

# Metastability

in a system of interacting nonlinear diffusions

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Seminar über Stochastische Prozesse, Zürich, November 2006

## Metastability in physics

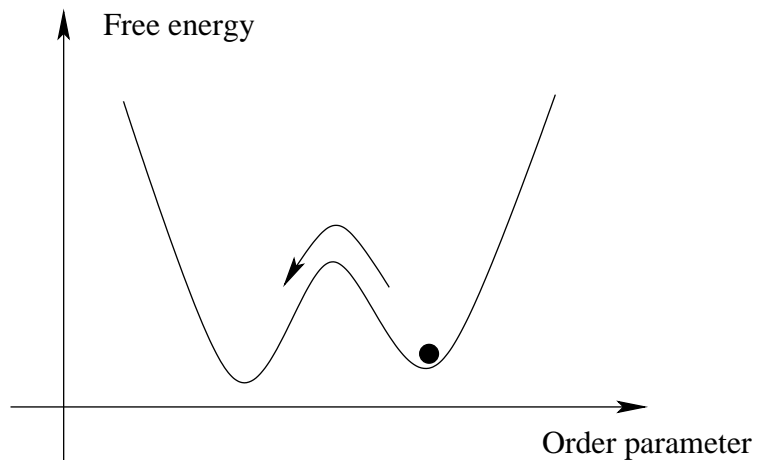
Examples:

- 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

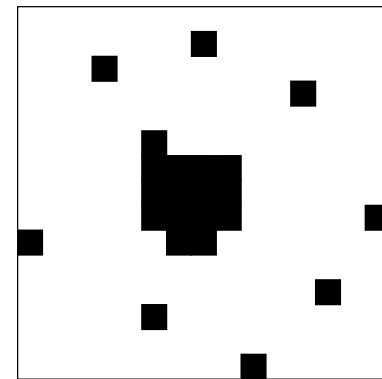
- ▷ Lattice:  $\Lambda \subset \mathbb{Z}^d$
- ▷ Configuration space:  $\mathcal{X} = S^\Lambda$ ,  $S$  finite set (e.g.  $\{-1, 1\}$ )
- ▷ Hamiltonian:  $H : \mathcal{X} \rightarrow \mathbb{R}$  (e.g. Ising or lattice gas)
- ▷ Gibbs measure:  $\mu_\beta(x) = e^{-\beta H(x)} / Z_\beta$
- ▷ Dynamics: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

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

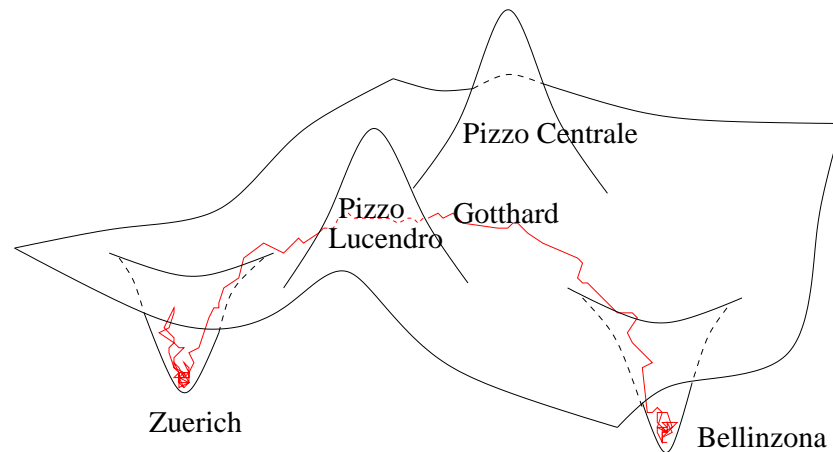
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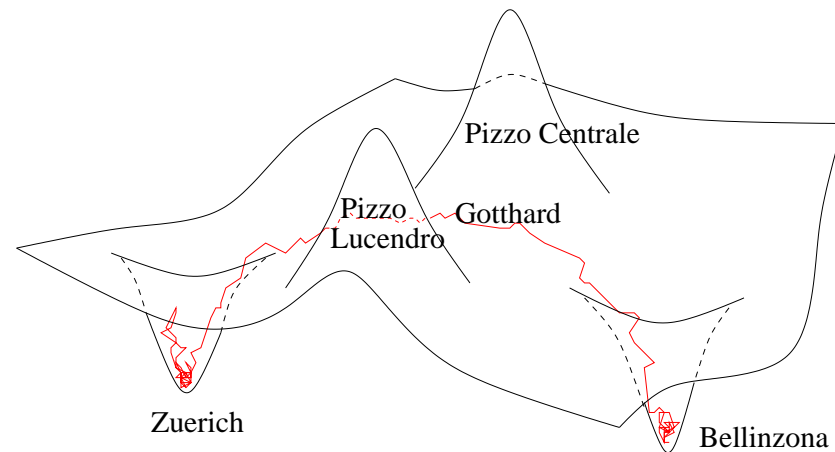
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$\tau$ : transition time between potential wells (first-hitting time)

