Metastability
in a system of interacting nonlinear diffusions

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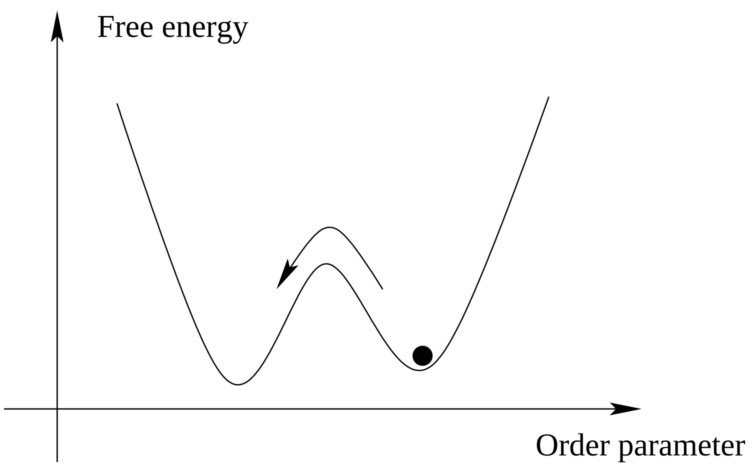
Applications of spatio-temporal
dynamical systems in biology
Nice, June 19, 2008

Metastability in physics

Examples:

- Supercooled liquid
- Supersaturated gas
- Wrongly magnetised ferromagnet

▷ Near first-order phase transition
▷ Nucleation implies crossing energy barrier

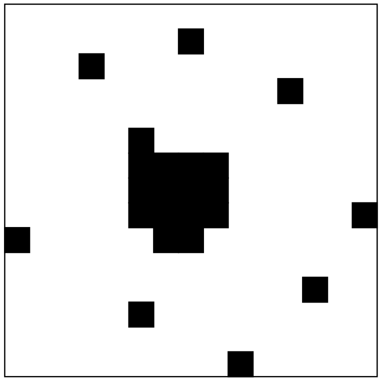


Metastability in stochastic lattice models

▷ Lattice: $\Lambda \subset\subset \mathbb{Z}^d$
▷ Configuration space: $\mathcal{X} = S^\Lambda$, S finite set (e.g. $\{-1, 1\}$)
▷ Hamiltonian: $H : \mathcal{X} \to \mathbb{R}$ (e.g. Ising or lattice gas)
▷ Gibbs measure: $\mu_\beta(x) = \mathrm{e}^{-\beta H(x)} / Z_\beta$
▷ 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

$$\mathrm{d}x^\sigma(t) = -\nabla V(x^\sigma(t))\,\mathrm{d}t + \sigma\,\mathrm{d}B(t)$$

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

Invariant measure:

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

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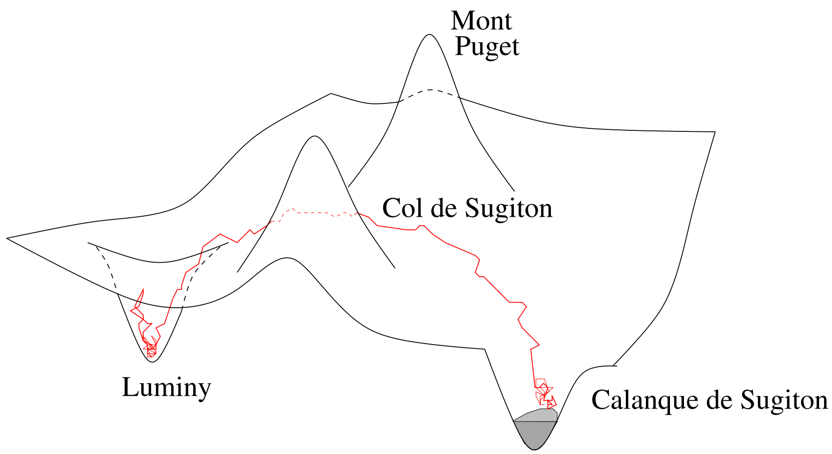

τ: transition time between potential wells (first-hitting time)

"Eyring–Kramers law" (Eyring 1935, Kramers 1940)

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

Metastability in reversible diffusions

- Large deviations (Wentzell & Freidlin 1969):

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

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

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

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):

$$\lim_{\sigma\to 0} \mathbb{P}^x\Big\{\tau > t\mathbb{E}^x[\tau]\Big\} = \mathrm{e}^{-t}$$

