

Metastability

in a chain of coupled nonlinear diffusions

Nils Berglund

Centre de Physique Théorique - CNRS

Marseille Luminy

<http://berglund.univ-tln.fr>

Joint work with:

[Bastien Fernandez](#), CPT, Marseille

[Barbara Gentz](#), University of Bielefeld

Stochastic Analysis Seminar,

Warwick, 13 June 2007

Metastability in physics

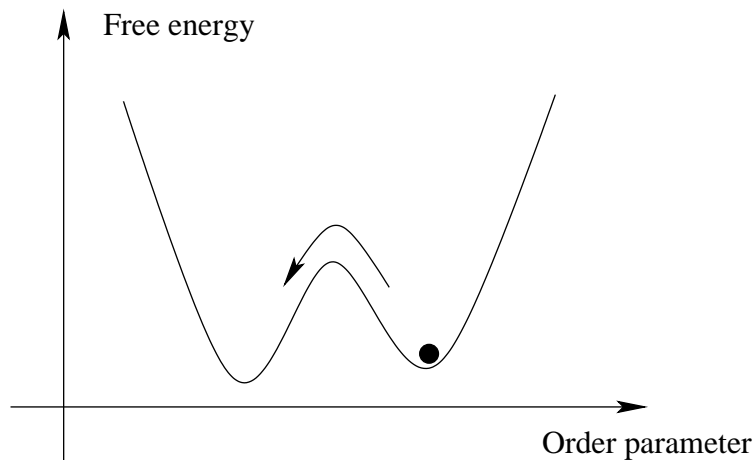
Examples:

- Supercooled liquid
- Supersaturated gas
- Wrongly magnetised ferromagnet

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

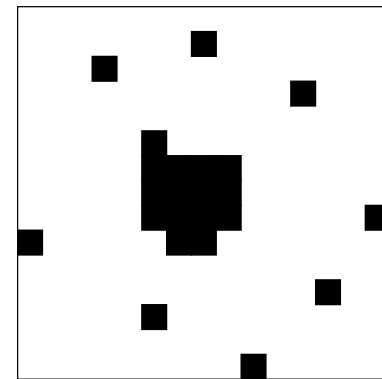
- ▷ Lattice: $\Lambda \subset \mathbb{Z}^d$
- ▷ Configuration space: $\mathcal{X} = S^\Lambda$, S finite set (e.g. $\{-1, 1\}$)
- ▷ Hamiltonian: $H : \mathcal{X} \rightarrow \mathbb{R}$ (e.g. Ising or lattice gas)
- ▷ Gibbs measure: $\mu_\beta(x) = e^{-\beta H(x)} / Z_\beta$
- ▷ Dynamics: Markov chain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

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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:

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

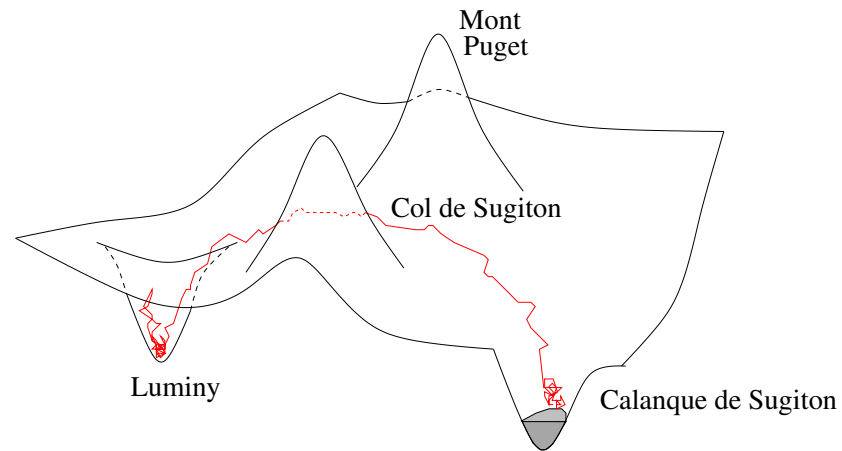
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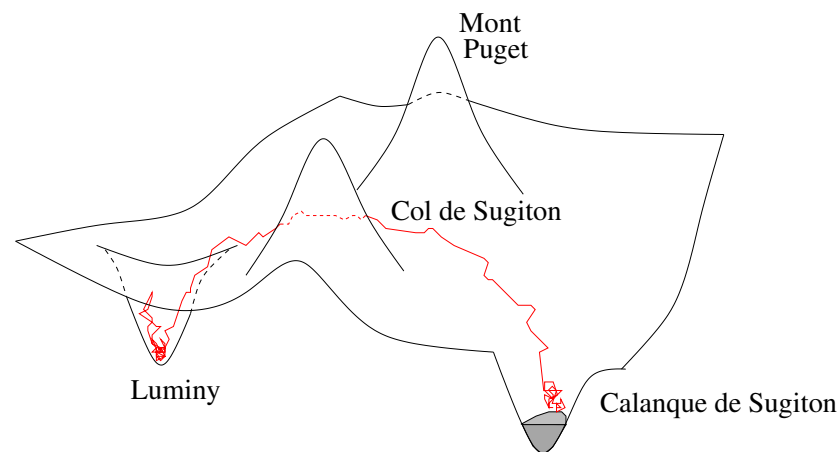
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τ : transition time between potential wells (first-hitting time)

