Interface dynamics of a metastable mass-conserving diffusion

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Definition of the model

Consider the potential

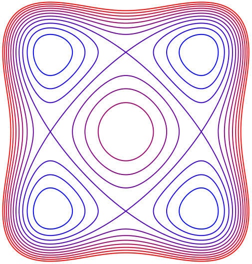
$$V_\gamma(x) = \sum_{i=1}^{N} \frac{1}{4}x_i^4 - \frac{1}{2}x_i^2 + \frac{\gamma}{4}\sum_{i=1}^{N}(x_{i+1} - x_i)^2,$$

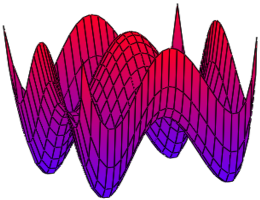
where $N \geq 2$, $\gamma \geq 0$ and $x_{N+1} = x_1$. It defines a diffusion process

$$\mathrm{d}x_t = -\nabla V_\gamma(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t \;,$$

where W_t is an N-dimensional Wiener process and $\varepsilon \geq 0$.

Definition of the model

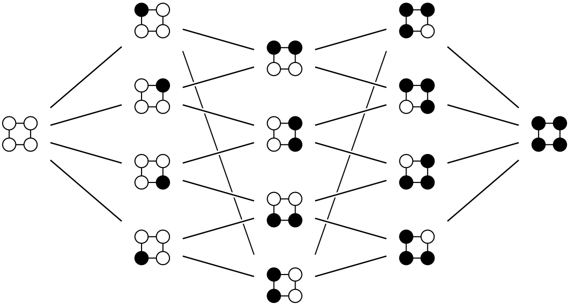




- Know set of stationary points $\mathcal{S}$ of V_γ, especially local minima and 1-saddles.
- Asymmetric case (no G st $\forall g \in G, V \circ g = V$) : Bovier, Gayrard, Klein(2005)
- Difficulty : for V_γ we can take $G = D_N \times \mathbb{Z}/_{2\mathbb{Z}} = \langle R, S, C \rangle$.

Without conservation law

N. Berglund, B. Fernandez, B. Gentz (2007)



- For $\gamma = 0$: $\mathcal{S} = \{-1, 0, 1\}^N$, $\mathcal{S}_0 = \{-1, 1\}^N$.
- There exists $\gamma^*(N) \geq \frac{1}{4}$ st transition graph $\mathcal{G}$ is the same $\forall \gamma \in [0, \gamma^*(N))$.

Uncoupled case with constraint

$$S = \{x \in \mathbb{R}^N \ : \ \sum_{i=1}^{N} x_i = 0\}.$$

$$\nabla V_0(x) = \lambda \mathbf{1} \ \Leftrightarrow \ \forall i \in [\![1, N]\!], \ x_i^3 - x_i = \lambda$$

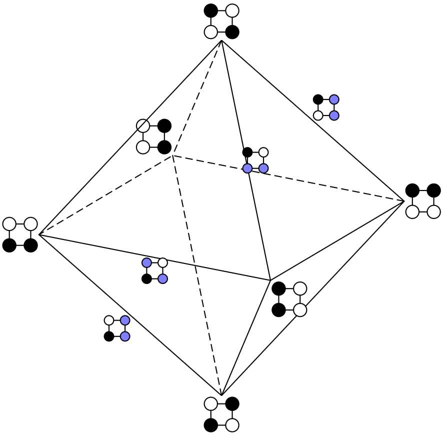
Assume $|\lambda| < \lambda_c = \frac{2}{3\sqrt{3}}$, denote $\alpha_0, \alpha_1, \alpha_2$ the distinct roots of $X^3 - X - \lambda$. Let a_j be the number of occurrences of α_j, and reorder the α_j st $a_0 \leqslant a_1 \leqslant a_2$. Denote such a stationary point by the triple (a_0, a_1, a_2).

Proposition (N. Berglund, S.D.)