Metastability in reversible diffusions

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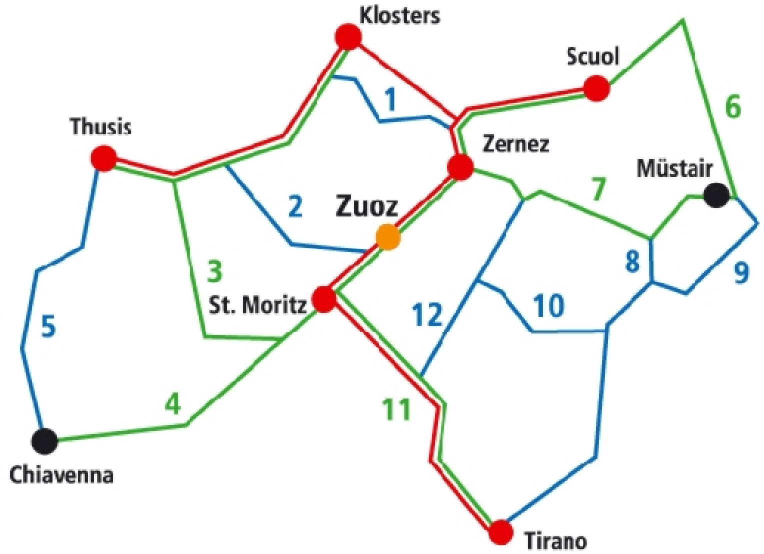

Rot Rhätische Bahn
Grün ganzjährig offen
Blau Wintersperre

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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Gradient System: $\mathrm{d}x^\sigma(t) = -\nabla V_\gamma(x^\sigma(t))\,\mathrm{d}t + \sigma\,\mathrm{d}B(t)$

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

The model

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$\triangleright$ Interacting diffusions

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

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▷ Interacting diffusions

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▷ Scaling regimes: γ and σ may depend on N

▷ Weak coupling γ: $x_i \to \pm 1$, 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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Theorem: $\forall N$, $\exists \gamma^\star(N) > 1/4$ s.t. points of each $S_k(\gamma)$ continuous in γ for $0 \leqslant \gamma < \gamma^\star(N)$

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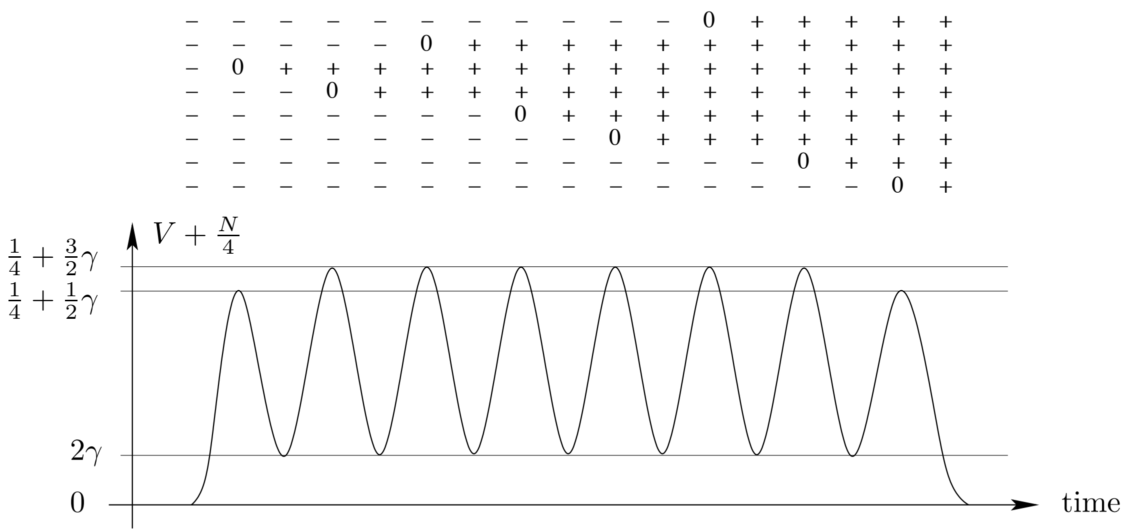
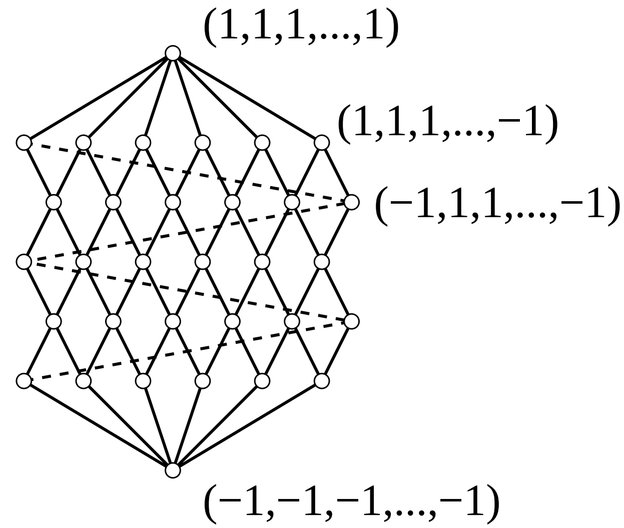
▷ $0 < \gamma \ll 1$:

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

Ising-like dynamics





Strong coupling: Synchronisation

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

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

Theorem:

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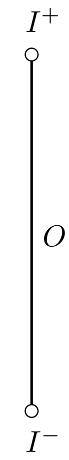

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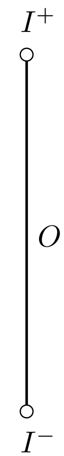