- 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  $\tau$

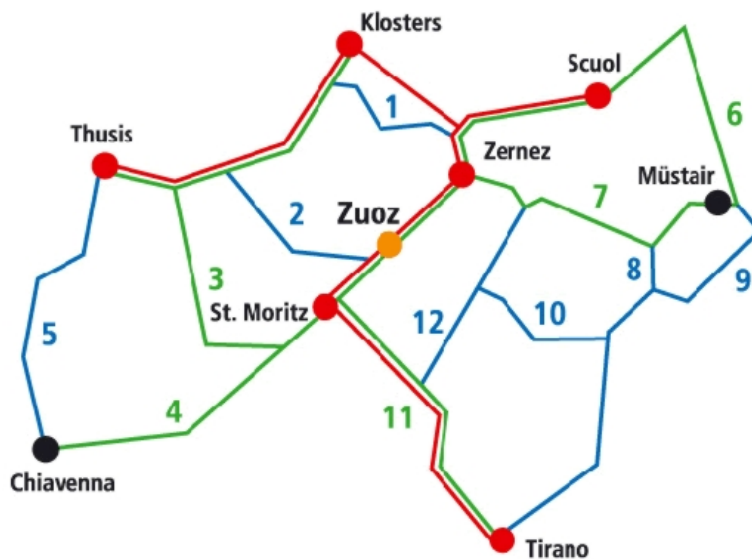


## Metastability in reversible diffusions

- ▷ 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  $\gamma$  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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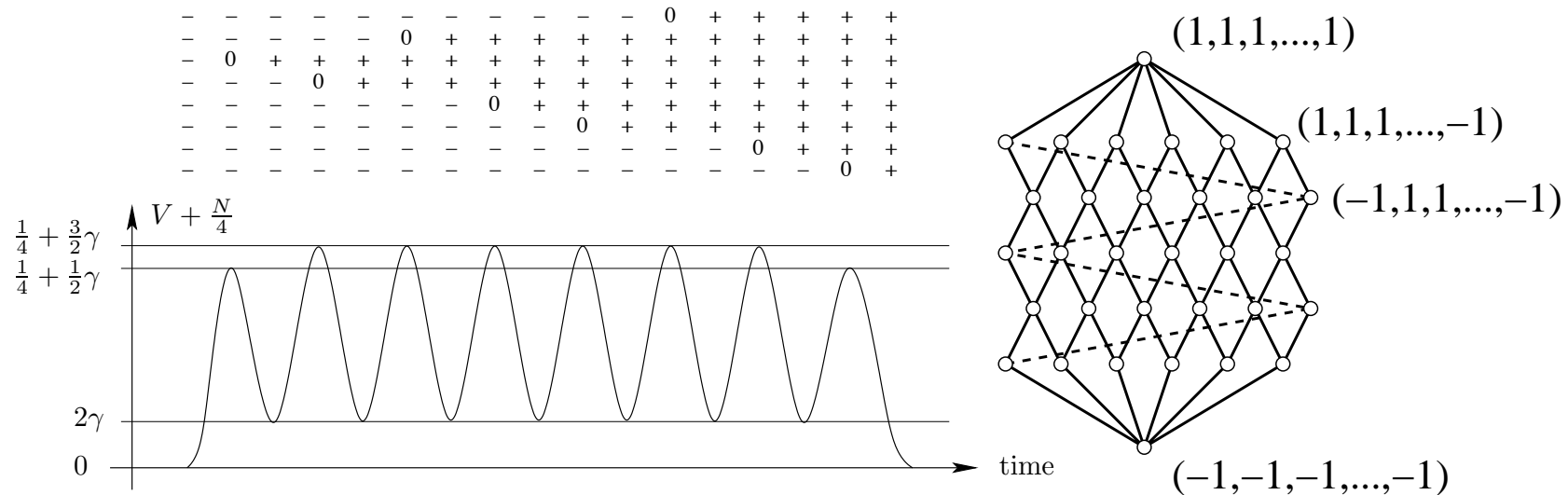
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▷  $0 < \gamma \ll 1$ :