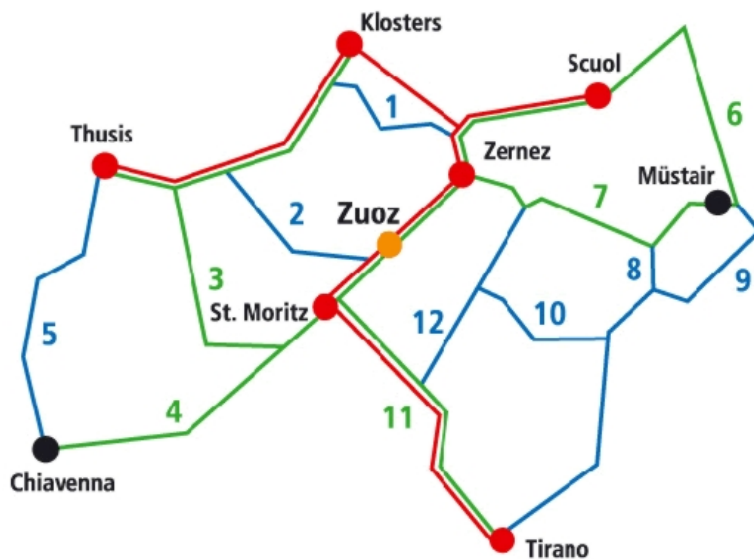
- Large deviations (Wentzell & Freidlin): $\lim_{\sigma \rightarrow 0} \sigma^2 \log(\mathbb{E}\{\tau\})$
- Analytic (Miclo, Mathieu, Kolokoltsov): spectrum of generator
- Variational (Bovier *et al*): spectrum and distribution of τ

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

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

Weak coupling

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

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Theorem: $\forall N, \exists \gamma^*(N) > 0$ s.t. points of each $S_k(\gamma)$ continuous in γ for $0 \leq \gamma < \gamma^*(N)$

$$\frac{1}{4} \leq \inf_{N \geq 2} \gamma^*(N) \leq \gamma^*(3) = \frac{1}{3}(\sqrt{3 + 2\sqrt{3}} - \sqrt{3}) = 0.2701\dots$$

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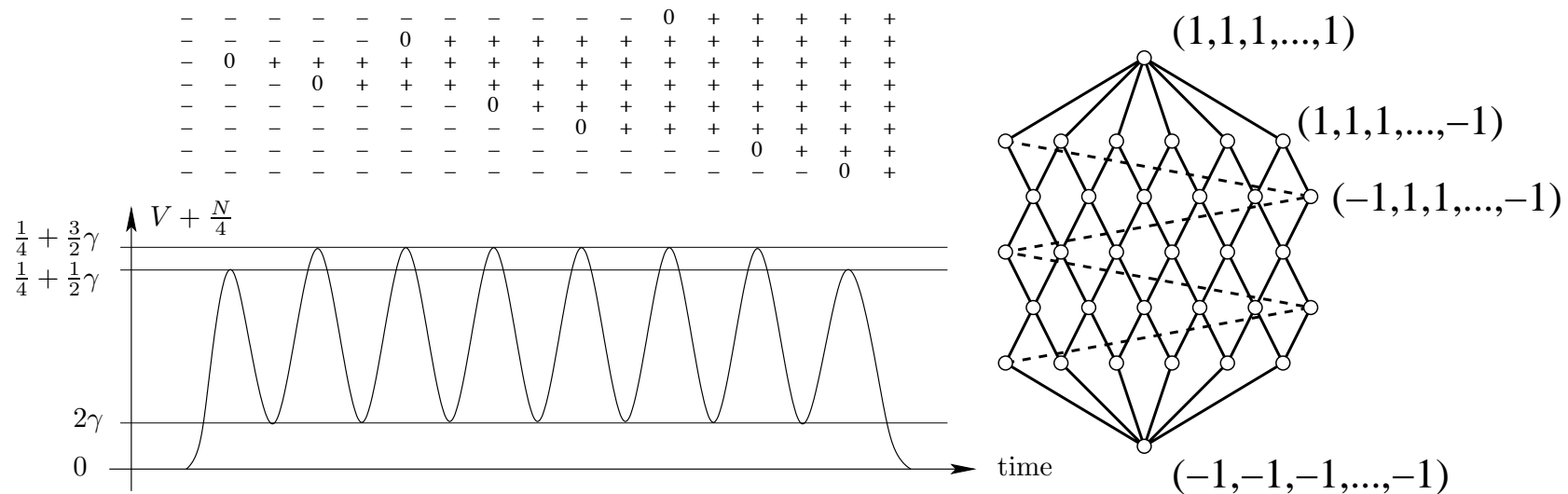
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▷ $0 < \gamma \ll 1$:

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



Strong coupling: Synchronisation

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

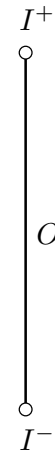
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Let $\gamma_1 = \frac{1}{1 - \cos(2\pi/N)} \left(= \frac{N^2}{2\pi^2} [1 - \mathcal{O}(N^{-2})] \right)$

Theorem:

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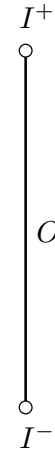
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Proof:

