Metastability

in a system of interacting nonlinear diffusions

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Metastability in physics

Examples:

- Supercooled liquid
- Supersaturated gas
- Wrongly magnetised ferromagnet

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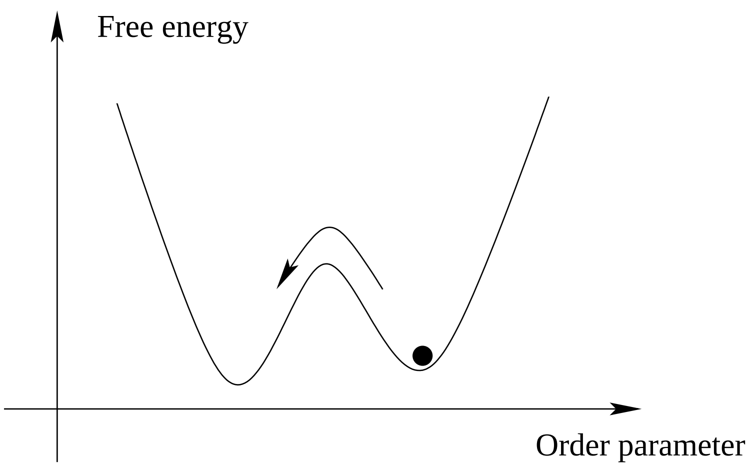
▷ Near first-order phase transition
▷ Nucleation implies crossing energy barrier



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)

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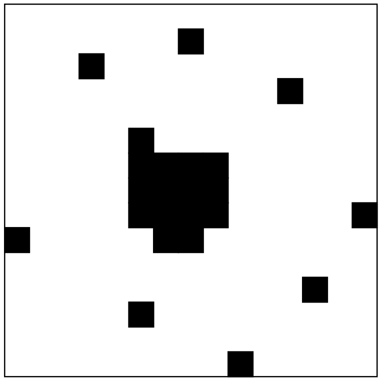
Results (for $\beta \gg 1$) on

- 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

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

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

Invariant measure:

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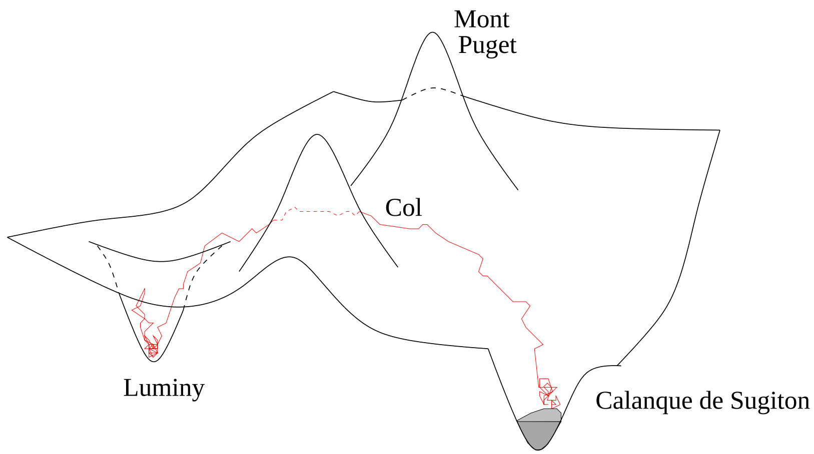

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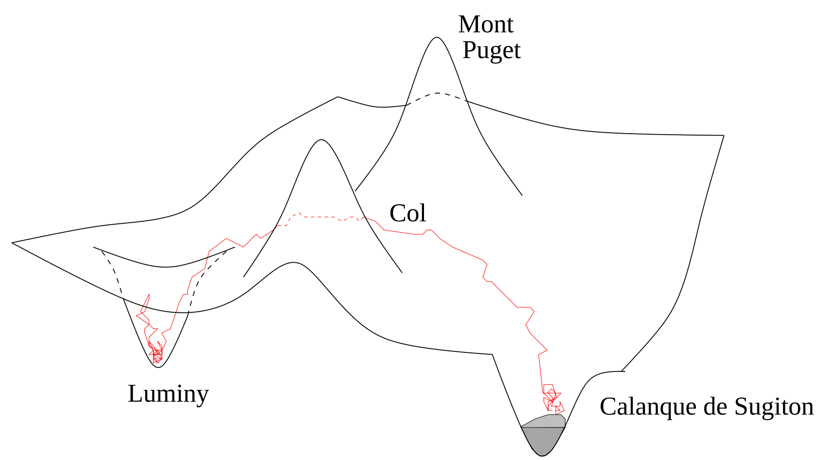

