

Métastabilité

dans un système de diffusions couplées

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Travail en commun avec:

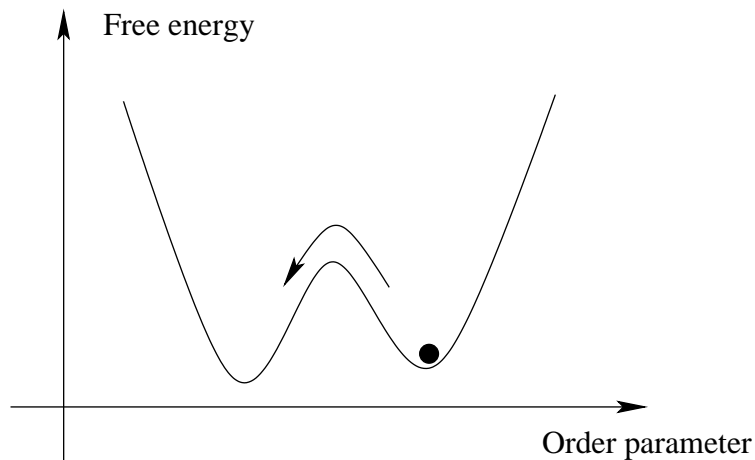
[Bastien Fernandez](#), CPT, Marseille
[Barbara Gentz](#), University of Bielefeld

Séminaire de probabilités
Paris 6 & 7, Chevalleret, 27 mai 2008

Metastability in physics

Examples:

- Supercooled liquid
 - Supersaturated gas
 - Wrongly magnetised ferromagnet
- ▷ Near first-order phase transition
- ▷ Nucleation implies crossing energy barrier

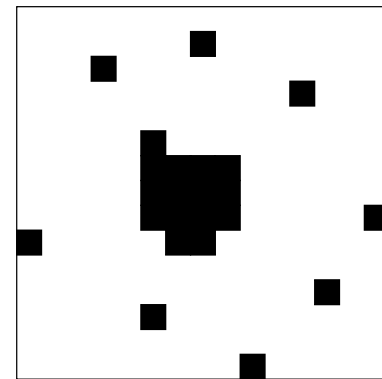


Metastability in stochastic lattice models

- ▷ Lattice: $\Lambda \subset \mathbb{Z}^d$
- ▷ Configuration space: $\mathcal{X} = S^\Lambda$, S finite set (e.g. $\{-1, 1\}$)
- ▷ Hamiltonian: $H : \mathcal{X} \rightarrow \mathbb{R}$ (e.g. Ising or lattice gas)
- ▷ Gibbs measure: $\mu_\beta(x) = e^{-\beta H(x)} / Z_\beta$
- ▷ Dynamics: Markov chain with invariant measure μ_β (e.g. Metropolis: Glauber or Kawasaki)

Results (for $\beta \gg 1$) on

- Transition time between $+$ and $-$ or empty and full configuration
- Transition path
- Shape of critical droplet



- ▷ Frank den Hollander, *Metastability under stochastic dynamics*, Stochastic Process. Appl. **114** (2004), 1–26.
- ▷ Enzo Olivieri and Maria Eulália Vares, *Large deviations and metastability*, Cambridge University Press, Cambridge, 2005.

Metastability in reversible diffusions

$$dx^\sigma(t) = -\nabla V(x^\sigma(t)) dt + \sigma dB(t)$$

- ▷ $V : \mathbb{R}^d \rightarrow \mathbb{R}$: potential, growing at infinity
- ▷ $dB(t)$: d -dim Brownian motion on $(\Omega, \mathcal{F}, \mathbb{P})$

Invariant measure:

$$\mu_\sigma(x) = \frac{e^{-2V(x)/\sigma^2}}{Z_\sigma}$$

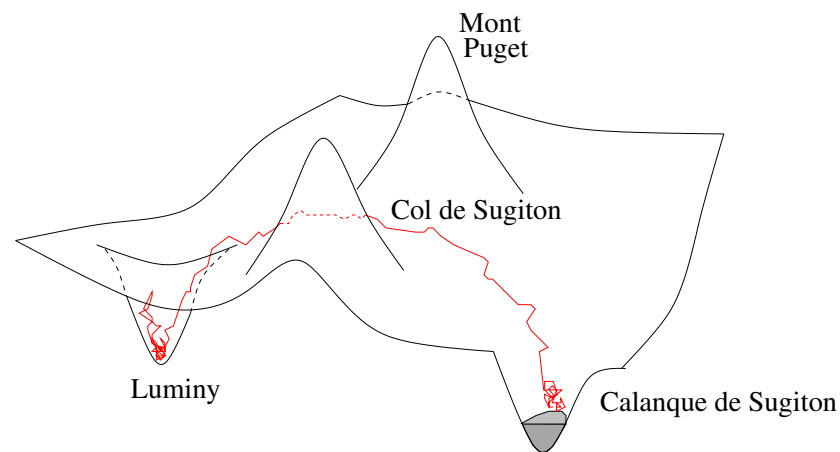
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τ : transition time between potential wells (first-hitting time)

“Eyring–Kramers law” (Eyring 1935, Kramers 1940)

- Dim 1: $\mathbb{E}^x[\tau] \simeq \frac{2\pi}{\sqrt{V''(x)|V''(z)|}} e^{2[V(z)-V(x)]/\sigma^2}$
- Dim ≥ 2 : $\mathbb{E}^x[\tau] \simeq \frac{2\pi}{|\lambda_1(z)|} \sqrt{\frac{\det(\nabla^2 V(z))}{\det(\nabla^2 V(x))}} e^{2[V(z)-V(x)]/\sigma^2}$

Metastability in reversible diffusions

- Large deviations (Wentzell & Freidlin 1969):

$$\lim_{\sigma \rightarrow 0} \sigma^2 \log(\mathbb{E}^x[\tau]) = 2[V(z) - V(x)]$$