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

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

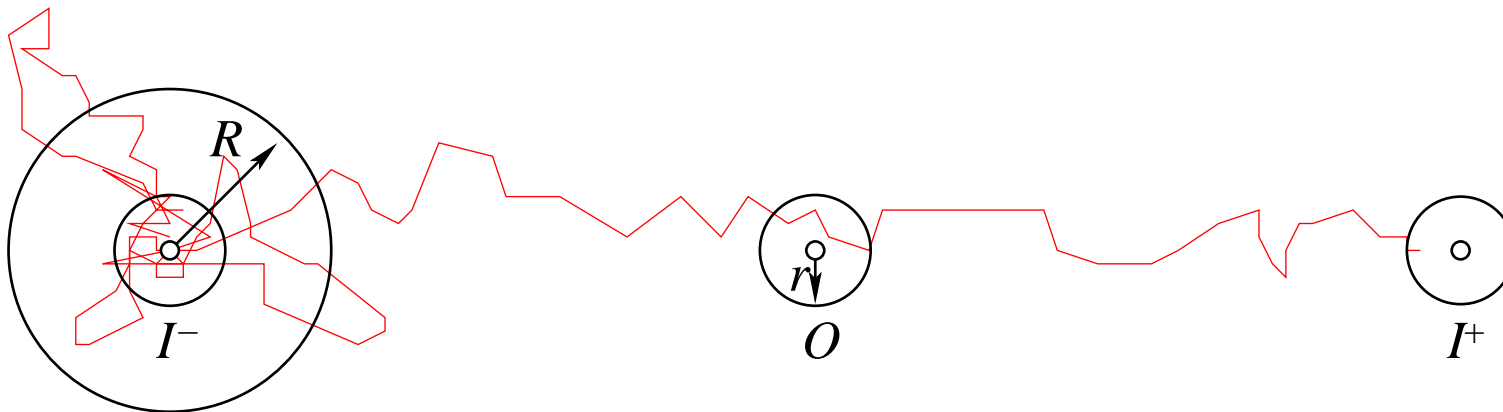
- Let $\tau_+ = \tau^{\text{hit}}(\mathcal{B}(I^+, r))$. Then $\forall \delta > 0$,

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

$$\lim_{\sigma \rightarrow 0} \sigma^2 \log \mathbb{E}^{x_0} \{ \tau_+ \} = \frac{1}{2}$$

- 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

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

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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 $H \triangleleft G$: $\text{Fix}(H) = \{x \in \mathcal{X} : hx = x \forall h \in H\}$

Properties:

$$|C_x| |O_x| = |G|$$

$$C_{gx} = gC_x g^{-1}$$

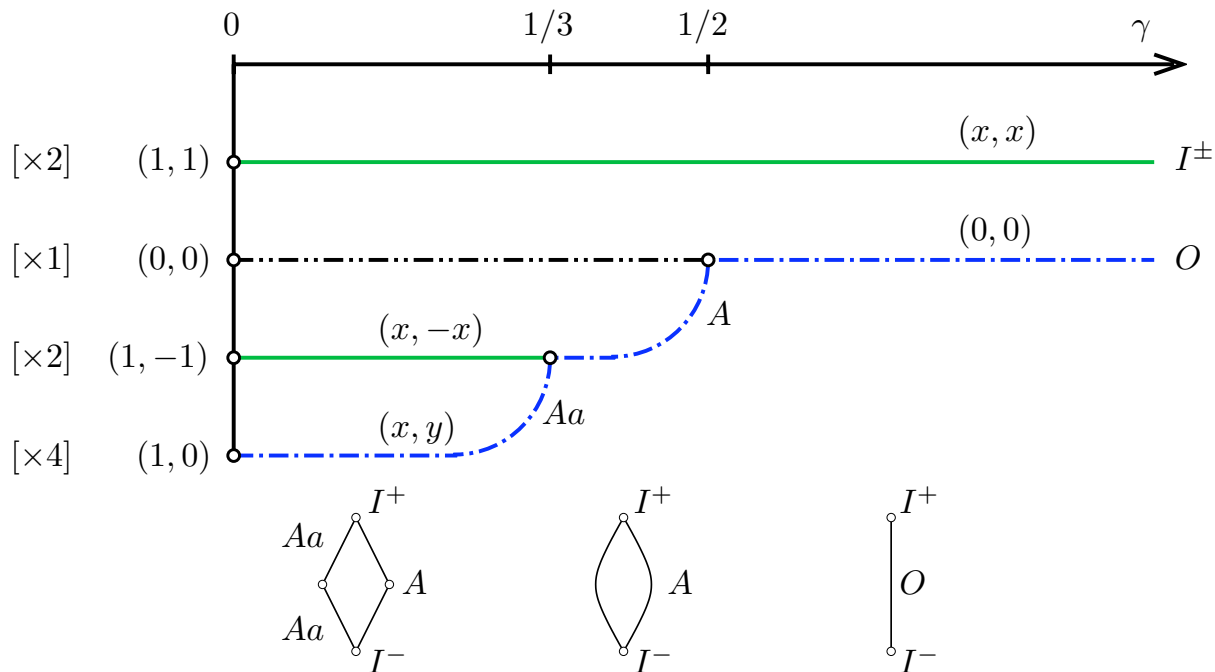
$$\text{Fix}(gHg^{-1}) = g \text{Fix}(H)$$