Theorem:

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Proof:

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

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

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

$$\frac{\mathrm{d}W(x)}{\mathrm{d}t} = \langle x-Rx, \frac{\mathrm{d}}{\mathrm{d}t}(x-Rx)\rangle \leqslant \langle x-Rx, A(x-Rx)\rangle \leqslant (1-\frac{\gamma}{\gamma_1})\|x-Rx\|^2$$

Strong coupling: Synchronisation

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

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

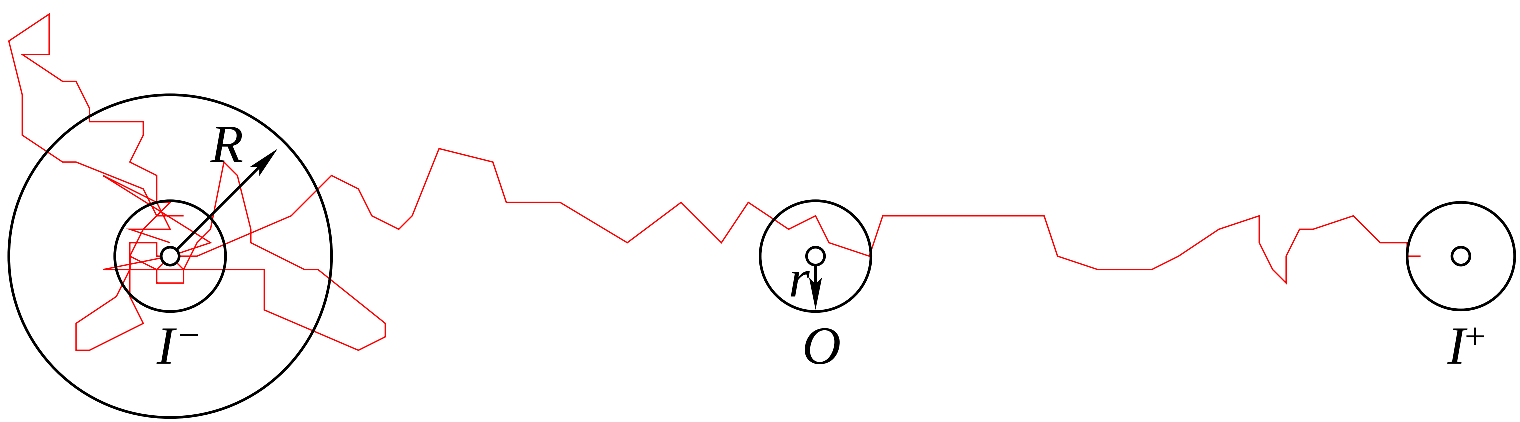
- Let $\tau_+ = \tau^{\text{hit}}(\mathcal{B}(I^+, r))$. Then $\forall \delta > 0$,

$$\lim_{\sigma\to 0} \mathbb{P}^{x_0}\Big\{ \mathrm{e}^{(N/2-\delta)/\sigma^2} \leqslant \tau_+ \leqslant \mathrm{e}^{(N/2+\delta)/\sigma^2} \Big\} = 1$$

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

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

$$\lim_{\sigma\to 0} \mathbb{P}^{x_0}\Big\{ \tau_O < \tau_+ \Bigm| \tau_+ < \tau_- \Big\} = 1$$



Symmetry groups

Potential V_γ invariant by

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

$\Rightarrow V_\gamma$ 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 $\mathcal{X}$, $\mathcal{S}$, $\mathcal{S}_k \; \forall k$

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

$N = 2$

$z^\star$	$O_{z^\star}$	$C_{z^\star}$	$\mathrm{Fix}(C_{z^\star})$
$(0,0)$	$\{(0,0)\}$	G	$\{(0,0)\}$
$(1,1)$	$\{(1,1),(-1,-1)\}$	$D_2 = \{\mathrm{id}, S\}$	$\{(x,x)\}_{x\in\mathbb{R}} = \mathcal{D}$
$(1,-1)$	$\{(1,-1),(-1,1)\}$	$\{\mathrm{id}, CS\}$	$\{(x,-x)\}_{x\in\mathbb{R}}$
$(1,0)$	$\{\pm(1,0),\pm(0,1)\}$	$\{\mathrm{id}\}$	$\{(x,y)\}_{x,y\in\mathbb{R}} = \mathcal{X}$