- Analytic (Helffer, Sjöstrand 85, Miclo 95, Mathieu 95, Kolokol'tsov 96, . . .):
low-lying spectrum of generator
- Potential theory/variational (Bovier, Eckhoff, Gaynard, Klein 2004):

$$\mathbb{E}^x[\tau] = \frac{2\pi}{|\lambda_1(z)|} \sqrt{\frac{\det(\nabla^2 V(z))}{\det(\nabla^2 V(x))}} e^{2[V(z) - V(x)]/\sigma^2} \left[1 + \mathcal{O}(\sigma |\log \sigma|^{1/2}) \right]$$

and similar asymptotics for eigenvalues of generator

- Witten complex (Helffer, Klein, Nier 2004):
full asymptotic expansion of prefactor
- Distribution of τ (Day 1983, Bovier *et al* 2005):

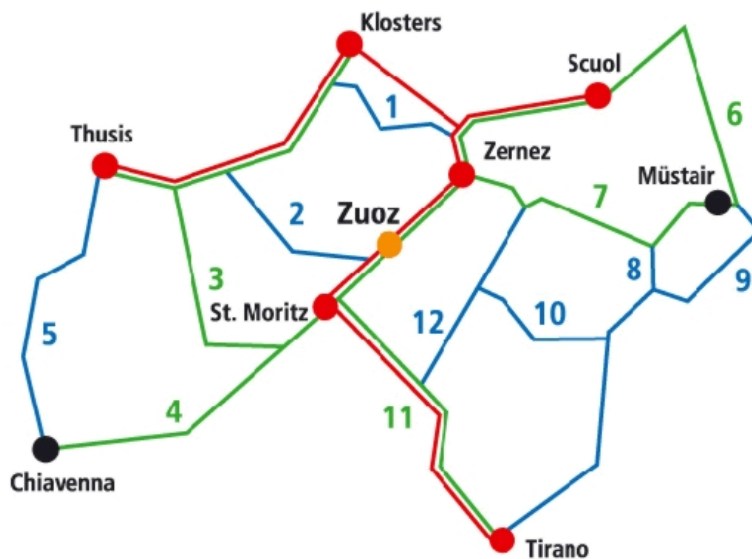
$$\lim_{\sigma \rightarrow 0} \mathbb{P}^x \left\{ \tau > t \mathbb{E}^x[\tau] \right\} = e^{-t}$$

Metastability in reversible diffusions

- ▷ Stationary pts: $\mathcal{S} = \{x : \nabla V(x) = 0\}$
- ▷ Saddles of index k : $\mathcal{S}_k = \{x \in \mathcal{S} : \text{Hess } V(x) \text{ has } k \text{ ev } < 0\}$
- ▷ Graph $\mathcal{G} = (\mathcal{S}_0, \mathcal{E})$, $x \leftrightarrow y$ if $x, y \in \text{unst. manif. of } s \in \mathcal{S}_1$
- ▷ $x_t \sim$ markovian jump process on \mathcal{G}

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Rot Rhätische Bahn
Grün ganzjährig offen
Blau Wintersperre

Nr.	Pass	Land	Passhöhe (m.ü.M.)
1	Flüela	CH	2383
2	Albula	CH	2312
3	Julier	CH	2284
4	Maloja	CH	1815
5	Splügen	I - CH	2115
6	Reschen	A - I	1507
7	Ofen	CH	2149
8	Umbrail	CH - I	2502
9	Stilfserjoch	I	2757
10	Foscagno	I	2291
11	Bernina	CH - I	2323
12	Fla. di Livigno	I	2315

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- Local bistable potential $U(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2 - hx$

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$$dx_i(t) = f(x_i(t)) dt + \frac{\gamma}{2} [x_{i+1}(t) - 2x_i(t) + x_{i-1}(t)] dt$$

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$$\text{Gradient System: } dx^\sigma(t) = -\nabla V_\gamma(x^\sigma(t)) dt + \sigma dB(t)$$

$$\text{Potential: } V_\gamma(x) = \sum_{i \in \Lambda} U(x_i) + \frac{\gamma}{4} \sum_{i \in \Lambda} (x_{i+1} - x_i)^2$$

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▷ Interacting diffusions

(Dawson, Gärtner, Deuschel, Cox, Greven, Shiga, Klenke, Fleischmann, Méléard, Kondratiev, Röckner, Carmona, Xu . . .)

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▷ Scaling regimes: γ and σ may depend on N

▷ Weak coupling γ : $x_i \rightarrow \pm 1$, Ising-like behaviour

▷ Large N , $\gamma \sim N^2$: continuum limit, Ginzburg–Landau SPDE

$$\partial_t u(\varphi, t) = f(u(\varphi, t)) + \tilde{\gamma} \partial_{\varphi\varphi} u(\varphi, t) + \text{noise}$$

$$(\varphi \in \mathbb{S}^1)$$

Symmetric local dynamics: Assume $h = 0$

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Weak coupling

▷ $\gamma = 0$: $\mathcal{S} = \{-1, 0, 1\}^\Lambda$, $\mathcal{S}_0 = \{-1, 1\}^\Lambda$, $\mathcal{G} = \text{hypercube}$.

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Theorem: $\forall N, \exists \gamma^*(N) > 1/4$ s.t. points of each $\mathcal{S}_k(\gamma)$ continuous in γ for $0 \leq \gamma < \gamma^*(N)$