$$N = 2$$

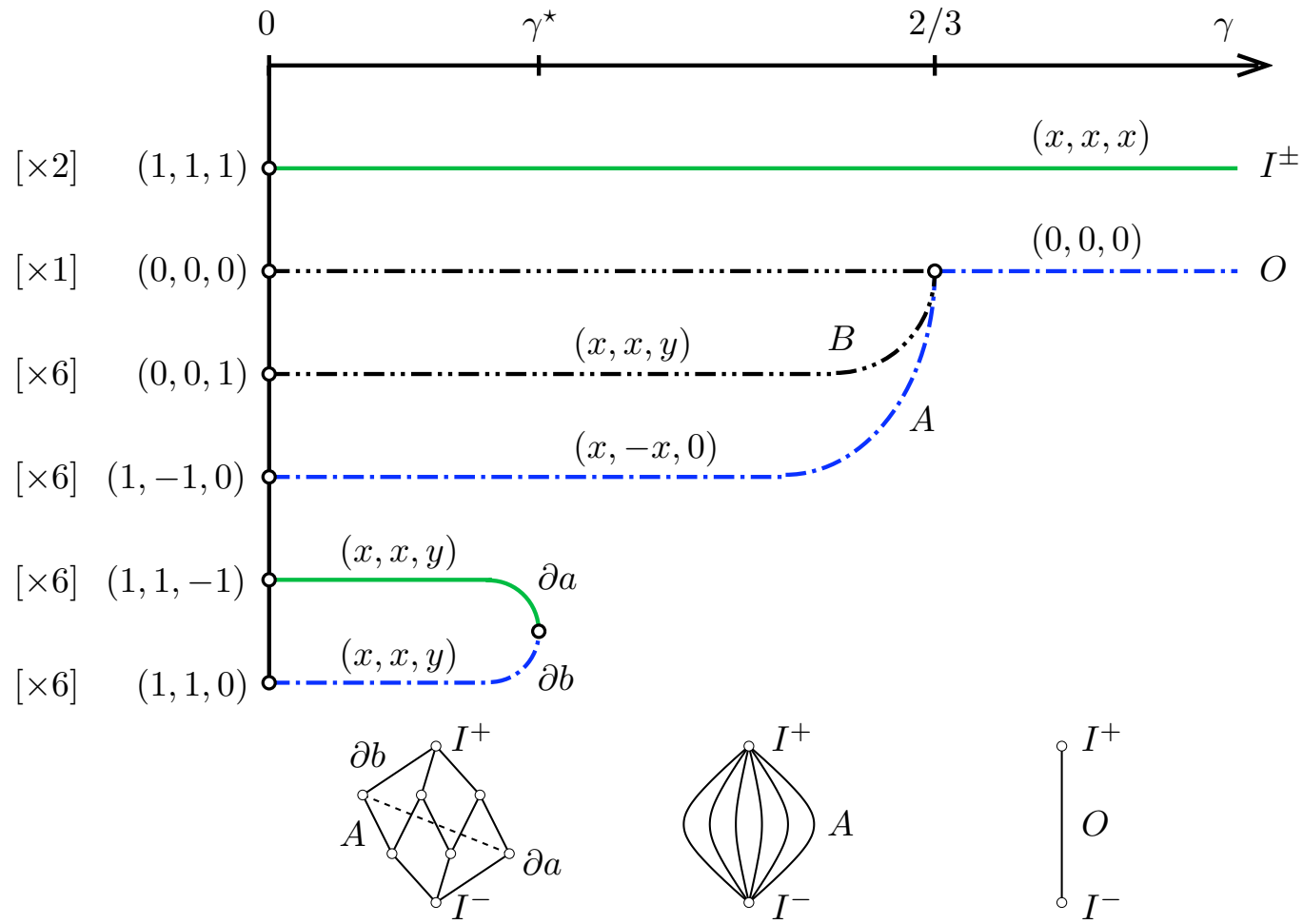
z^*	O_{z^*}	C_{z^*}	$\text{Fix}(C_{z^*})$
$(0, 0)$	$\{(0, 0)\}$	G	$\{(0, 0)\}$
$(1, 1)$	$\{(1, 1), (-1, -1)\}$	$D_2 = \{\text{id}, S\}$	$\{(x, x)\}_{x \in \mathbb{R}} = \mathcal{D}$