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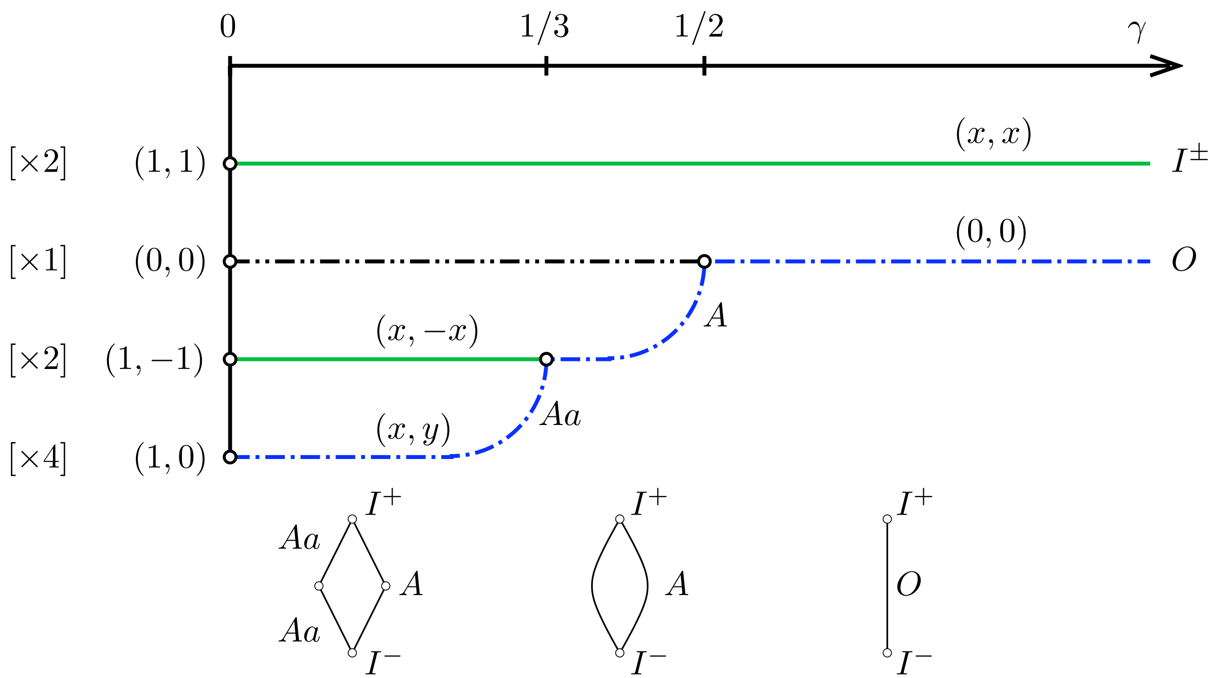