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



## Strong coupling: Synchronisation

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

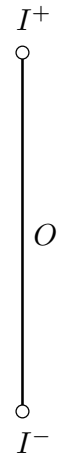
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**Theorem:**

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



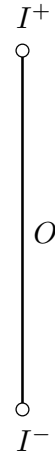
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**Proof:**

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

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

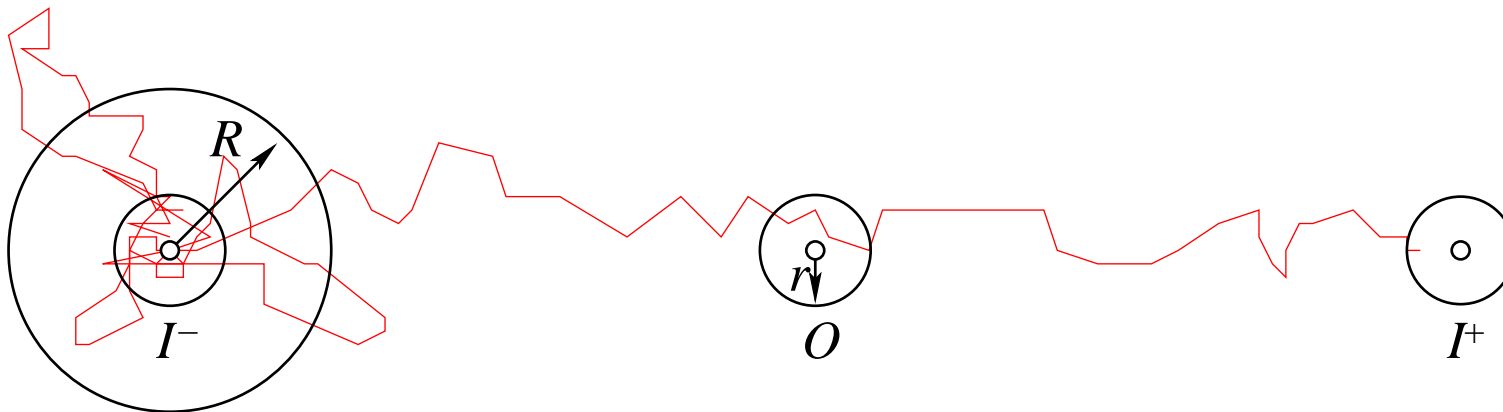
- Let  $\tau_+ = \tau^{\text{hit}}(\mathcal{B}(I^+, r))$ . Then  $\forall \delta > 0$ ,

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

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

- 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  $V_\gamma$  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:

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

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

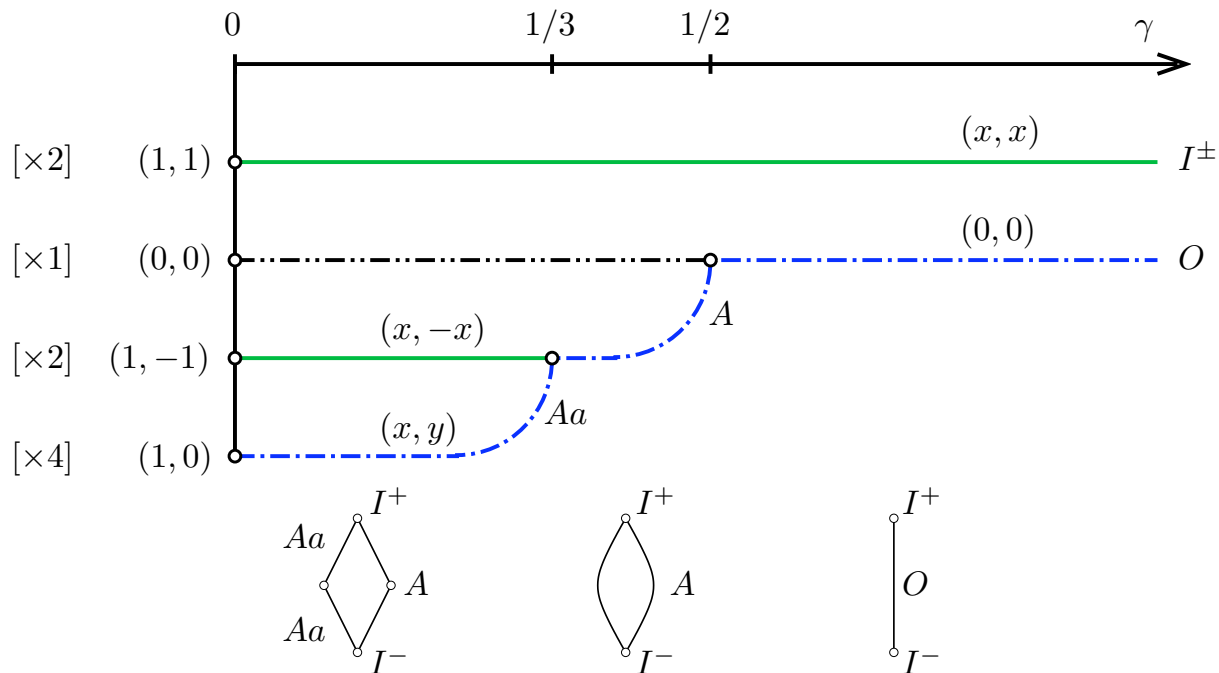
$$\text{Fix}(gHg^{-1}) = g \text{Fix}(H)$$