$(1, -1)$	$\{(1, -1), (-1, 1)\}$	$\{\text{id}, CS\}$	$\{(x, -x)\}_{x \in \mathbb{R}}$
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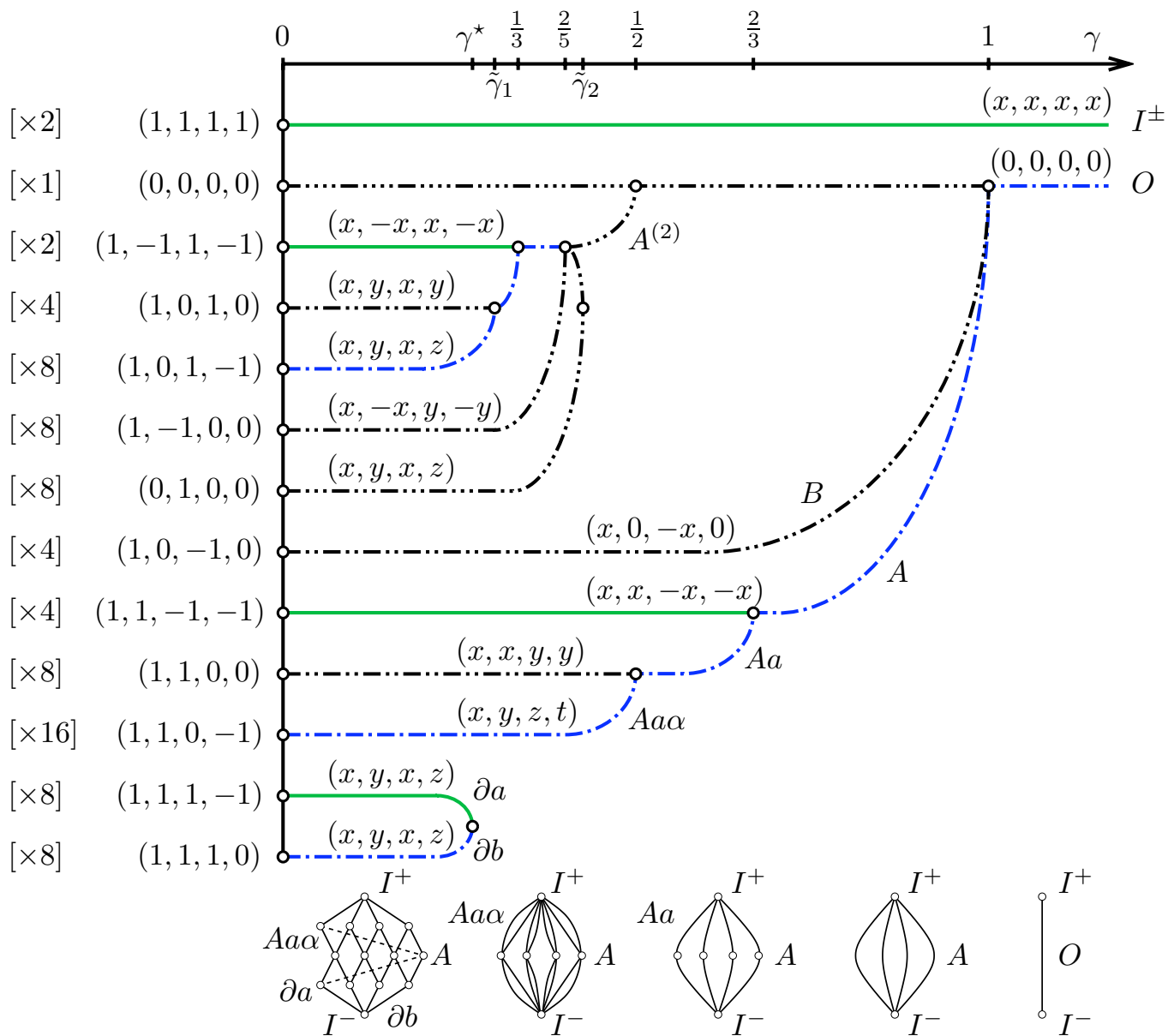
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$N = 3$