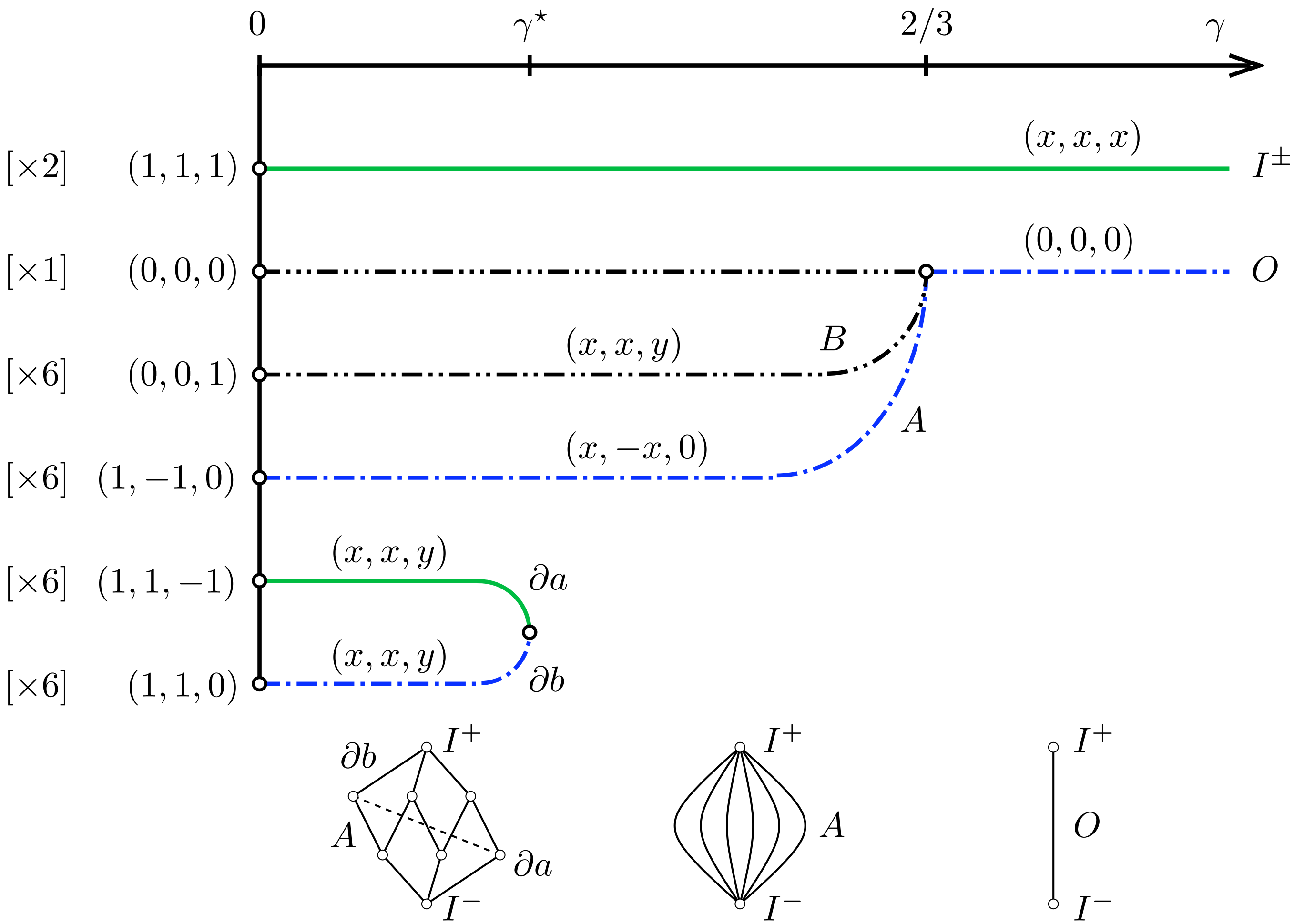
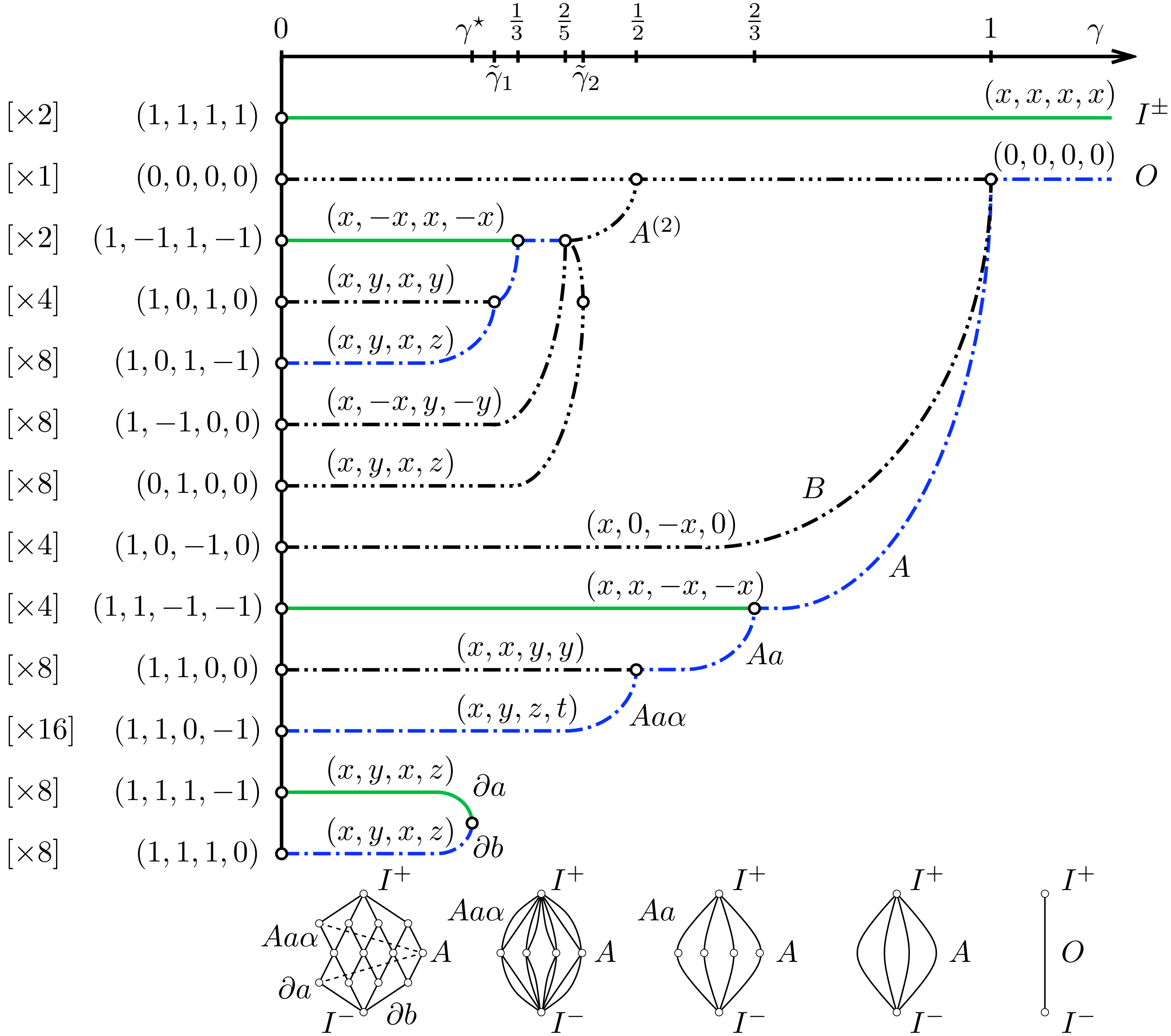