$N = 2$

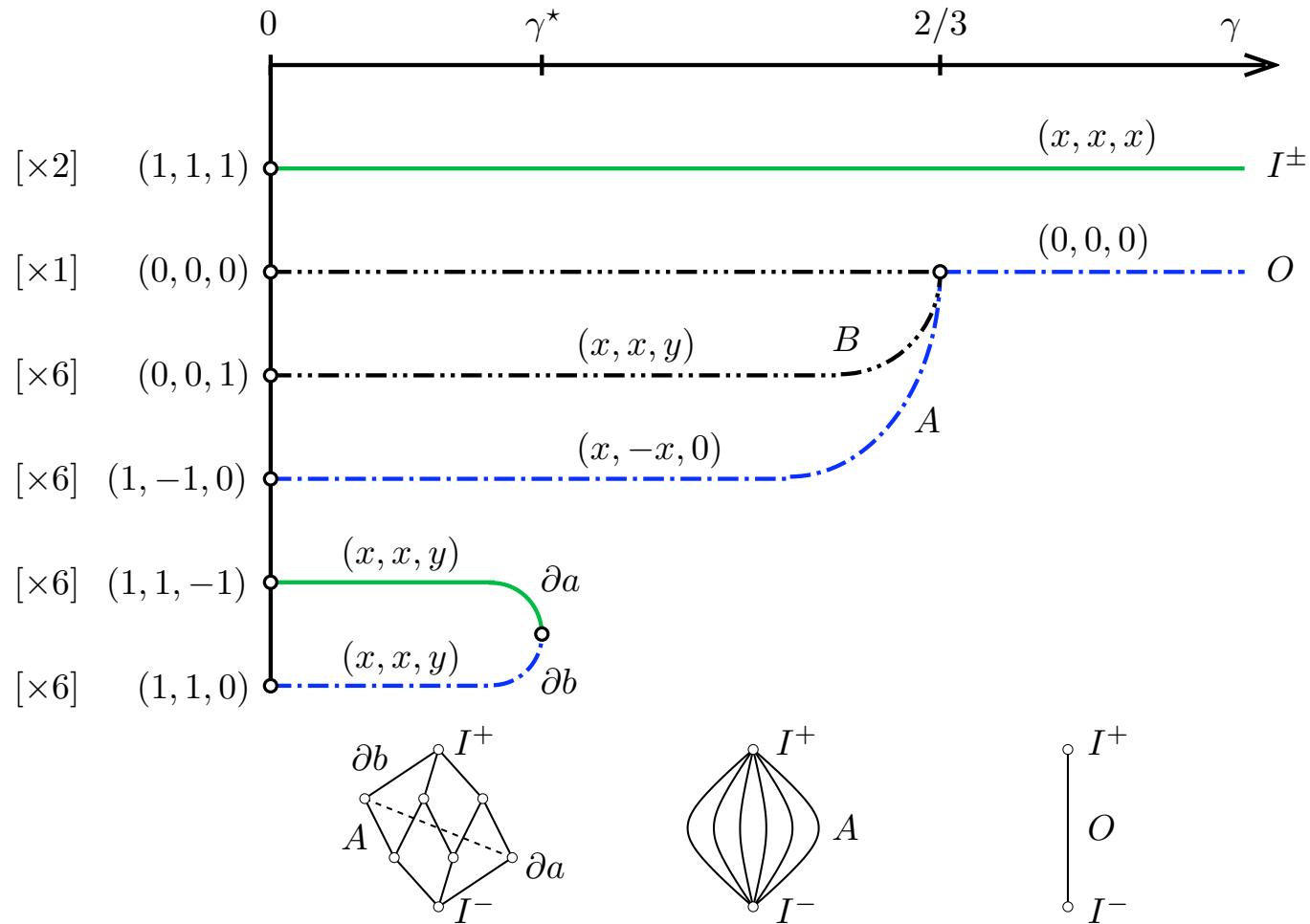
$z^*$	$O_{z^*}$	$C_{z^*}$	$\text{Fix}(C_{z^*})$
$(0, 0)$	$\{(0, 0)\}$	$G$	$\{(0, 0)\}$
$(1, 1)$	$\{(1, 1), (-1, -1)\}$	$D_2 = \{\text{id}, S\}$	$\{(x, x)\}_{x \in \mathbb{R}} = \mathcal{D}$