$$N = 4$$



Desynchronisation

Theorem: \forall even N , $\exists \delta(N) > 0$ 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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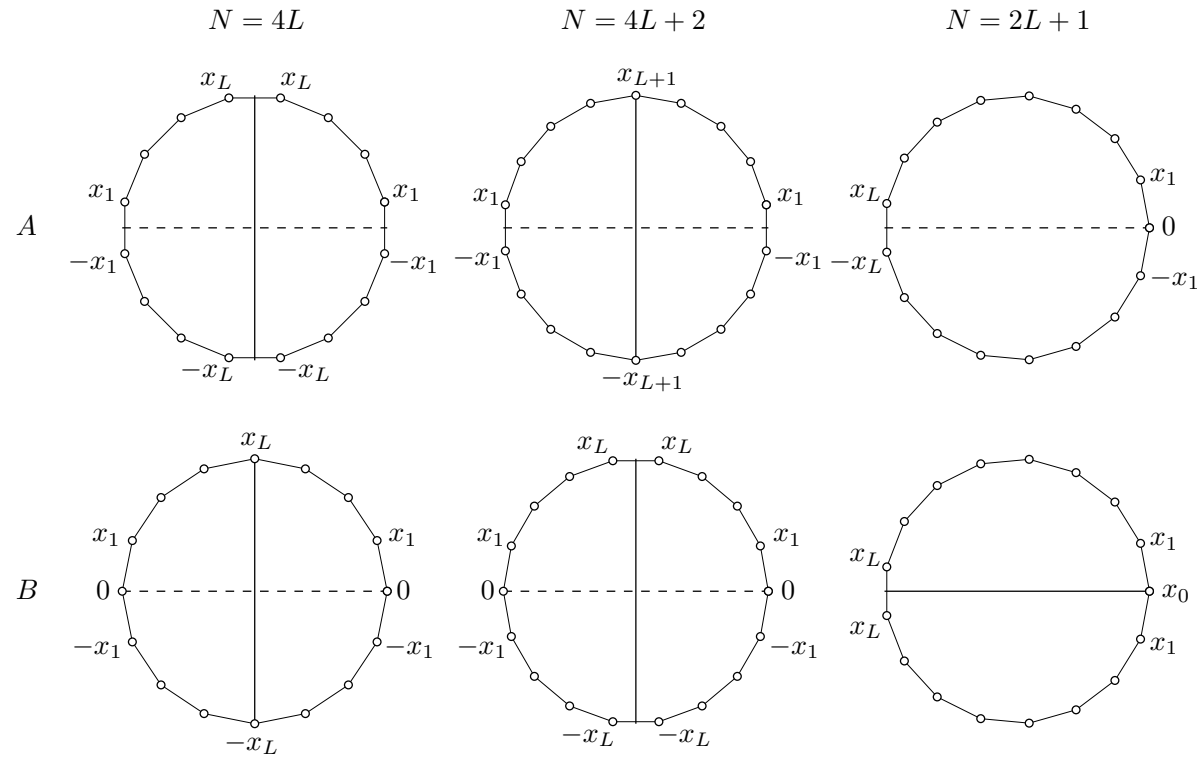
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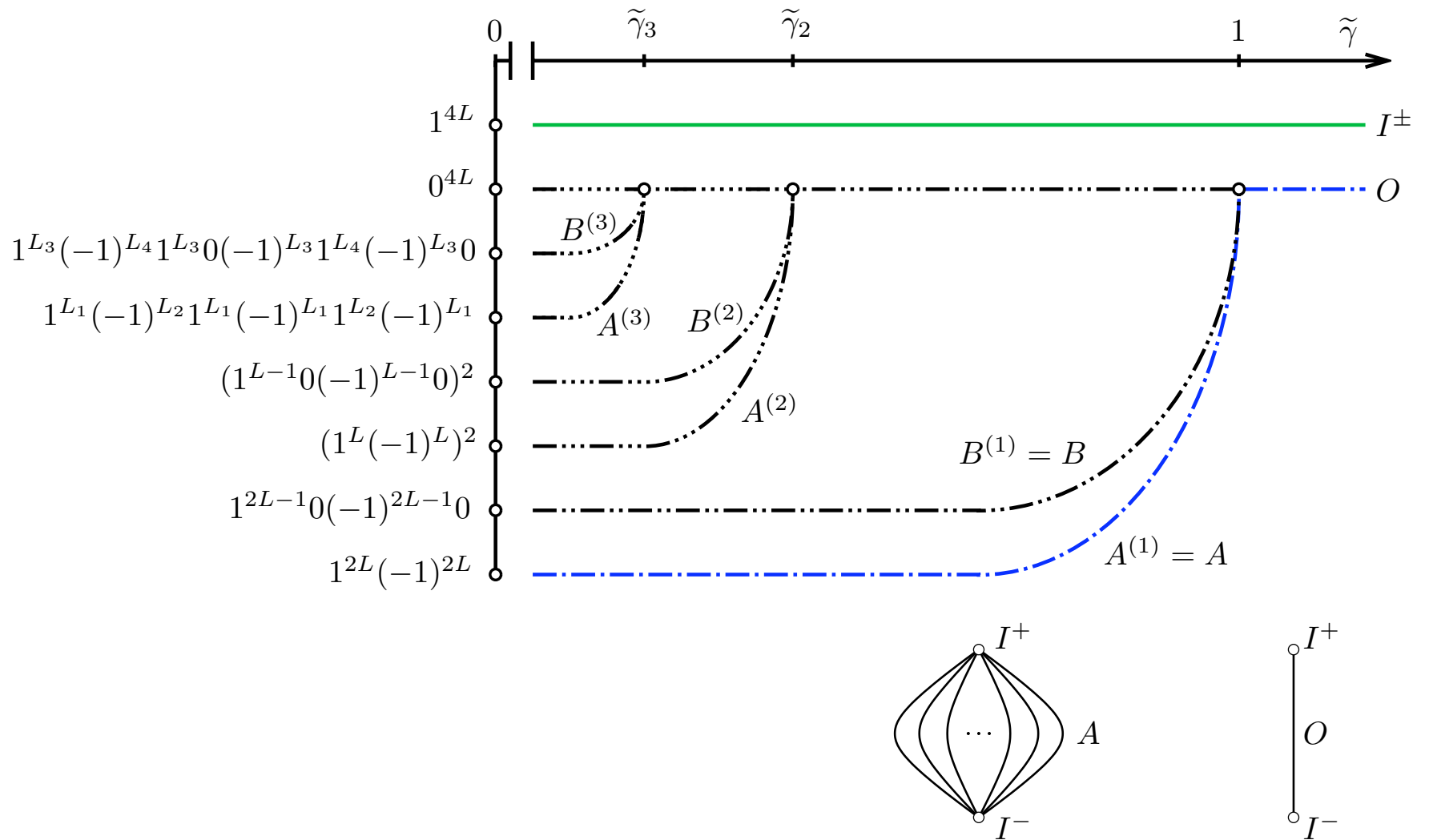
- ▷ N odd: similar result, $|\mathcal{S}| \geq 4N + 3$
- ▷ Similar corollary τ , with $\tau_0 \mapsto \tau_{UgA}$
- ▷ A and B have particular symmetries

Symmetries



N	x	$\text{Fix}(C_x)$
$4L$	A	$(x_1, \dots, x_L, x_L, \dots, x_1, -x_1, \dots, -x_L, -x_L, \dots, -x_1)$
	B	$(x_1, \dots, x_L, \dots, x_1, 0, -x_1, \dots, -x_L, \dots, -x_1, 0)$
$4L + 2$	A	$(x_1, \dots, x_{L+1}, \dots, x_1, -x_1, \dots, -x_{L+1}, \dots, -x_1)$
	B	$(x_1, \dots, x_L, x_L, \dots, x_1, 0, -x_1, \dots, -x_L, -x_L, \dots, -x_1, 0)$
$2L + 1$	A	$(x_1, \dots, x_L, -x_L, \dots, -x_1, 0)$
	B	$(x_1, \dots, x_L, x_L, \dots, x_1, x_0)$