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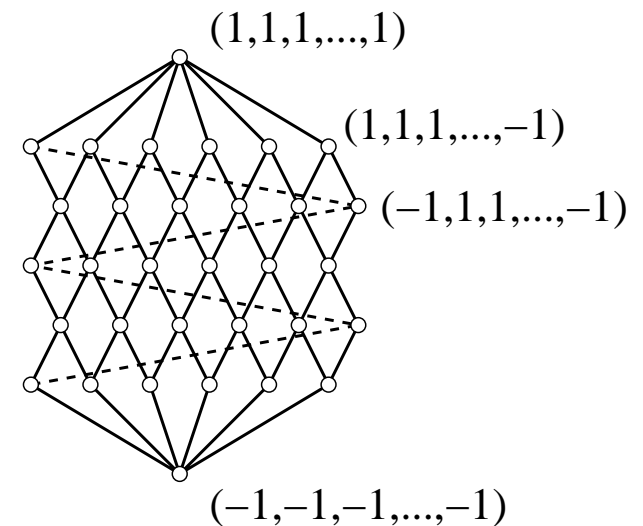
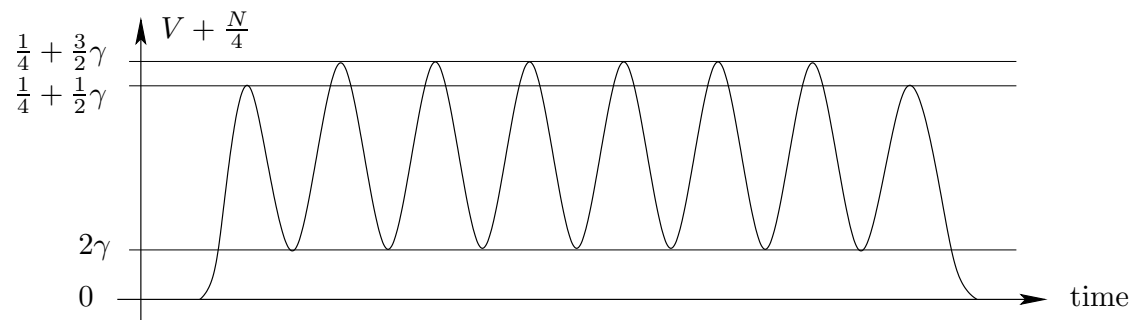
Theorem: $\forall N, \exists \gamma^*(N) > 1/4$ s.t. points of each $\mathcal{S}_k(\gamma)$ continuous in γ for $0 \leq \gamma < \gamma^*(N)$

▷ $0 < \gamma \ll 1$:

$$V_\gamma(x^*(\gamma)) = V_0(x^*(0)) + \frac{\gamma}{4} \sum_{i \in \Lambda} (x_{i+1}^*(0) - x_i^*(0))^2 + \mathcal{O}(\gamma^2)$$

Ising-like dynamics

-	-	-	-	-	-	-	-	-	-	0	+	+	+	+	+
-	0	+	+	+	+	+	+	+	+	+	+	+	+	+	+
-	-	-	0	+	+	+	+	+	+	+	+	+	+	+	+
-	-	-	-	-	-	0	+	+	+	+	+	+	+	+	+
-	-	-	-	-	-	-	-	0	+	+	+	+	+	+	+
-	-	-	-	-	-	-	-	-	-	-	0	+	+	+	+



Strong coupling: Synchronisation

- Remarks:
- $I^\pm = \pm(1, 1, \dots, 1) \in \mathcal{S}_0 \forall \gamma$
 - $O = (0, 0, \dots, 0) \in \mathcal{S} \forall \gamma$

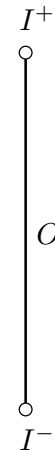
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Let $\gamma_1 = \frac{1}{1 - \cos(2\pi/N)} \quad \left(= \frac{N^2}{2\pi^2} [1 - \mathcal{O}(N^{-2})] \right)$

Theorem:

- $\mathcal{S} = \{I^-, I^+, O\} \Leftrightarrow \gamma \geq \gamma_1$
- $\mathcal{S}_1 = \{O\} \Leftrightarrow \gamma > \gamma_1$



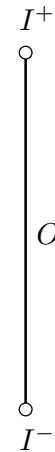
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Proof:

$$\dot{x} = Ax - F(x), \quad A = \begin{pmatrix} 1-\gamma & \gamma/2 & & \gamma/2 \\ \gamma/2 & \ddots & \ddots & \\ & \ddots & \ddots & \gamma/2 \\ \gamma/2 & & \gamma/2 & 1-\gamma \end{pmatrix}, \quad F_i(x) = x_i^3$$

Lyapunov function: $W(x) = \frac{1}{2} \sum_{i \in \Lambda} (x_i - x_{i+1})^2 = \frac{1}{2} \|x - Rx\|^2$

$$Rx = (x_2, \dots, x_N, x_1)$$

$$\frac{dW(x)}{dt} = \langle x - Rx, \frac{d}{dt}(x - Rx) \rangle \leq \langle x - Rx, A(x - Rx) \rangle \leq \left(1 - \frac{\gamma}{\gamma_1}\right) \|x - Rx\|^2$$

Strong coupling: Synchronisation

Remark: $V(O) - V(I^-) = V(O) - V(I^+) = N/4$

Corollary: $\forall N, \forall \gamma > \gamma_1(N), \forall 0 < r < R \leq \frac{1}{2}, \forall x_0 \in \mathcal{B}(I^-, r)$:

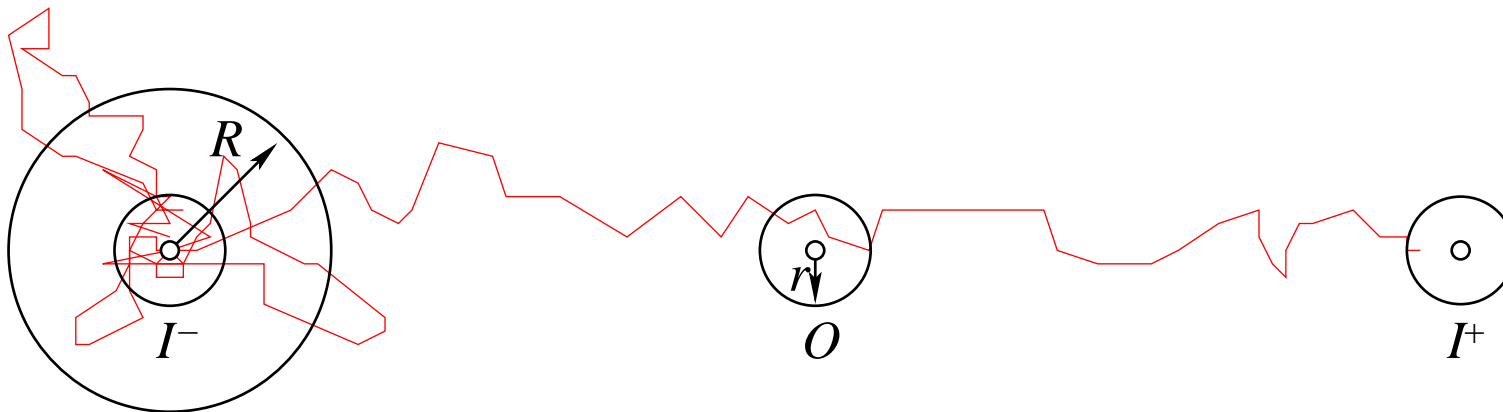
- Let $\tau_+ = \tau^{\text{hit}}(\mathcal{B}(I^+, r))$. Then $\forall \delta > 0$,