$(1, -1)$	$\{(1, -1), (-1, 1)\}$	$\{\text{id}, CS\}$	$\{(x, -x)\}_{x \in \mathbb{R}}$
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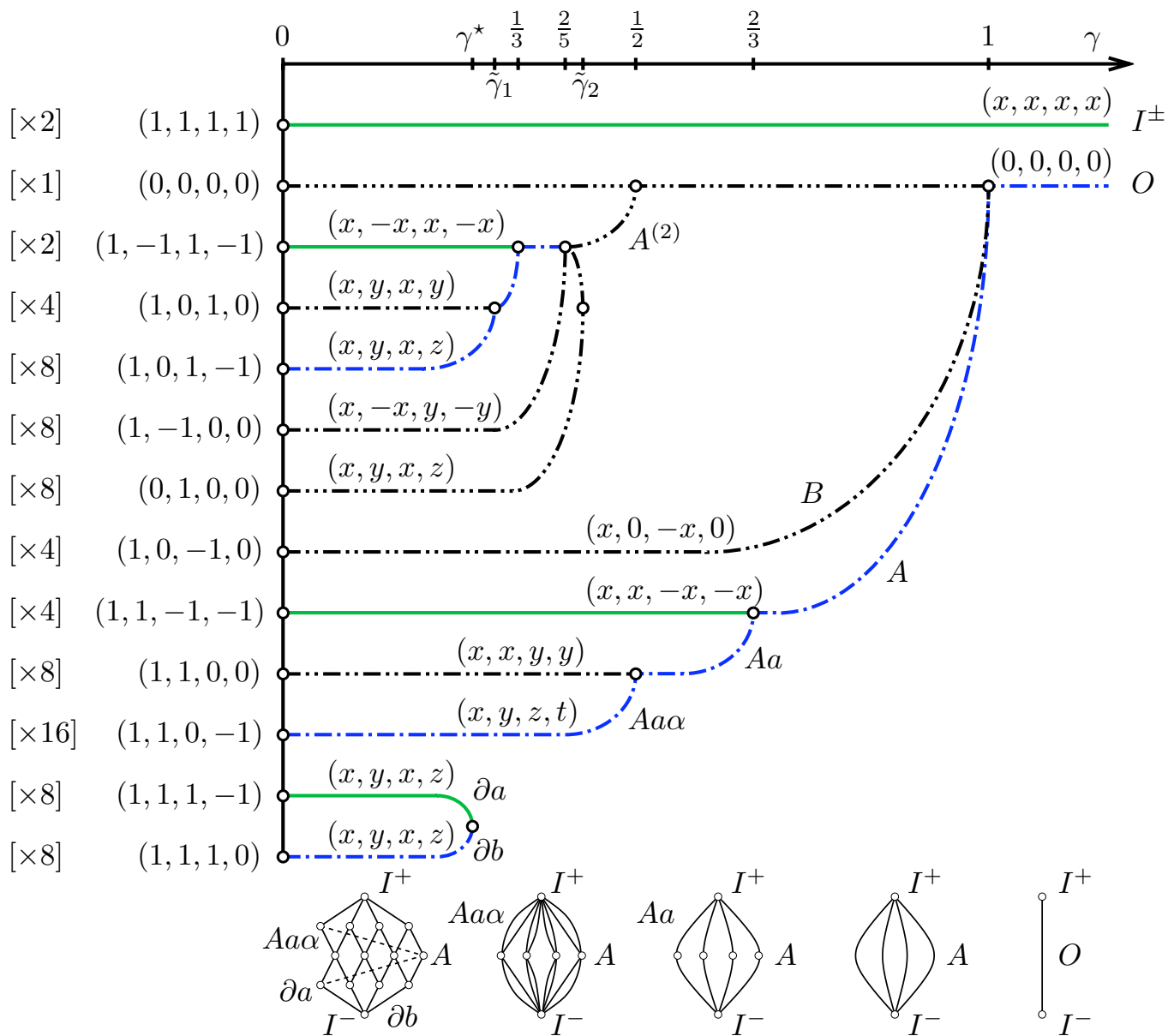
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$N = 3$