Assume that N is not a multiple of 3, and let $x^\star$ be a critical point with triple (a_0, a_1, a_2). Then

- *if $2a_1 > a_0 + a_2$, then $x^\star$ is a stationary point of index a_0 ;*
- *if $2a_1 < a_0 + a_2$, then $x^\star$ is a stationary point of index $a_2 - 1$.*

Uncoupled case example : $N = 4$



$\bullet = 1$, $\circ = -1$ and $\color{blue}\bullet = 0$.

Uncoupled case

Consider the case where $N = 2M$ is even, $N \geq 8$ and N is not a multiple of 3. 1-saddles correspond to triples $(1, a, N - a - 1)$. Write $k_{\max} = \lfloor N/6 \rfloor$ and

- B_k set of all local minima with triple $(0, M - k, M + k)$, where $k \in [\![0, k_{\max}]\!]$;
- C_k the set of all 1-saddles with triple $(1, M - k, M + k - 1)$, where $k \in [\![1, k_{\max}]\!]$.

$\forall k$, $\exists \gamma * (k)$ indep. of N st. B_k, C_k persist.

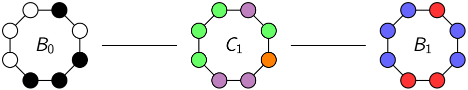
Uncoupled case

Theorem (N. Berglund, S.D.)

Each 1-saddle in C_k connects exactly one local minimum in B_{k-1} with one local minimum in B_k. More precisely, if the coordinates of the saddle have values $\alpha'_0, \alpha'_1, \alpha'_2$, and those of the local minima are respectively α_1, α_2 and α''_1, α''_2, then the connection rules are given by

$$\begin{aligned} \alpha_1 \longleftrightarrow \alpha'_0 \longleftrightarrow \alpha''_2 &\qquad 1 \text{ coordinate },\\ \alpha_1 \longleftrightarrow \alpha'_1 \longleftrightarrow \alpha''_1 &\qquad M-k \text{ coordinates },\\ \alpha_2 \longleftrightarrow \alpha'_2 \longleftrightarrow \alpha''_2 &\qquad M+k-1 \text{ coordinates }. \end{aligned}$$

Uncoupled case example : $N = 8$



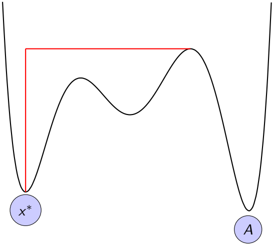
The coordinates for family B_0 corresponding to the triple $(0, 4, 4)$ are ● $= 1$ and ○ $= -1$. Those for C_1 corresponding to the triple $(1, 3, 4)$ are 🟠 $= -1/\sqrt{7}$, 🟣 $= 3/\sqrt{7}$ and 🟢 $= -2/\sqrt{7}$. Those for B_1 corresponding to the triple $(0, 3, 5)$ are 🔴 $= 5/\sqrt{19}$ and 🔵 $= -3/\sqrt{19}$.

Communication height

Let $x^\star$ be a local minimum of V and let $A \subset \mathbb{R}^N$. The *communication height* from $x^\star$ to A is the nonnegative number

$$H(x^\star, A) = \inf_{\gamma : x^\star \to A} \sup_{t \in [0,1]} V(\gamma(t)) - V(x^\star) ,$$

where the infimum runs over all continuous paths $\gamma : [0,1] \to \mathbb{R}^N$ such that $\gamma(0) = x^\star$ and $\gamma(1) \in A$. Any path γ realising that is called a *minimal path* from $x^\star$ to A.



Metastable hierarchy

Definition (Metastable hierarchy of a partition)

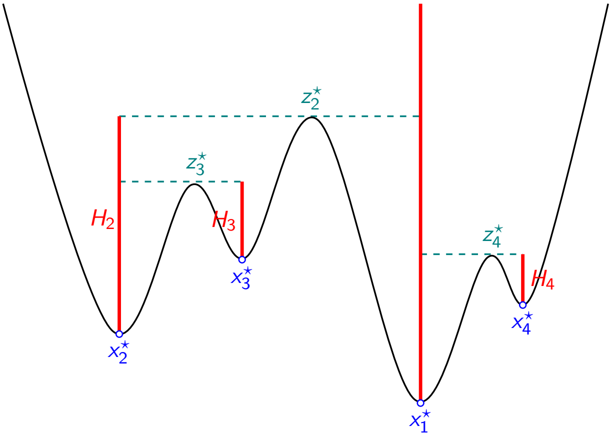
A partition $\mathcal{S}_0 = P_1 \cupdot P_2 \cupdot \ldots \cupdot P_m$ of the set $\mathcal{S}_0$ of local minima of V is said to form a *metastable hierarchy* if there exists a constant $\theta > 0$ such that for all $k \in [\![2, m]\!]$, one has