$N = 3$



0
$\gamma^\star$
2/3
γ
[×2] (1, 1, 1)
[×1] (0, 0, 0)
[×6] (0, 0, 1)
[×6] (1, −1, 0)
[×6] (1, 1, −1)
[×6] (1, 1, 0)
(x, x, x)
$I^\pm$
(0, 0, 0)
O
(x, x, y)
B
A
(x, −x, 0)
(x, x, y)
∂a
(x, x, y)
∂b
∂b
I^+
A
∂a
I^-
I^+
A
I^-
I^+
O
I^-

$N = 4$



0
$\gamma^\star$
$\frac{1}{3}$
$\frac{2}{5}$
$\frac{1}{2}$
$\frac{2}{3}$
1
γ
$\tilde{\gamma}_1$
$\tilde{\gamma}_2$
[×2] (1, 1, 1, 1)
[×1] (0, 0, 0, 0)
[×2] (1, −1, 1, −1)
[×4] (1, 0, 1, 0)
[×8] (1, 0, 1, −1)
[×8] (1, −1, 0, 0)
[×8] (0, 1, 0, 0)
[×4] (1, 0, −1, 0)
[×4] (1, 1, −1, −1)
[×8] (1, 1, 0, 0)
[×16] (1, 1, 0, −1)
[×8] (1, 1, 1, −1)
[×8] (1, 1, 1, 0)
(x, x, x, x)
$I^\pm$
$(0, 0, 0, 0)$
O
$(x, -x, x, -x)$
$A^{(2)}$
(x, y, x, y)
(x, y, x, z)
$(x, -x, y, -y)$
(x, y, x, z)
B
$(x, 0, -x, 0)$
A
$(x, x, -x, -x)$
Aa
(x, x, y, y)
(x, y, z, t)
$Aa\alpha$
(x, y, x, z)
∂a
(x, y, x, z)
∂b
I^+
$Aa\alpha$
A
∂a
I^-
∂b
I^+
$Aa\alpha$
A
I^-
I^+
Aa
A
I^-
I^+
A
I^-
I^+
O
I^-

Desynchronisation

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

$$\begin{aligned}
\mathcal{S}_0 &= O_{I^+} = \{I^+, I^-\} \\
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\mathcal{S}_3 &= O_O = \{O\}
\end{aligned}$$

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

with

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

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

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

N large

Recall $\gamma_1(N) \asymp N^2$
Assume $\gamma > const\, N^2$, 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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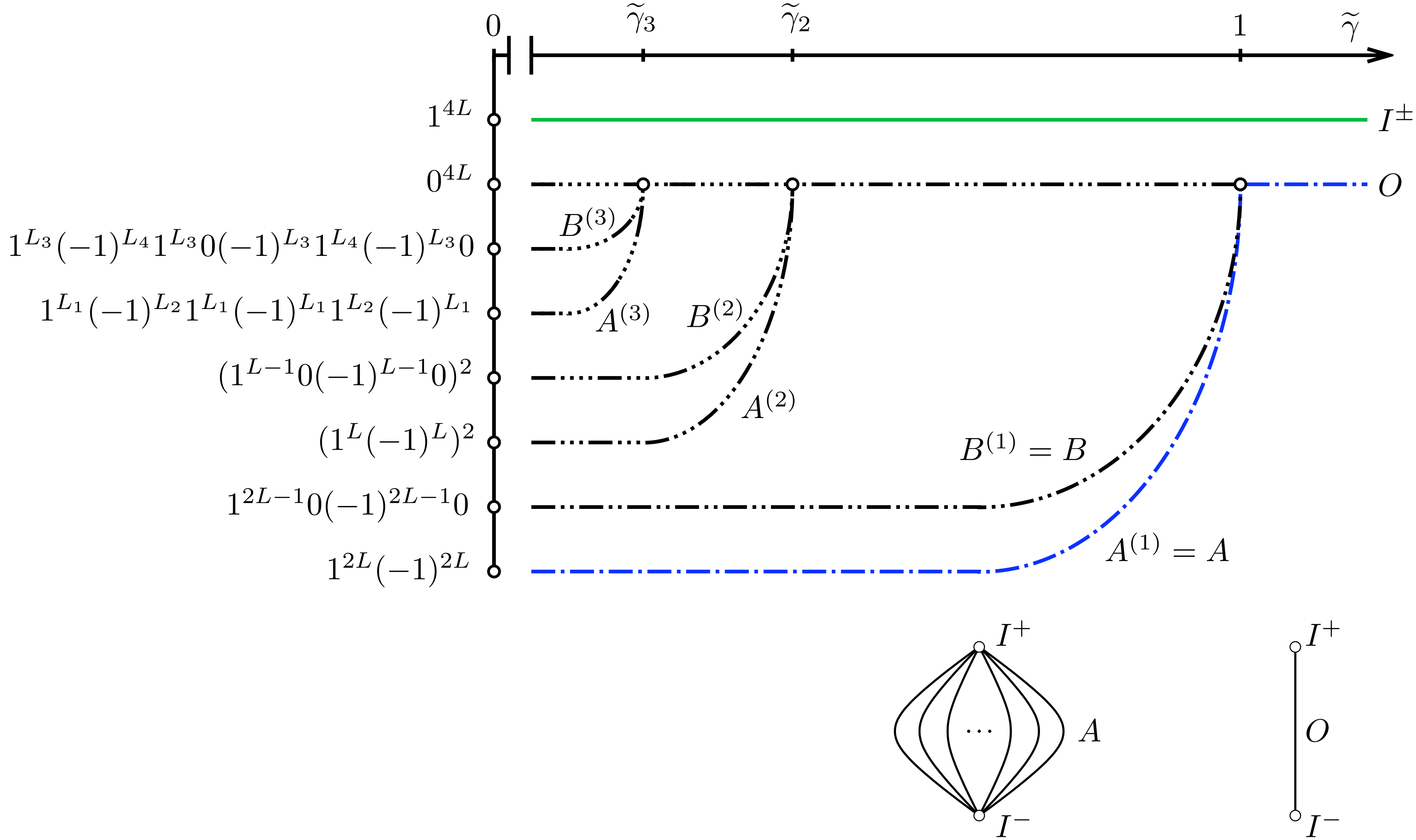
$$x \in \mathcal{S} \quad \Leftrightarrow \quad f(x_n) + \frac{\gamma}{2}\Big[x_{n+1} - 2x_n + x_{n-1}\Big] = 0$$