$$\lim_{\sigma \rightarrow 0} \mathbb{P}^{x_0} \left\{ e^{(N/2 - \delta)/\sigma^2} \leq \tau_+ \leq e^{(N/2 + \delta)/\sigma^2} \right\} = 1$$

$$\lim_{\sigma \rightarrow 0} \sigma^2 \log \mathbb{E}^{x_0} \{ \tau_+ \} = \frac{N}{2}$$

- Let $\tau_O = \tau^{\text{hit}}(\mathcal{B}(O, r))$,
and $\tau_- = \inf \{ t > \tau^{\text{exit}}(\mathcal{B}(I^-, R)) : x_t \in \mathcal{B}(I^-, r) \}$. Then

$$\lim_{\sigma \rightarrow 0} \mathbb{P}^{x_0} \left\{ \tau_O < \tau_+ \mid \tau_+ < \tau_- \right\} = 1$$



Symmetry groups

Potential V_γ invariant by

- $R(x_1, \dots, x_N) = (x_2, \dots, x_N, x_1)$
- $S(x_1, \dots, x_N) = (x_N, x_{N-1}, \dots, x_1)$
- $C(x_1, \dots, x_N) = -(x_1, \dots, x_N)$

$\Rightarrow V_\gamma$ invariant by group $G = D_N \times \mathbb{Z}_2$ generated by R, S, C

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$\Rightarrow V_\gamma$ invariant by group $G = D_N \times \mathbb{Z}_2$ generated by R, S, C
 G acts as **group of transformations** on \mathcal{X} , $S, S_k \forall k$

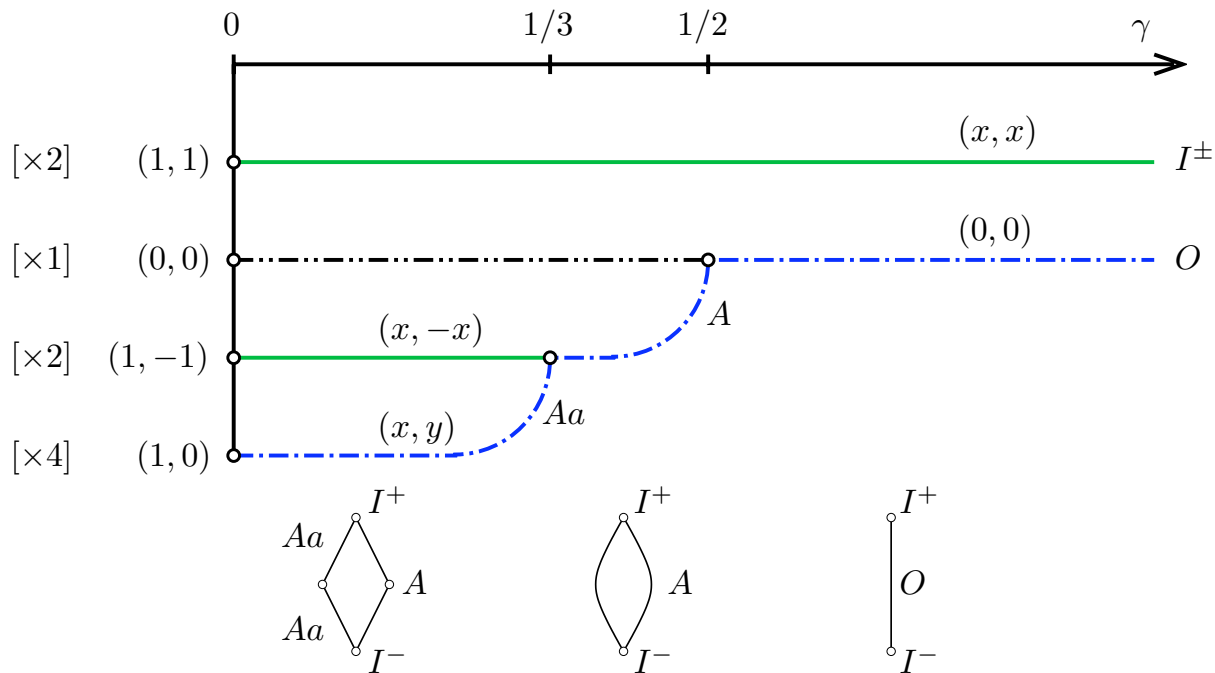
- **Orbit** of $x \in \mathcal{X}$: $O_x = \{gx : g \in G\}$
- **Isotropy group** of $x \in \mathcal{X}$: $C_x = \{g \in G : gx = x\} \triangleleft G$
- **Fixed-point space** of $H \triangleleft G$: $\text{Fix}(H) = \{x \in \mathcal{X} : hx = x \forall h \in H\}$