$$H\left(x^\star, \bigcup_{i=1}^{k-1} P_i\right) \leqslant \min_{y^\star \in P_\ell} H\left(y^\star, \bigcup_{i=1}^{k} P_i \setminus P_\ell\right) - \theta$$

for all $x^\star \in P_k$ and all $\ell \in [\![1, k-1]\!]$. In this case, we write

$$P_1 \prec P_2 \prec \cdots \prec P_m .$$

Metastable hierarchy



Metastable hierarchy

Theorem (A. Bovier, V. Gayrard and M.Klein (2005))

- *Metastable order* $x_1^\star \prec \cdots \prec x_m^\star$
- τ_k *first-hitting time of the* ε*-neighbourhood of* $\{x_1^\star, \ldots, x_k^\star\}$
- λ_k *the* k*th smallest eigenvalue of* $-\mathcal{L}$
- $z_k^\star$ *is a unique* 1*-saddle for any minimal path from* $x_k^\star$ *to* $\{x_1^\star, \ldots, x_{k-1}^\star\}$

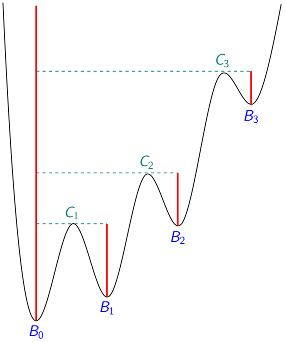
Then for each $k \in [\![2, m]\!]$, *one has*

$$\mathbb{E}^{x_k^\star}[\tau_{k-1}] = \frac{2\pi}{|\lambda_-(z_k^\star)|}\sqrt{\frac{|\det \nabla^2 V(z_k^\star)|}{\det \nabla^2 V(x_k^\star)}}\, \mathrm{e}^{[V(z_k^\star)-V(x_k^\star)]/\varepsilon}\left[1+\mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|^{3/2})\right].$$

Furthermore, $\lambda_1 = 0$ *and there exists a constant* $\theta_1 > 0$ *such that*

$$\lambda_k = \frac{1}{\mathbb{E}^{x_k^\star}[\tau_{k-1}]}\left[1+\mathcal{O}(\mathrm{e}^{-\theta_1/\varepsilon})\right]$$

Hierarchy on B_k



Theorem (N. Berglund, S.D.)

If $\gamma = 0$, *then* $B_0 \prec B_1 \prec \cdots \prec B_{k_{\max}}$.

Hierarchy on B_0

$$V_\gamma(x^\star(\gamma)) = V_0(x^\star(0)) + \frac{\gamma}{4}\sum_{i=1}^{N}\left(x^\star_{i+1}(0) - x^\star_i(0)\right)^2 + \mathcal{O}(\gamma^2)\,.$$

$$I_{1/-1}(x^\star) = \sum_{i=1}^{N} 1_{\{x^\star_i(0)\neq x^\star_{i+1}(0)\}}$$

Lemma

$x^\star$ a critical point in B_0 and $M = \frac{N}{2} \geqslant 4$. Then :

1. *The total number of interfaces $I_{1/-1}(x^\star)$ is even.*
2. *If $I_{1/-1}(x^\star) = 2$, then $x^\star$ has a cluster of M particles.*
3. *If $I_{1/-1}(x^\star) > M$, then $x^\star$ has at least one isolated site.*
4. *If $I_{1/-1}(x^\star) \in [\![4, M]\!]$, then $x^\star$ can has isolated sites or no.*

Hierarchy on B_0

Proposition (N.Berglund, S.D.)