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

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

- ▷ 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


0
$\widetilde{\gamma}_3$
$\widetilde{\gamma}_2$
1
$\widetilde{\gamma}$
1^{4L}
0^{4L}
$1^{L_3}(-1)^{L_4}1^{L_3}0(-1)^{L_3}1^{L_4}(-1)^{L_3}0$
$1^{L_1}(-1)^{L_2}1^{L_1}(-1)^{L_1}1^{L_2}(-1)^{L_1}$
$(1^{L-1}0(-1)^{L-1}0)^2$
$(1^{L}(-1)^{L})^2$
$1^{2L-1}0(-1)^{2L-1}0$
$1^{2L}(-1)^{2L}$
$I^{\pm}$
O
$B^{(3)}$
$A^{(3)}$
$B^{(2)}$
$A^{(2)}$
$B^{(1)} = B$
$A^{(1)} = A$
I^+
$\cdots$
A
I^-
I^+
O
I^-

N large

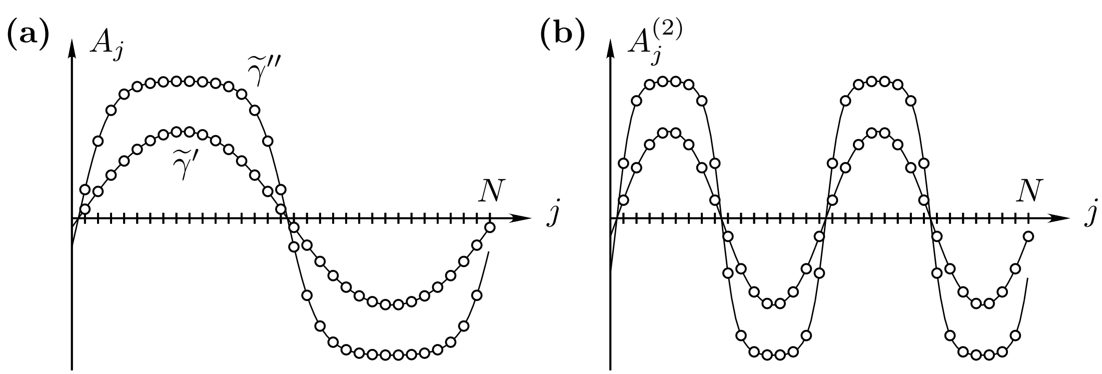
Let $\widetilde{\gamma} = \frac{\gamma}{\gamma_1} = \gamma(1 - \cos(2\pi/N))$,

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

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

$$\begin{aligned} \mathcal{S}_0 &= O_{I^+} = \{I^+, I^-\} & & \\ \mathcal{S}_{2m-1} &= O_{A^{(m)}} & & m = 1, \dots, M \\ \mathcal{S}_{2m} &= O_{B^{(m)}} & & m = 1, \dots, M\ , \\ \mathcal{S}_{2M+1} &= O_O = \{O\} & & \end{aligned}$$