$N = 2$

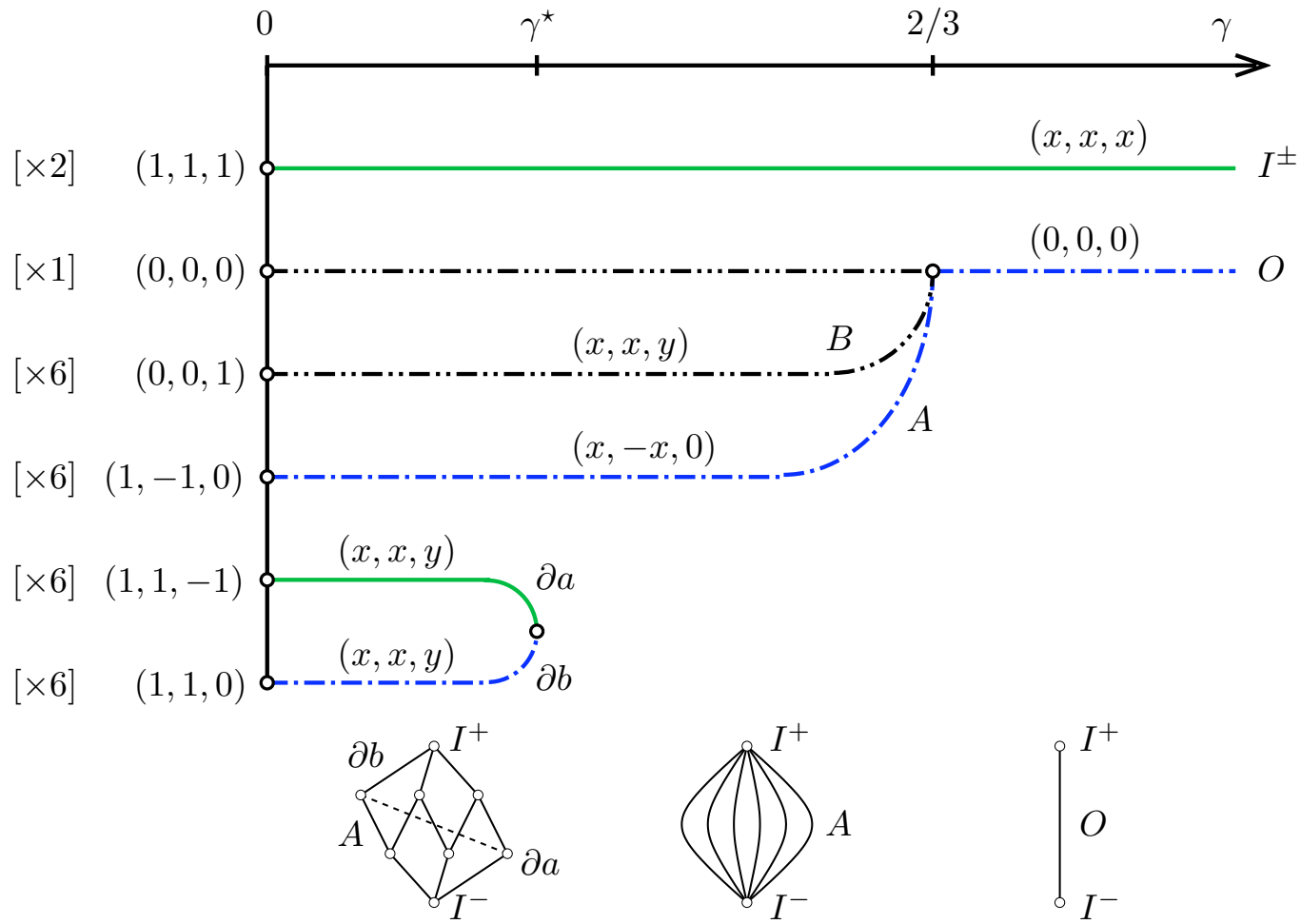
z^*	O_{z^*}	C_{z^*}	$\text{Fix}(C_{z^*})$
$(0, 0)$	$\{(0, 0)\}$	G	$\{(0, 0)\}$
$(1, 1)$	$\{(1, 1), (-1, -1)\}$	$D_2 = \{\text{id}, S\}$	$\{(x, x)\}_{x \in \mathbb{R}} = \mathcal{D}$
$(1, -1)$	$\{(1, -1), (-1, 1)\}$	$\{\text{id}, CS\}$	$\{(x, -x)\}_{x \in \mathbb{R}}$
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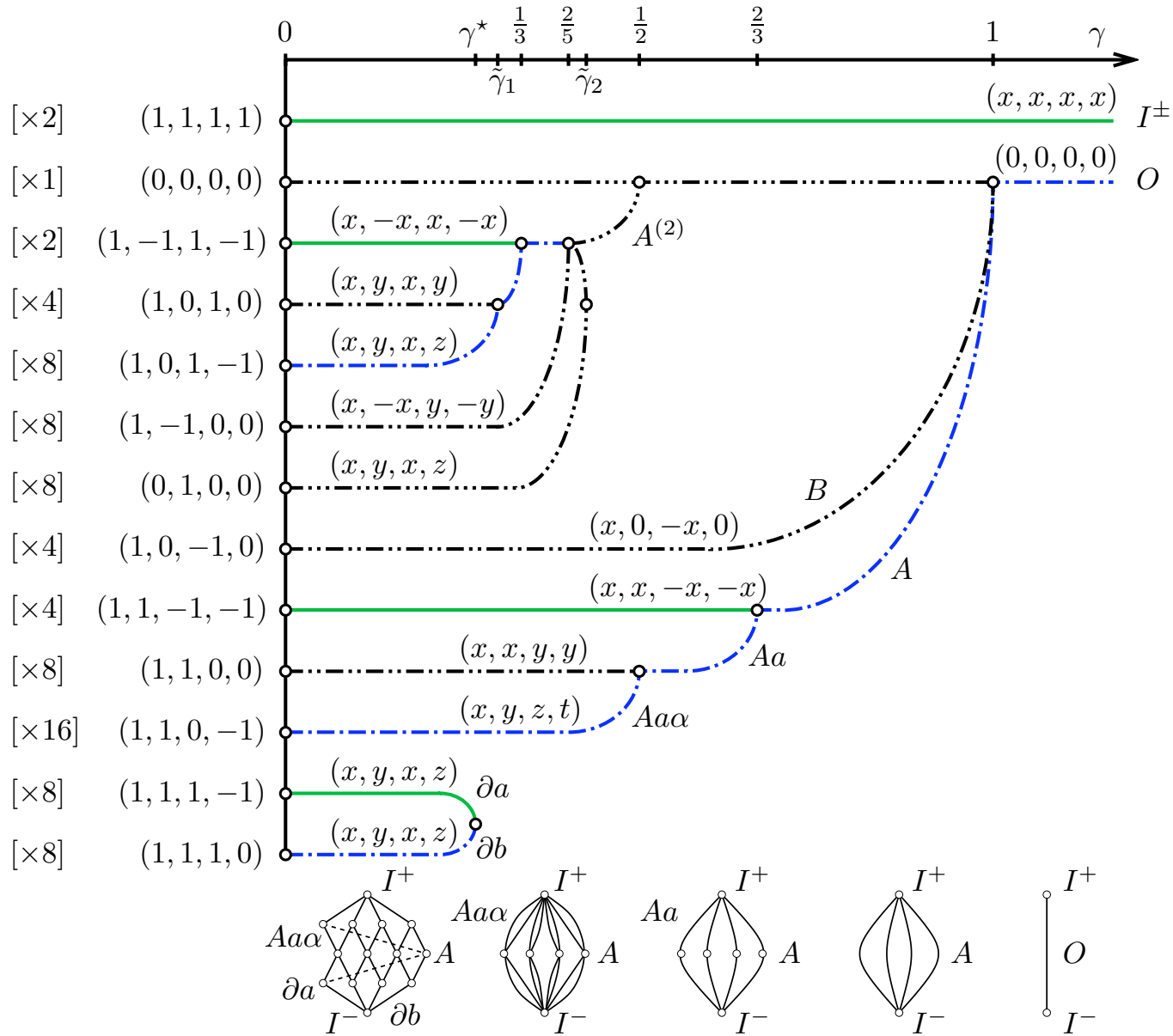
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$N = 3$