$$N = 4$$



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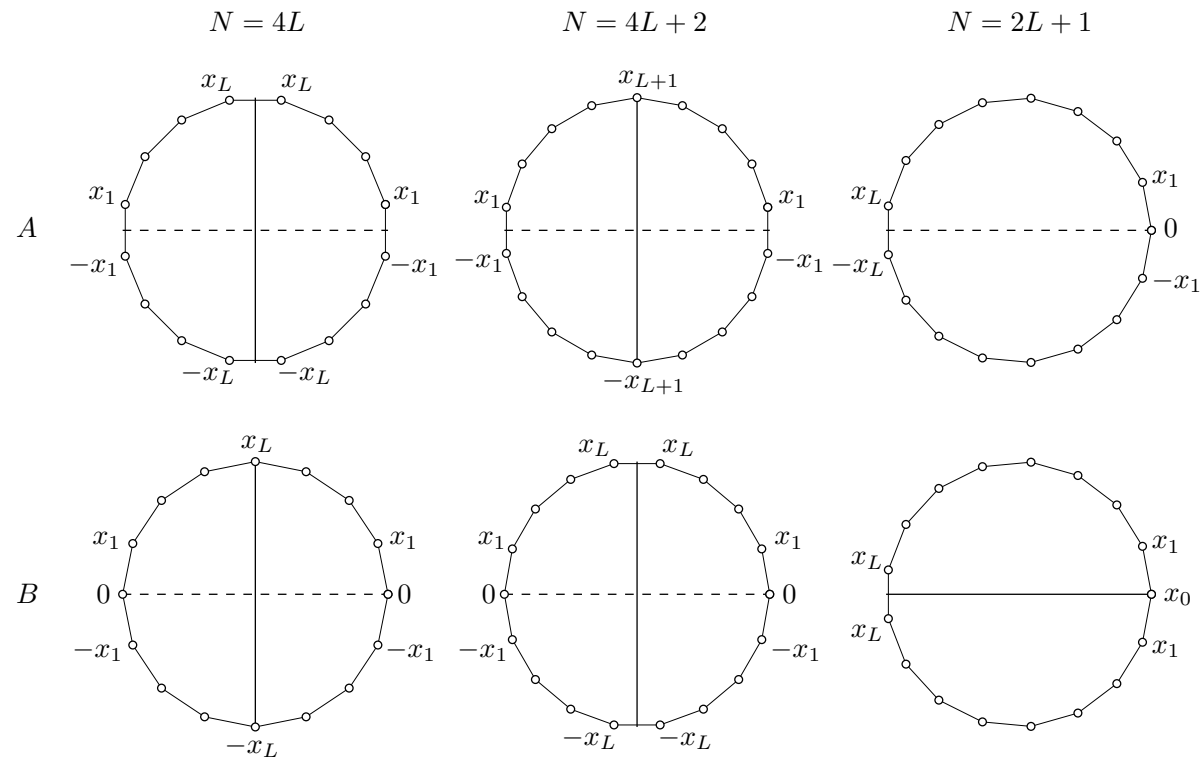
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- ▷  $N$  odd: similar result,  $|\mathcal{S}| \geq 4N + 3$
- ▷ Similar corollary  $\tau$ , with  $\tau_0 \mapsto \tau_{UgA}$
- ▷  $A$  and  $B$  have particular symmetries



