+) = S(\widehat{\sigma}) - S(\phi^-)$. We define

$$\frac{\mathrm{Det}\mathcal{H}_{\widehat{\sigma}}S}{\mathrm{Det}\mathcal{H}_{\phi^-}S} = \prod_{k\geqslant 0}\frac{\lambda_k(\widehat{\sigma})}{\lambda_k(\phi^-)}$$

which converge since $\lambda_k = c\gamma k^2 + O(1)$ for $k \geqslant 0$.

Example Allen-Cahn (Neumann b.c.) for $\gamma > \gamma_0 = \frac{1}{\pi^2}$: we have $\phi^+ = \mathbb{1}$, $\phi^- = -\mathbb{1}$ and $\widehat{s} = 0$. We get

$$S(\phi) = \int_0^1 \frac{\gamma}{2}\phi'^2(x) + \frac{1}{4}\phi(x)^4 - \frac{1}{2}\phi(x)^2 \mathrm{d}x$$
$$\mathcal{H}_\phi S h = -\gamma h'' + (3\phi^2 - 1)h.$$

We obtain

$$S(\phi^\pm) = -\frac{1}{4} \qquad S(\widehat{\sigma}) = 0$$
$$\mathcal{H}_{\phi^\pm} S h = -\gamma h'' + 2h \qquad \mathcal{H}_{\widehat{\sigma}} S h = -\gamma h'' - h$$
$$\lambda_k(\phi^\pm) = \gamma\pi^2 k^2 + 2 \qquad \lambda_k(\widehat{\sigma}) = \gamma\pi^2 k^2 - 1 \qquad k \geqslant 0$$

Functional determinants, Levit Smilansky 1977, Dreyfus Dym 1978

For $\hat{s}$, f^- solutions of

$$\mathcal{H}_{\hat{\sigma}} S\hat{s} = 0 \qquad \hat{s}(0) = 1 \qquad \hat{s}'(0) = 0$$
$$\mathcal{H}_{\phi^-} Sf^- = 0 \qquad f^-(0) = 1 \qquad {f^-}'(0) = 0$$

then

$$f^-(x) = \mathrm{ch}\left(\sqrt{\frac{2}{\gamma}}x\right), \qquad \widehat{s}(x) = \cos\left(\frac{x}{\sqrt{\gamma}}\right).$$

For Neumann boundary conditions,

$$\frac{\mathrm{Det}\mathcal{H}_{\hat{\sigma}} S}{\mathrm{Det}\mathcal{H}_{\phi^-} S} = \frac{\hat{s}'(1)}{{f^-}'(1)} = -\frac{1}{\sqrt{2}}\frac{\sin\left(\frac{1}{\sqrt{\gamma}}\right)}{\mathrm{sh}\left(\sqrt{\frac{2}{\gamma}}\right)}.$$

Analogue representation for Dirichlet boundary conditions.

Finite Difference Approximation

Main principle: use Eyring-Kramers Formula in dimension N then $N \to +\infty$.
We construct a diffusion in $\mathbb{R}^N$ such that $Y_t^i \approx u(\frac{i}{N}, tN)$.

$$S_N(y) = \frac{1}{N} \sum_{i=1}^{N} \frac{\gamma}{2} N^2 (y_{i+1} - y_i)^2 + V(y_i) \quad (y_i = \phi(i/N))$$

$$\begin{aligned} \mathrm{d}Y_t &= -\nabla S_N(Y_t)\mathrm{d}t + \sqrt{2\varepsilon}\mathrm{d}B_t \\ &= \frac{N\gamma}{2}\left[Y_t^{i+1} - 2Y_t^i + Y_t^{i-1}\right]\mathrm{d}t - \frac{1}{N}V'(Y_t^i)\mathrm{d}t + \sqrt{2\varepsilon}\mathrm{d}B_t^i. \end{aligned}$$

B_t defined from the white noise

$$B_t^i = \sqrt{N} W\left(\left[\frac{i}{N}, \frac{i+1}{N}\right[\times [0, t[\right).$$

We approximate u with u^N the linear interpolation s.t. $u^N(\frac{i}{N}, tN) = Y_t^i$.

Main steps

Aim: interchange of limits ($\varepsilon \to 0$ and $N \to \infty$)

1. for a fixed ε, convergence of u^N to u, thus convergence of the expected transition time

$$\lim_{N\to\infty} \mathbb{E}_{\phi_N^-}\left[\tau_\varepsilon^N\left(B^+\right)\right] = \mathbb{E}_{\phi^-}\left[\tau_\varepsilon\left(B^+\right)\right].$$

2. for fixed N, calculation of the transition time $a_N(\varepsilon)$

$$\left|\frac{1}{a_N(\varepsilon)}\mathbb{E}_{\phi_N^-}\left[\tau_\varepsilon^N\left(B^+\right)\right] - 1\right| = \psi(\varepsilon, N) < \Psi(\varepsilon) = O(\sqrt{\varepsilon}\,|\ln(\varepsilon)|^{3/2})$$

where $\Psi(\varepsilon)$ *does not depend on* N.

3. the limit $a(\varepsilon)$ of $a_N(\varepsilon)$ gives the precise asymptotics

$$a(\varepsilon) = \lim_{N\to\infty} a_N(\varepsilon).$$

Step 2

Aim: calculation of $a_N(\varepsilon)$ with error bounds uniformly in the dimension

1. using potential theory

$$\left|\frac{1}{a_N(\varepsilon)}\mathbb{E}_{\nu_N^-}\left[\tau_\varepsilon^N\left(B^+\right)\right]-1\right|=\psi_1(\varepsilon,N)<\Psi_1(\varepsilon)$$

where ν_N^- is the equilibrium probability on ∂B_N^-.