$N = 4$



Desynchronisation

Theorem: \forall even $N \geq 4$, $\exists \delta(N) > 0$ s.t. for $\gamma_1 - \delta(N) < \gamma < \gamma_1$, $|\mathcal{S}| = 2N + 3$, and can be decomposed as

$$\mathcal{S}_0 = O_{I^+} = \{I^+, I^-\}$$

$$\mathcal{S}_1 = O_A = \{A, RA, \dots, R^{N-1}A\}$$

$$\mathcal{S}_2 = O_B = \{B, RB, \dots, R^{N-1}B\}$$

$$\mathcal{S}_3 = O_O = \{O\}$$

with

$$A_j(\gamma) = \frac{2}{\sqrt{3}} \sqrt{1 - \frac{\gamma}{\gamma_1}} \sin\left(\frac{2\pi}{N}\left(j - \frac{1}{2}\right)\right) + \mathcal{O}\left(1 - \frac{\gamma}{\gamma_1}\right)$$

$$\frac{V_\gamma(A)}{N} = -\frac{1}{6}\left(1 - \frac{\gamma}{\gamma_1}\right)^2 + \mathcal{O}\left(\left(1 - \frac{\gamma}{\gamma_1}\right)^3\right)$$

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- ▷ N odd: similar result, $|\mathcal{S}| \geq 4N + 3$
- ▷ Similar corollary for τ , with $\tau_0 \mapsto \tau_{UgA}$
- ▷ A and B have particular symmetries

N large

Recall $\gamma_1(N) \asymp N^2$

Assume $\gamma > \text{const } N^2$, let $\tilde{\gamma} = \gamma/\gamma_1$

Equation \rightarrow Ginzburg–Landau SPDE

$$\partial_t u(\varphi, t) = f(u(\varphi, t)) + \tilde{\gamma} \partial_{\varphi\varphi} u(\varphi, t) + \text{noise}$$

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$$x \in \mathcal{S} \quad \Leftrightarrow \quad f(x_n) + \frac{\gamma}{2} [x_{n+1} - 2x_n + x_{n-1}] = 0$$

$$\Leftrightarrow \quad \begin{cases} x_{n+1} = x_n + \varepsilon w_n - \frac{1}{2} \varepsilon^2 f(x_n) \\ w_{n+1} = w_n - \frac{1}{2} \varepsilon [f(x_n) + f(x_{n+1})] \end{cases}$$

$$\varepsilon = \sqrt{\frac{2}{\gamma}} \simeq \frac{2\pi}{N\sqrt{\tilde{\gamma}}} \ll 1$$

▷ Area-preserving map

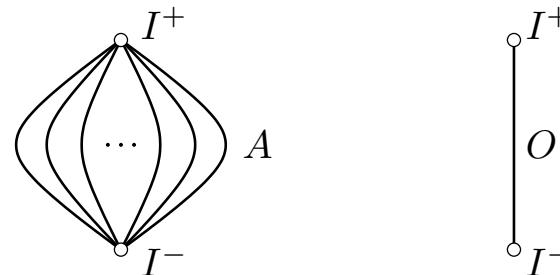
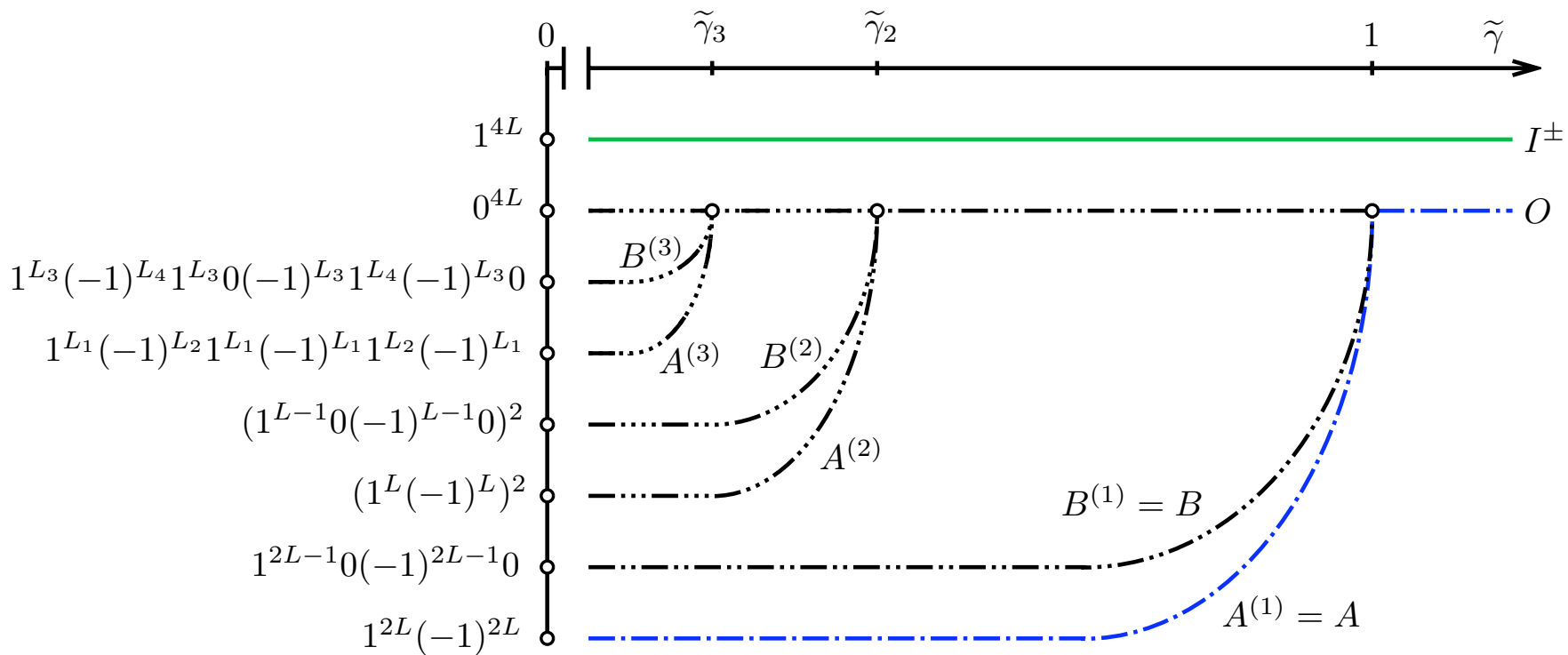
▷ Discretisation of $\ddot{x} = -f(x)$