# 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

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

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

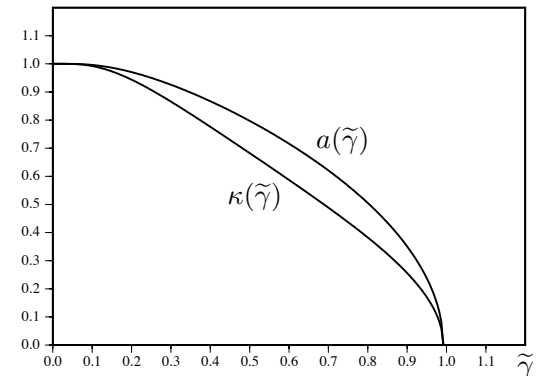
**Theorem:**  $\forall M \geq 1, \exists N_M < \infty$  s.t. for  $N \geq N_M$  and  $\tilde{\gamma}_{M+1} < \tilde{\gamma} < \tilde{\gamma}_M$ ,  $\mathcal{S}$  can be decomposed as

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

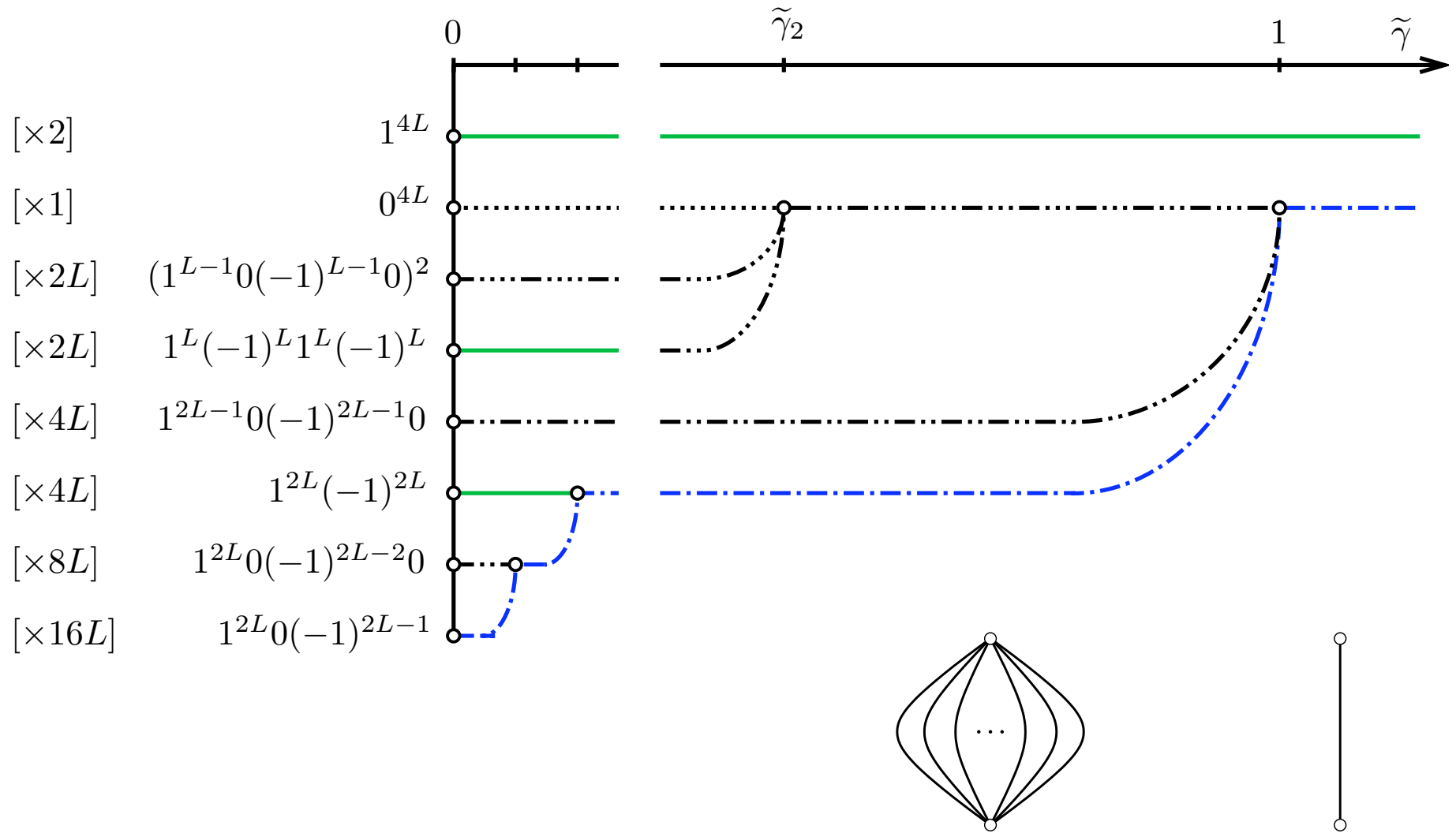
with  $A_j^{(m)}(\tilde{\gamma}) = a(m^2\tilde{\gamma}) \operatorname{sn}\left(\frac{4K(\kappa(m^2\tilde{\gamma}))}{N}m\left(j - \frac{1}{2}\right), \kappa(m^2\tilde{\gamma})\right) + \mathcal{O}\left(\frac{M}{N}\right)$