Let $x_1^\star(\gamma), x_2^\star(\gamma) \in B_0$ and let $p = I_{1/-1}(x_1^\star(0))$. Then a transition between them is possible if and only if $x_2^\star(0)$ is obtained by interchanging a particle and a hole in $x_1^\star(0)$. Then

$$I_{1/-1}\big(x_2^\star(0)\big) \in \{p-4, p-2, p, p+2, p+4\} ,$$

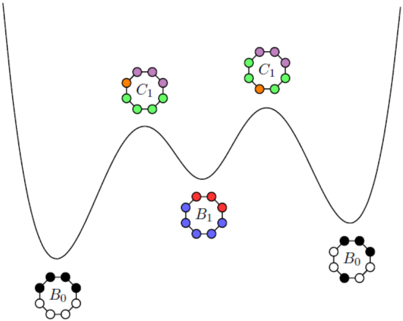
$$H\big(x_1^\star(\gamma), x_2^\star(\gamma)\big) = H^{(0)} + \gamma H^{(1)}\big(x_1^\star(0), x_2^\star(0)\big) + \mathcal{O}(\gamma^2) ,$$

where

$$H^{(0)} = V_0(C_1) - V_0(B_0) = \frac{M(M-1)}{4(M^2 - 3M + 3)} \tag{4.1}$$

depends only on $M = \frac{N}{2}$, while $H^{(1)}(x_1^\star(0), x_2^\star(0))$ also depends on p and on the number of interfaces of the two exchanged sites.

Hierarchy on B_0



Hierarchy on B_0

	Transition	Δp	$H^{(1)}(x_1^\star(0), x_2^\star(0))$	Saddle
I	⋯ ●●● ⋯ ○○○ ⋯	$+4$	$\frac{10M^2 - 36M + 36 - 3p}{4(M^2 - 3M + 3)}$	$[0, 2, p+2]$
II.a	⋯ ●●● ⋯ ○○● ⋯	$+2$	$\frac{2(M-3)^2 - 3p}{4(M^2 - 3M + 3)}$	$[0, 2, p]$
II.b	⋯ ●●○ ⋯ ○○○ ⋯			
II.c	⋯ ●●○○ ⋯			
III	⋯ ●●○ ⋯ ○○● ⋯	0	$\frac{-2M^2 + 6M - 3p}{4(M^2 - 3M + 3)}$	$[1, 1, p-1]$
IV.a	⋯ ●●● ⋯ ●○● ⋯	0	$\frac{-6M^2 + 12M - 3p}{4(M^2 - 3M + 3)}$	$[0, 2, p-2]$
IV.b	⋯ ○●○ ⋯ ○○○ ⋯			
IV.c	⋯ ●●○● ⋯			
IV.d	⋯ ○●○○ ⋯			
V.a	⋯ ●●○ ⋯ ●○● ⋯	-2		
V.b	⋯ ○●○ ⋯ ○○● ⋯			
V.c	⋯ ○●○● ⋯			
VI	⋯ ○●○ ⋯ ●○● ⋯	-4		

Hierarchy on B_0

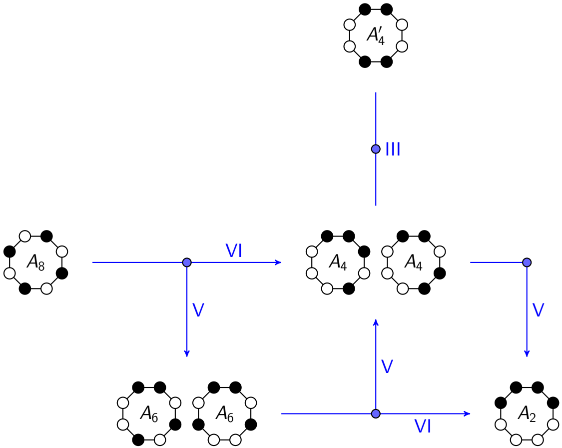
Theorem (N.Berglund, S.D.)