▷ Almost conserved quantity: $C(x, w) = \frac{1}{2}(x^2 + w^2) - \frac{1}{4}x^4$

$$C(x_{n+1}, w_{n+1}) = C(x_n, w_n) + \mathcal{O}(\varepsilon^3)$$

▷ Transf. to action–angle variables involves elliptic functions

N large



N large

Let $\tilde{\gamma} = \frac{\gamma}{\gamma_1} = \gamma(1 - \cos(2\pi/N))$,

$$\tilde{\gamma}_M = \frac{1 - \cos(2\pi/N)}{1 - \cos(2\pi M/N)} \quad \left(= \frac{1}{M^2} + \mathcal{O}\left(\frac{1}{N^2}\right) \right)$$

Theorem: $\forall M \geq 1, \exists N_M < \infty$ s.t. for $N \geq N_M$ and $\tilde{\gamma}_{M+1} < \tilde{\gamma} < \tilde{\gamma}_M$, \mathcal{S} can be decomposed as

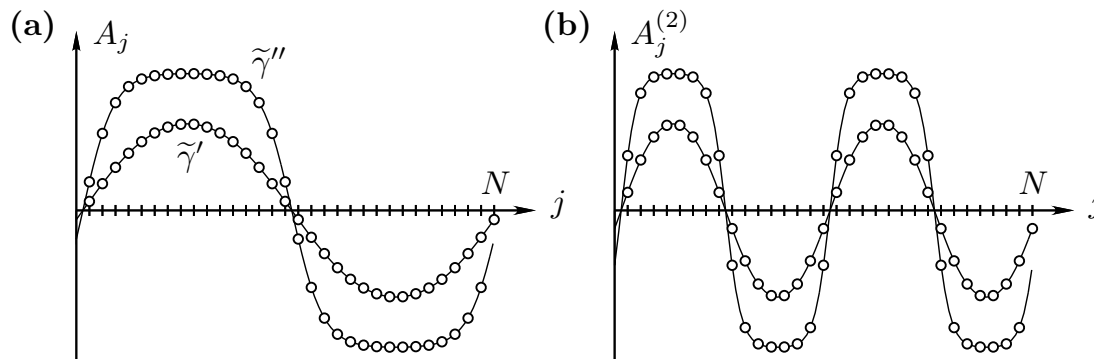
$$\mathcal{S}_0 = O_{I^+} = \{I^+, I^-\}$$

$$\mathcal{S}_{2m-1} = O_{A^{(m)}} \quad m = 1, \dots, M$$

$$\mathcal{S}_{2m} = O_{B^{(m)}} \quad m = 1, \dots, M,$$

$$\mathcal{S}_{2M+1} = O_O = \{O\}$$

with $A^{(m)}, B^{(m)}(\tilde{\gamma})$ known, given in terms of elliptic functions sn

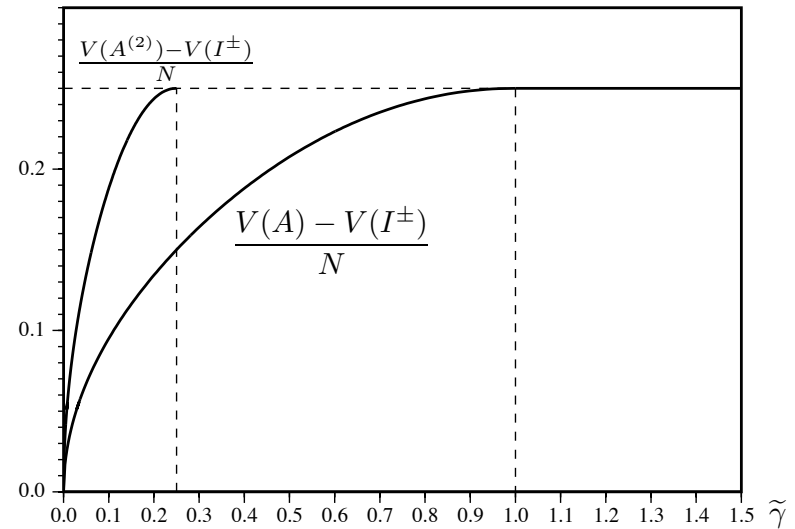


N large

Potential difference:

$$H(\tilde{\gamma}) = V(A) - V(I^\pm) \sim N$$

(explicit expression
in terms of elliptic integrals)