Case N large: bifurcation diagram ($N=4L$)



Case 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

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

$$\mathcal{S}_{2m-1} = O_{A(m)}$$

$$m = 1, \dots, M$$

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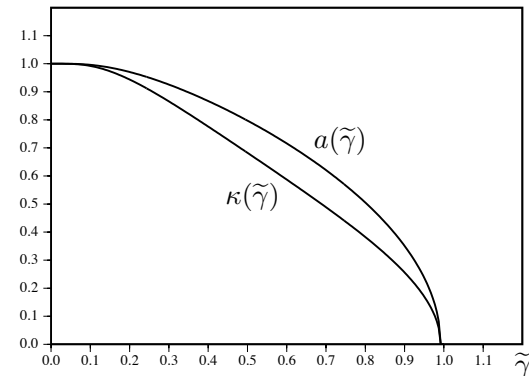
$$\mathcal{S}_{2M+1} = O_O = \{O\}$$

with $A_j^{(m)}(\tilde{\gamma}) = a(m^2\tilde{\gamma}) \operatorname{sn}\left(\frac{4K(\kappa(m^2\tilde{\gamma}))}{N}m\left(j - \frac{1}{2}\right), \kappa(m^2\tilde{\gamma})\right) + \mathcal{O}\left(\frac{M}{N}\right)$

and $\kappa(\tilde{\gamma})$, $a(\tilde{\gamma})$ implicitly defined by

$$\tilde{\gamma} = \frac{\pi^2}{4K(\kappa(\tilde{\gamma}))^2(1 + \kappa(\tilde{\gamma})^2)}$$

$$a(\tilde{\gamma})^2 = \frac{2\kappa(\tilde{\gamma})^2}{1 + \kappa(\tilde{\gamma})^2}$$



Case 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

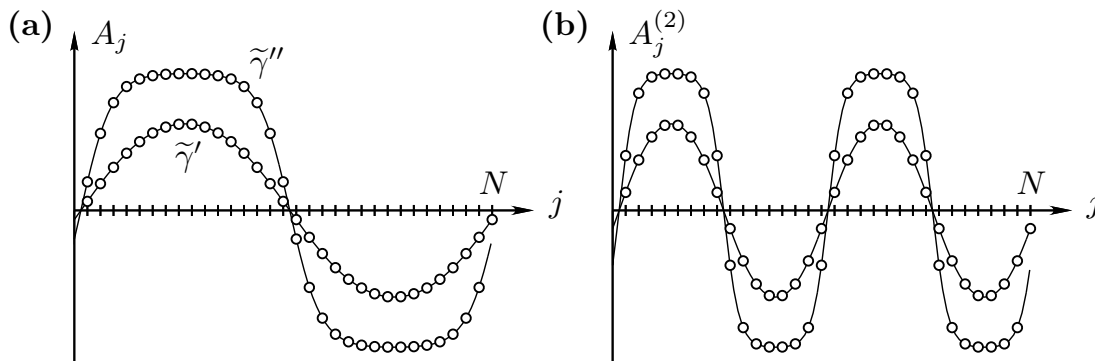
$$\mathcal{S}_0 = O_{I^+} = \{I^+, I^-\}$$

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

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

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

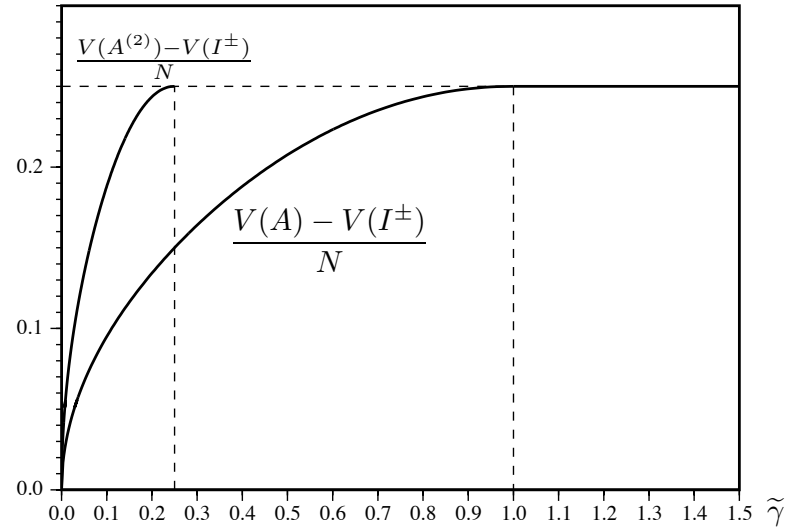
with $A_j^{(m)}(\tilde{\gamma}) = a(m^2\tilde{\gamma}) \operatorname{sn}\left(\frac{4K(\kappa(m^2\tilde{\gamma}))}{N}m\left(j - \frac{1}{2}\right), \kappa(m^2\tilde{\gamma})\right) + \mathcal{O}\left(\frac{M}{N}\right)$