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

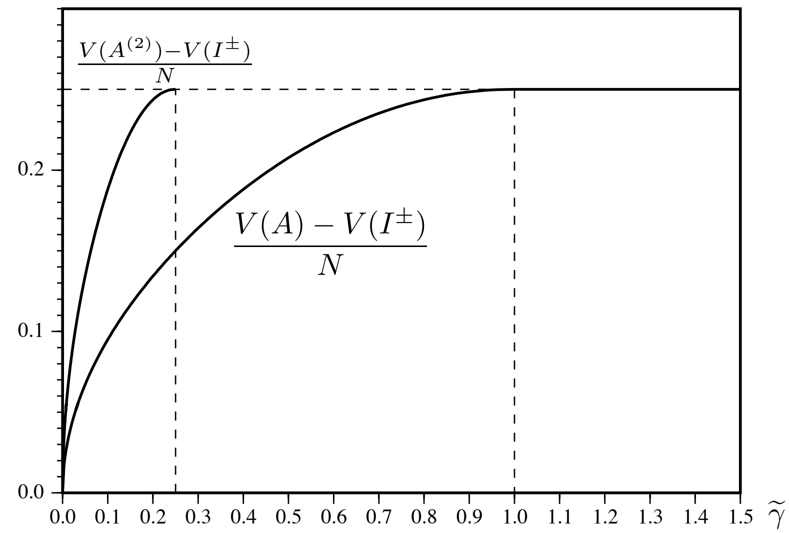


N large

Potential difference:

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

(explicit expression
in terms of elliptic integrals)



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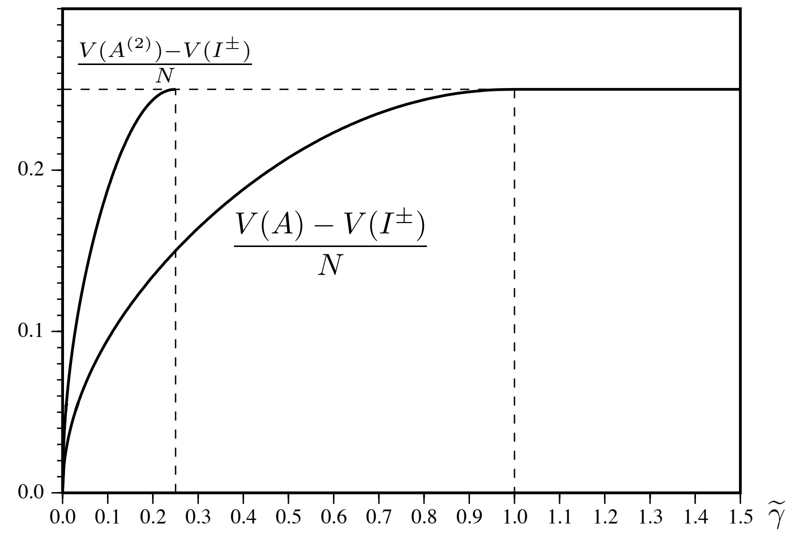

Corollary: $\forall 0 < \tilde{\gamma} \leqslant 1$, $\exists N_0(\tilde{\gamma})$ s.t. $\forall N \geqslant N_0(\tilde{\gamma})$, $\forall 0 < r < \frac{1}{2}$, $\forall x_0 \in \mathcal{B}(I^-, r)$:

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

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

- During a transition, path likely to pass close to one of the points of O_A:
  Let $\tau_A = \tau^{\text{hit}}(\bigcup_{g \in G} \mathcal{B}(gA, r))$,
  and $\tau_- = \inf\{t > \tau^{\text{exit}}(\mathcal{B}(I^-, R)) : x_t \in \mathcal{B}(I^-, r)\}$. Then

$$\lim_{\sigma \to 0} \mathbb{P}^{x_0}\Big\{\tau_A < \tau_+ \,\Big|\, \tau_+ < \tau_-\Big\} = 1$$

Beyond exponential asymptotics

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

▷ Work by Barret & Bovier

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

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▷ Work by Barret & Bovier

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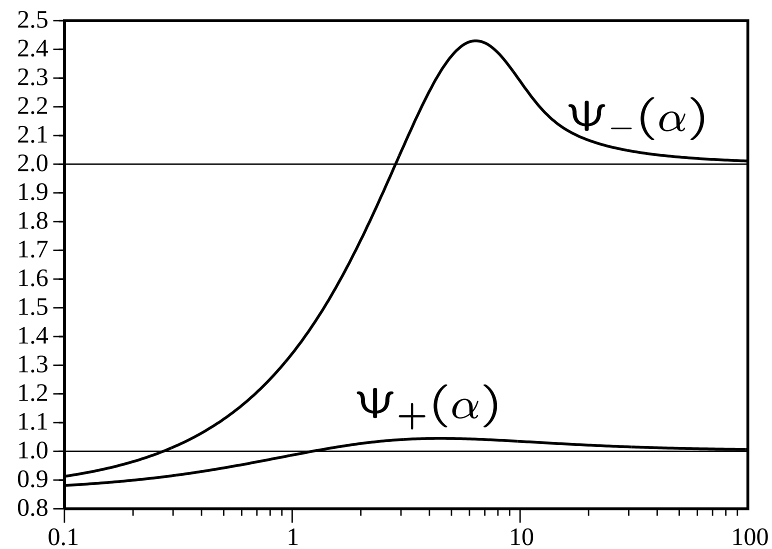
Theorem: Let $\nabla^2 V(z)$ have eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 \leqslant \dots \leqslant \lambda_N$, with $\lambda_1 < 0 < \lambda_3$. Then $\forall\, \lambda_2 \geqslant 0$,

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

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

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

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



Outlook

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

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References & ad

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