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

$$\begin{aligned} \tilde{\gamma} &= \frac{\pi^2}{4K(\kappa(\tilde{\gamma}))^2(1+\kappa(\tilde{\gamma})^2)} \\ a(\tilde{\gamma})^2 &= \frac{2\kappa(\tilde{\gamma})^2}{1+\kappa(\tilde{\gamma})^2} \end{aligned}$$



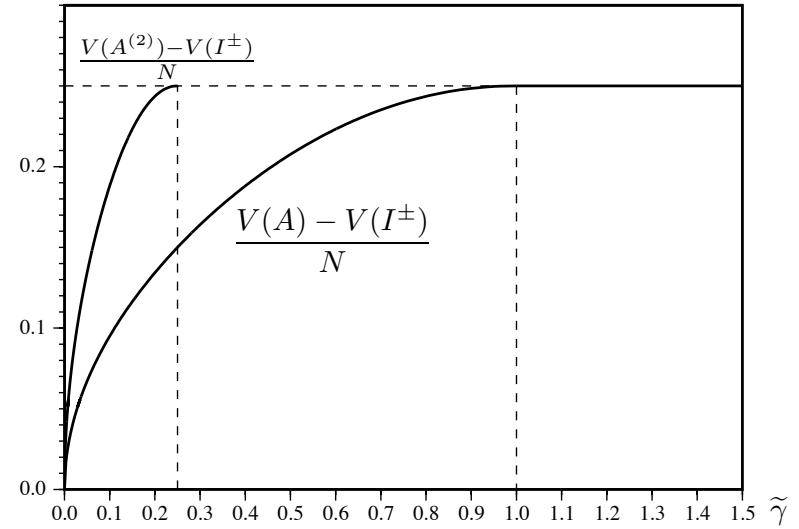
# Case $N$ large: bifurcation diagram ( $N=4L$ )



Potential difference:

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

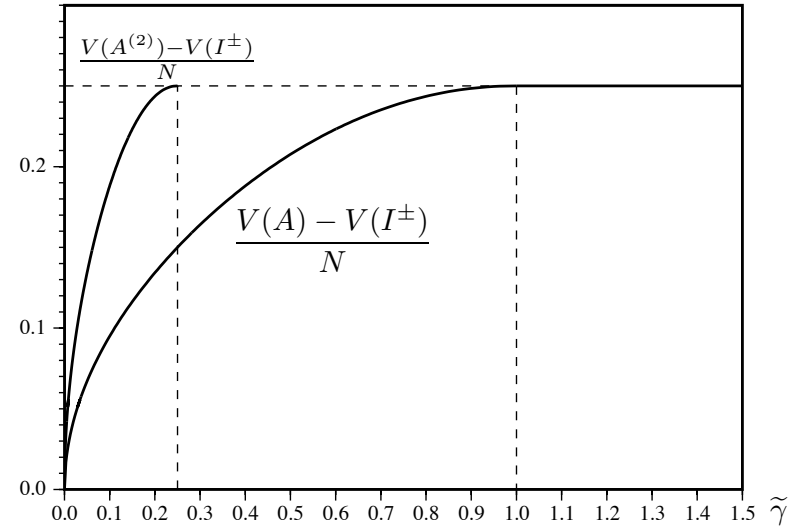
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**Corollary:**  $\forall 0 < \tilde{\gamma} \leq 1$ ,  $\exists N_0(\tilde{\gamma})$  s.t.  $\forall N \geq N_0(\tilde{\gamma})$ ,  
 $\forall 0 < r < R \leq \frac{1}{2}$ ,  $\forall x_0 \in \mathcal{B}(I^-, r)$ :

- 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  $(I, \psi)$ :

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

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



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

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

**Problem**: Show that there are only two orbits for each  $\nu$ .

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

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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  $(\psi_1, \dots, \psi_n)$ .