Potential difference:

$$\begin{aligned}
 H(\tilde{\gamma}) &= \frac{V(A) - V(I^\pm)}{N} \\
 &= \frac{1}{4} - \frac{1}{3(1+\kappa^2)} \left[\frac{2+\kappa^2}{1+\kappa^2} - 2 \frac{E(\kappa)}{K(\kappa)} \right] \\
 &\quad + \mathcal{O}\left(\frac{\kappa^2}{N}\right)
 \end{aligned}$$

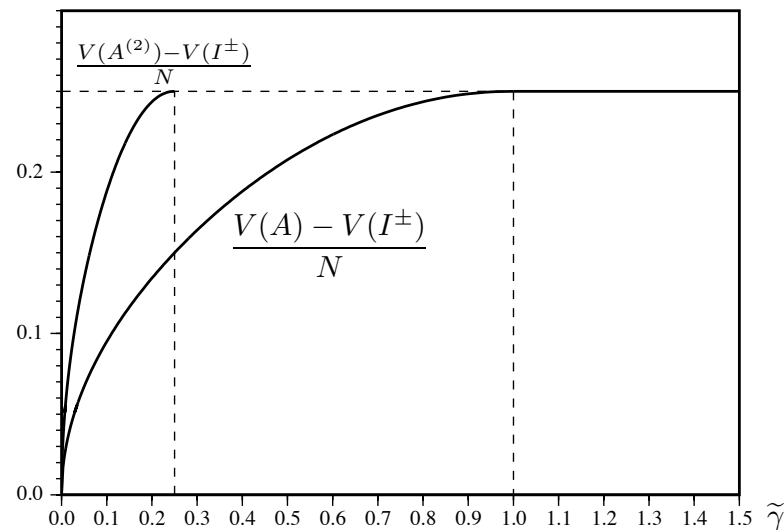
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Corollary: $\forall 0 < \tilde{\gamma} \leq 1$, $\exists N_0(\tilde{\gamma})$ s.t. $\forall N \geq N_0(\tilde{\gamma})$,
 $\forall 0 < r < R \leq \frac{1}{2}$, $\forall x_0 \in \mathcal{B}(I^-, r)$:

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

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

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

- 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

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

Ideas of the proof

$$\begin{aligned}x \in \mathcal{S} &\Leftrightarrow f(x_n) + \frac{\gamma}{2} [x_{n+1} - 2x_n + x_{n-1}] = 0 \\&\Leftrightarrow \begin{cases} x_{n+1} = x_n + \varepsilon w_n - \frac{1}{2} \varepsilon^2 f(x_n) \\ w_{n+1} = w_n - \frac{1}{2} \varepsilon [f(x_n) + f(x_{n+1})] \end{cases} \\ \varepsilon &= \sqrt{\frac{2}{\gamma}} \simeq \frac{2\pi}{N\sqrt{\tilde{\gamma}}} \ll 1\end{aligned}$$

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- ▷ Area-preserving map
- ▷ Discretisation of $\ddot{x} = -f(x)$
- ▷ Almost conserved quantity: $C(x, w) = \frac{1}{2}(x^2 + w^2) - \frac{1}{4}x^4$
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In action-angle variables (I, ψ) :

$$\begin{cases} \psi_{n+1} = \psi_n + \varepsilon \Omega(I_n) + \varepsilon^3 f(\psi_n, I_n, \varepsilon) & (\text{mod } 2\pi) \\ I_{n+1} = I_n + \varepsilon^3 g(\psi_n, I_n, \varepsilon) \end{cases}$$

$I = h(C)$, and $(\psi, C) \mapsto (x, w)$ involves elliptic functions.

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$$\begin{cases} \psi_n = \psi_0 + n\varepsilon\Omega(I_0) \\ I_n = I_0 \end{cases} \quad (\text{mod } 2\pi)$$

Orbit of period N if $N\varepsilon\Omega(I_0) = 2\pi M$, $M \in \{1, 2, \dots\}$.

$\nu = M/N$: **rotation number**, $j \mapsto x_j$ has $2M$ sign changes.

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▷ $\varepsilon > 0$: **Poincaré–Birkhoff theorem**: \exists at least two periodic orbits for each ν with $2\pi\nu/\varepsilon$ in range of Ω .

Problem: Show that there are only two orbits for each ν .

Ideas of the proof

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Generating function: $(\psi_n, \psi_{n+1}) \mapsto G(\psi_n, \psi_{n+1})$ such that

$$\partial_1 G(\psi_n, \psi_{n+1}) = -I_n \quad \partial_2 G(\psi_n, \psi_{n+1}) = I_{n+1}$$

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Property: Orbits of period N are stationary points of

$$G_N(\psi_1, \dots, \psi_N) = G(\psi_1, \psi_2) + G(\psi_2, \psi_3) + \dots + G(\psi_N, \psi_1 + 2\pi N\nu)$$

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In our case,

$$G(\psi_1, \psi_2) = \varepsilon G_0\left(\frac{\psi_2 - \psi_1}{\varepsilon}, \varepsilon\right) + 2\varepsilon^3 \sum_{p=1}^{\infty} \hat{G}_p\left(\frac{\psi_2 - \psi_1}{\varepsilon}, \varepsilon\right) \cos(p(\psi_1 + \psi_2))$$

- ▷ N particles “connected by springs” in a periodic ext. potential.
- ▷ Stationary pts can be analysed by Fourier transf. for (ψ_1, \dots, ψ_n) .

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