2. Then using the loss of memory of the initial condition uniformly in the dimension

$$\frac{1}{a_N(\varepsilon)}\left|\mathbb{E}_{\nu_N^-}\left[\tau_\varepsilon^N\left(B^+\right)\right]-\mathbb{E}_{\phi_N^-}\left[\tau_\varepsilon^N\left(B^+\right)\right]\right|<\Psi_2(\varepsilon).$$

Results from Martinelli, Scoppola, Olivieri on the loss of memory of the initial condition.

Step 2.1

From the potential theory, with $\mu_\varepsilon^N(\mathrm{d}z) = \exp(-S_N(z)/\varepsilon)\mathrm{d}z$ the reversible measure

$$\mathbb{E}_{\nu_-^N}(\tau_\varepsilon^N(B_N^+)) = \frac{\int_{(B_N^+)^c} h^*(z)\mu_\varepsilon^N(\mathrm{d}z)}{\mathrm{cap}(B_N^-, B_N^+)}.$$

The capacity satisfies

$$\mathrm{cap}(B_N^-, B_N^+) = \inf\left\{\mathcal{E}(h,h), h = \mathbb{1}_{B_-} \text{ on } B_- \cup B_+\right\} = \mathcal{E}(h^*, h^*).$$

$\mathcal{E}$ is the Dirichlet form

$$\mathcal{E}(h,h) = \varepsilon \int_{\mathbb{R}^N} \|\nabla h\|_2^2 \, \mathrm{d}\mu_\varepsilon^N$$

and $h^*(z) = \mathbb{P}_z[\tau_\varepsilon^N(B_N^-) < \tau_\varepsilon^N(B_N^+)]$.

Uniform upper bound for capacities

Aim: construction of a good test function h able to minimize $\mathcal{E}(h,h)$ well enough.
Heuristics: h must be close to h^*, therefore h must be nearly constant on the basins of attraction of B_N^- (≈ 1) and B_N^+ (≈ 0) and is steeper near the saddle $\widehat{\sigma}_N$.
Then a good choice of h leads to

$$\mathcal{E}(h,h) \leqslant \int_{C_\delta^N(\widehat{\sigma}_N)} \|\nabla h(z)\|_2^2 \, e^{-\frac{S_N(z)}{\varepsilon}} \mathrm{d}z + \int_{S_N(z) > S_N(\widehat{\sigma}_N)+\eta} \|\nabla h(z)\|_2^2 \, e^{-\frac{S_N(z)}{\varepsilon}} \mathrm{d}z.$$

The second integral gives a negligible contribution. The first, I_1, can be evaluated using Laplace's method: approximate S_N by a quadratic potential (i.e. the Hessian form).

The set $C_\delta^N(\widehat{\sigma}_N)$ is such that, for all N, $z \in C_\delta^N(\widehat{\sigma}_N)$

$$\left| S_N(z) - S_N(\widehat{\sigma}_N) - \frac{1}{2} HS^N(z - \widehat{\sigma}_N) \right| \leqslant C\delta^3.$$

One possible choice is to take (in the orthonormal basis of HS^N associated to eigenvalues $(\lambda_k^N)_{0 \leqslant k \leqslant N-1}$ in increasing order)

$$C_\delta^N(\widehat{\sigma}_N) = \widehat{\sigma}_N + \prod_{k=0}^{N-1} \left[-\frac{\delta r_k}{\sqrt{|\lambda_k^N|}}, \frac{\delta r_k}{\sqrt{|\lambda_k^N|}} \right]$$

where $\sum_{k \geqslant 1} \frac{r_k^{3/2}}{k^{3/2}} < \infty$. Then we choose $h(z) = h_0(\widehat{y}_0)$ where $\widehat{y}_0$ is the coordinate associated to λ_0^N (unique negative eigenvalue).

We obtain

$$I_1 = \int_{C_\delta^N(\widehat{\sigma}_N)} h_0'(\widehat{y}_0)^2 e^{-\frac{S_N(\widehat{y})}{\varepsilon}} \mathrm{d}\widehat{y}$$

$$\leqslant e^{-\frac{S^N(\widehat{\sigma}_N)}{\varepsilon}} \int_{-\delta\alpha_0}^{\delta\alpha_0} h_0'(\widehat{y}_0)^2 e^{|\lambda_0^N|\widehat{y}_0^2/2\varepsilon} \mathrm{d}\widehat{y}_0 \times \prod_{k=1}^{N-1} \int_{\mathbb{R}} e^{-|\lambda_{N,k}|{y_k}^2/2\varepsilon} \mathrm{d}y_k$$

$$\times \left(1 + 2C\frac{\delta^3}{\varepsilon}\right).$$

Then optimizing h_0 and setting $\delta = O(\sqrt{\varepsilon |\ln \varepsilon|})$

$$I_1 \leqslant \sqrt{2\pi\varepsilon}^{N-2} \frac{\left|\lambda_0^N\right| e^{-\frac{S_N(\widehat{\sigma}_N)}{\varepsilon}}}{\sqrt{|\det(HS^N(\widehat{\sigma}_N))|}} (1 + O(\sqrt{\varepsilon}\,|\ln(\varepsilon)|^{3/2})).$$