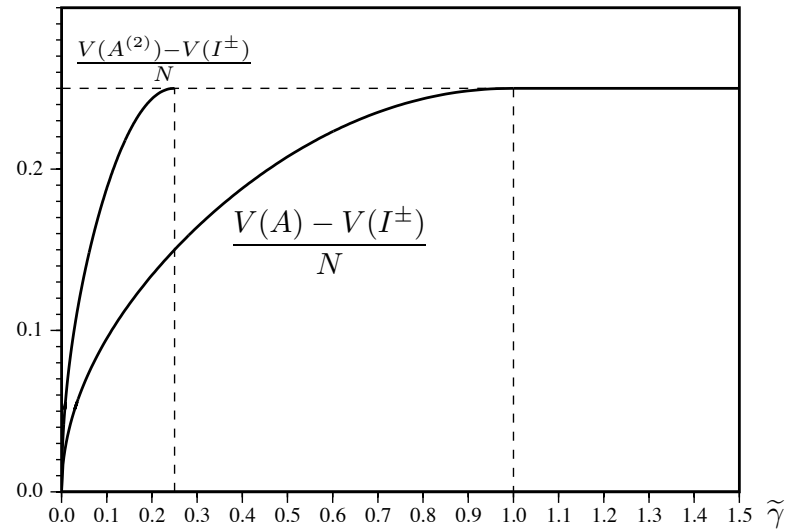


N large

Potential difference:

$$H(\tilde{\gamma}) = V(A) - V(I^\pm) \sim N$$

(explicit expression
in terms of elliptic integrals)



Corollary: $\forall 0 < \tilde{\gamma} \leq 1, \exists N_0(\tilde{\gamma})$ s.t. $\forall N \geq N_0(\tilde{\gamma}),$

$\forall 0 < r < \frac{1}{2}, \forall x_0 \in \mathcal{B}(I^-, r):$

- Let $\tau_+ = \tau^{\text{hit}}(\mathcal{B}(I^+, r))$. Then

$$\lim_{\sigma \rightarrow 0} \sigma^2 \log \mathbb{E}^{x_0} \{\tau_+\} = 2H(\tilde{\gamma}) \quad \Rightarrow \quad \mathbb{E}^{x_0} \{\tau_+\} \simeq e^{2H(\tilde{\gamma})/\sigma^2}$$

- During a transition, path likely to pass close to one of the points of O_A :

Let $\tau_A = \tau^{\text{hit}}(\cup_{g \in G} \mathcal{B}(gA, r)),$

and $\tau_- = \inf\{t > \tau^{\text{exit}}(\mathcal{B}(I^-, R)) : x_t \in \mathcal{B}(I^-, r)\}$. Then

$$\lim_{\sigma \rightarrow 0} \mathbb{P}^{x_0} \left\{ \tau_A < \tau_+ \mid \tau_+ < \tau_- \right\} = 1$$

Beyond exponential asymptotics

Recall Kramers' law $\mathbb{E}^x[\tau] \simeq \frac{2\pi}{|\lambda_1(z)|} \sqrt{\frac{\det(\nabla^2 V(z))}{\det(\nabla^2 V(x))}} e^{2[V(z)-V(x)]/\sigma^2}$

▷ Work by Barret & Bovier

What happens at bifurcations, e.g. when $\det(\nabla^2 V(z)) = 0$?

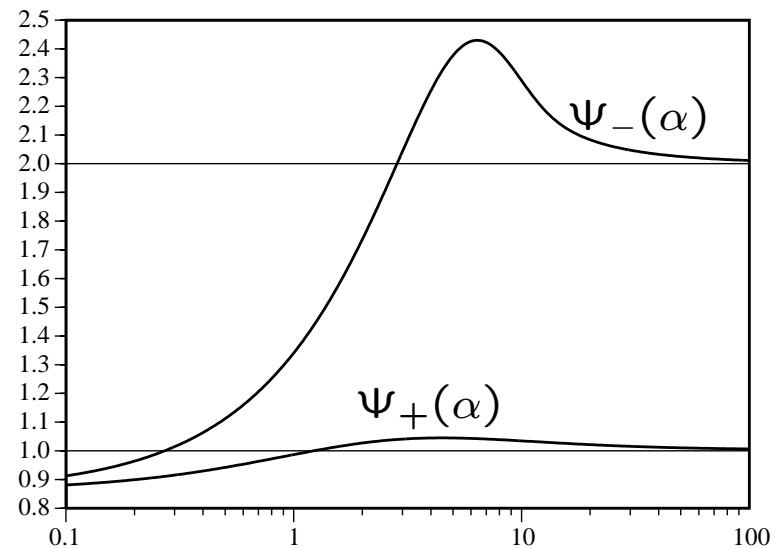
Theorem: Let $\nabla^2 V(z)$ have eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 \leq \dots \leq \lambda_N$, with $\lambda_1 < 0 < \lambda_3$. Then $\forall \lambda_2 \geq 0$,

$$\mathbb{E}^x[\tau_D] = 2\pi \sqrt{\frac{[\lambda_2 + c\sigma]\lambda_3 \dots \lambda_d}{|\lambda_1| \det \nabla^2(V(x))}} \frac{e^{2[V(z)-V(x)]/\sigma^2}}{\Psi_+(\lambda_2/c\sigma)} [1 + \mathcal{O}(\sigma^{1/2} |\log \sigma|^{1/4})]$$

where c related to $V''''(z)$ and

$$\Psi_+(\alpha) = \sqrt{\frac{\alpha(1+\alpha)}{8\pi}} e^{\alpha^2/16} K_{1/4}\left(\frac{\alpha^2}{16}\right)$$

Similar expression for $\lambda_2 < 0$ involving $I_{\pm 1/4}(\alpha^2/64)$



Outlook

- Asymmetric potential (magnetic field)
- Continuum limit $N \rightarrow \infty$ (SPDE)
- Inhomogeneous noise intensity (heat flow)
- Time-dependent magnetic field (hysteresis)

References

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