Let M' be the largest even number less or equal $M = \frac{N}{2}$. Then

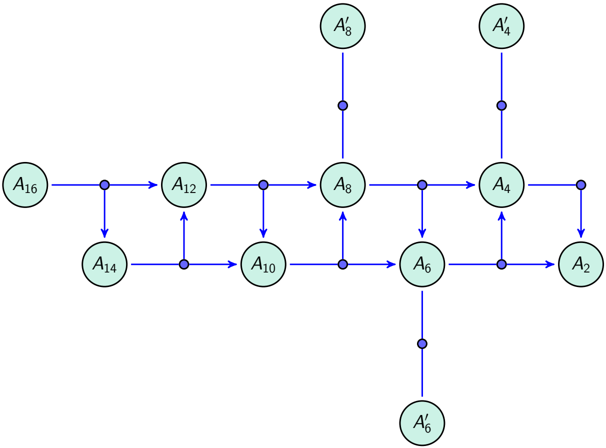
$$A_2 \prec A'_4 \prec A'_6 \prec \cdots \prec A'_{M'-2} \prec A'_{M'} \prec A_4 \prec A_6 \prec \cdots \prec A_{N-2} \prec A_N \ .$$

defines a metastable order of the families A_p and A'_p.

Hierarchy on B_0 example : $N = 8$



Hierarchy on B_0 example : $N = 16$



Spectral Gap

Theorem (N.Berglund, S.D.)

If ε is small enough, then the spectral gap of $-\mathcal{L}$ is given by

$$\lambda_2 = 4\sin^2\left(\frac{\pi}{N}\right)\frac{|\lambda_-(z^\star)|}{2\pi}\sqrt{\frac{\det \nabla^2 V_\gamma(x^\star)}{|\det \nabla^2 V_\gamma(z^\star)|}}\,\mathrm{e}^{-[V_\gamma(z^\star)-V_\gamma(x^\star)]/\varepsilon}\left[1+\mathcal{O}(\sqrt{\varepsilon}|\log\varepsilon|^3)\right]$$

where $x^\star$ is any configuration in A_2, and $z^\star$ is any saddle in C_1 whose limit as $\gamma \to 0$ has exactly 3 interfaces. Moreover

$$V_\gamma(z^\star) - V_\gamma(x^\star) = \frac{1}{4} + \frac{1}{2}\gamma + \mathcal{O}(N^{-1}) + \mathcal{O}(\gamma^2)$$

$$|\lambda_-(z^\star)|\sqrt{\frac{\det \nabla^2 V_\gamma(x^\star)}{|\det \nabla^2 V_\gamma(z^\star)|}} = \sqrt{2} + \mathcal{O}(N^{-1}) + \mathcal{O}(\gamma).$$

Thank you for your attention.

Weak positive coupling case

Theorem (N. Berglund, S.D.)

There exists a constant $c > 0$, independent of N, such that the stationary points of the families B_k and C_k persist for

$$\gamma \leqslant c\left(\frac{1}{6} - \frac{k}{N}\right)^2 ,$$

without changing their index. In the particular case of stationary points of the family B_0, we have the sharper result that they persist at least as long as $\gamma < \frac{7}{3} - \sqrt{5} \simeq 0.097$.

Hierarchy on B_k

Corollaire

For $k \in [\![1, k_{\max}]\!]$, let τ_{k-1} be the first-hitting time of the ε-neighbourhood of $B_0 \cup \cdots \cup B_{k-1}$. If the initial distribution μ of the system is concentrated on $B_k \cup \cdots \cup B_{k_{\max}}$ and invariant under G, then for $\gamma = 0$ one has

$$\mathbb{E}^{\mu}[\tau_{k-1}] = \frac{2\pi \, \mathrm{e}^{[V_0(z_k^\star) - V_0(x_k^\star)]/\varepsilon}}{|\lambda_-(z_k^\star)|(M+k)} \sqrt{\frac{|\det \nabla^2 V_0(z_k^\star)|}{\det \nabla^2 V_0(x_k^\star)}} \left[1 + \mathcal{O}(\sqrt{\varepsilon |\log \varepsilon|^3})\right] ,$$

where $x_k^\star$ is any local minimum in B_k and $z_k^\star$ is any saddle in C_k.