τ: transition time between potential wells (first-hitting time)

- Large deviations (Wentzell & Freidlin): $\lim_{\sigma\to0} \sigma^2 \log(\mathbb{E}\{\tau\})$
- Analytic (Miclo, Mathieu, Kolokoltsov): spectrum of generator
- Variational (Bovier *el al*): spectrum and distribution of τ

Metastability in reversible diffusions

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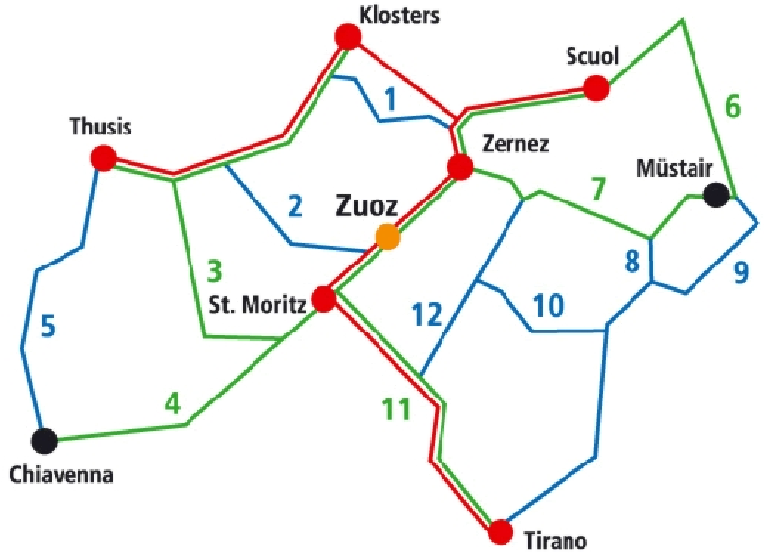

Rot	Rhätische Bahn
Grün	ganzjährig offen
Blau	Wintersperre

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 $U(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$

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

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

Weak coupling

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

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Theorem: $\forall N$, $\exists \gamma^\star(N) > 0$ s.t. points of each $S_k(\gamma)$ continuous in γ for $0 \leqslant \gamma < \gamma^\star(N)$
$\frac{1}{4} \leqslant \inf_{N \geqslant 2} \gamma^\star(N) \leqslant \gamma^\star(3) = \frac{1}{3}\Big(\sqrt{3 + 2\sqrt{3}} - \sqrt{3}\Big) = 0.2701\ldots$

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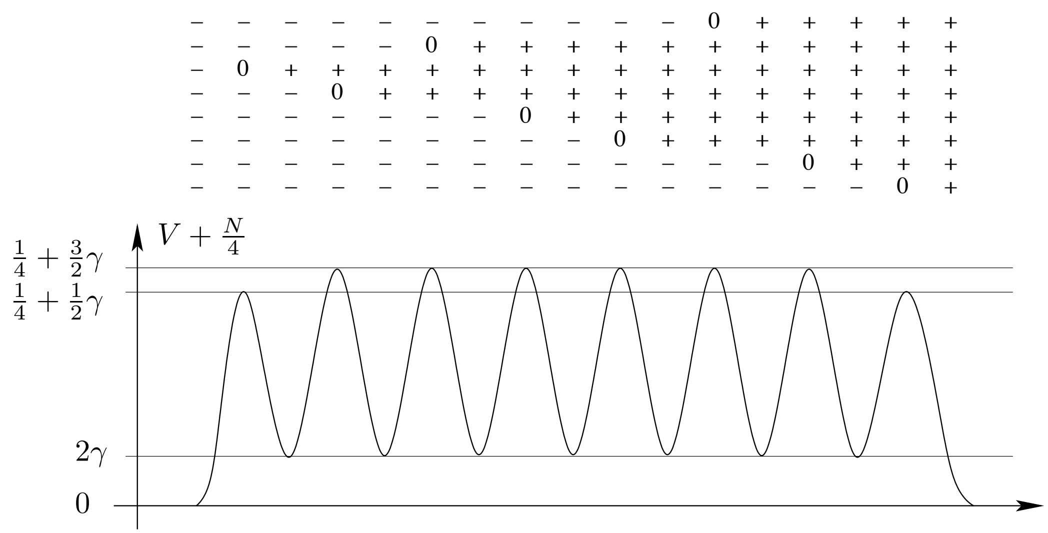
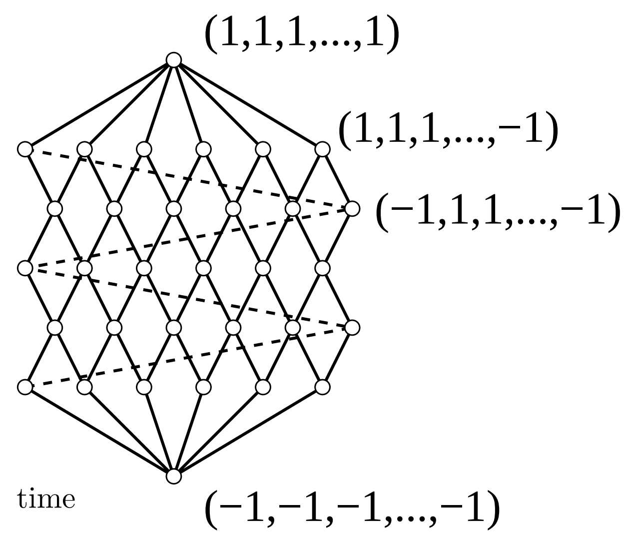
▷ $0 < \gamma \ll 1$:

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





Strong coupling: Synchronisation

Remarks:
- $I^{\pm} = \pm(1, 1, \ldots 1) \in \mathcal{S}_0 \ \forall \gamma$
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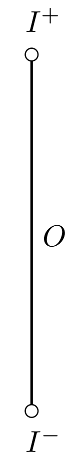
Let $\gamma_1 = \dfrac{1}{1 - \cos(2\pi/N)}$ $\quad \left(= \frac{N^2}{2\pi^2}\left[1 - \mathcal{O}(N^{-2})\right] \right)$



Theorem:

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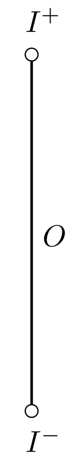

Theorem:

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

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

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

Strong coupling: Synchronisation

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

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

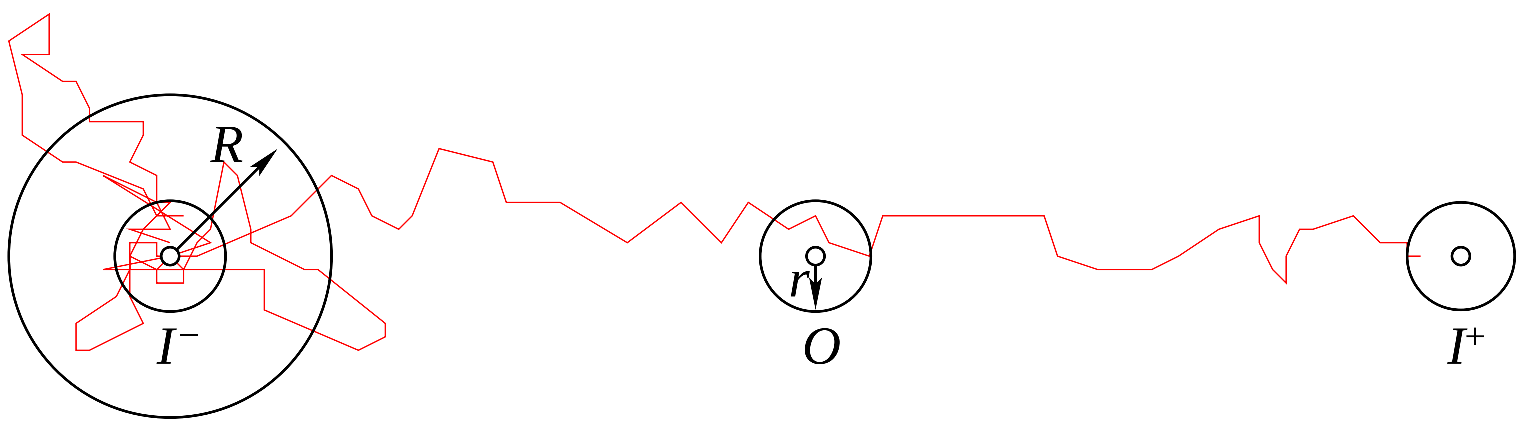
- Let $\tau_+ = \tau^{\text{hit}}(\mathcal{B}(I^+, r))$. Then $\forall \delta > 0$,

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

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

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

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



Symmetry groups

Potential V_γ invariant by

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

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

Properties:
$|C_x||O_x| = |G|$
$C_{gx} = gC_xg^{-1}$
$\mathrm{Fix}(gHg^{-1}) = g\,\mathrm{Fix}(H)$

$N = 2$

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

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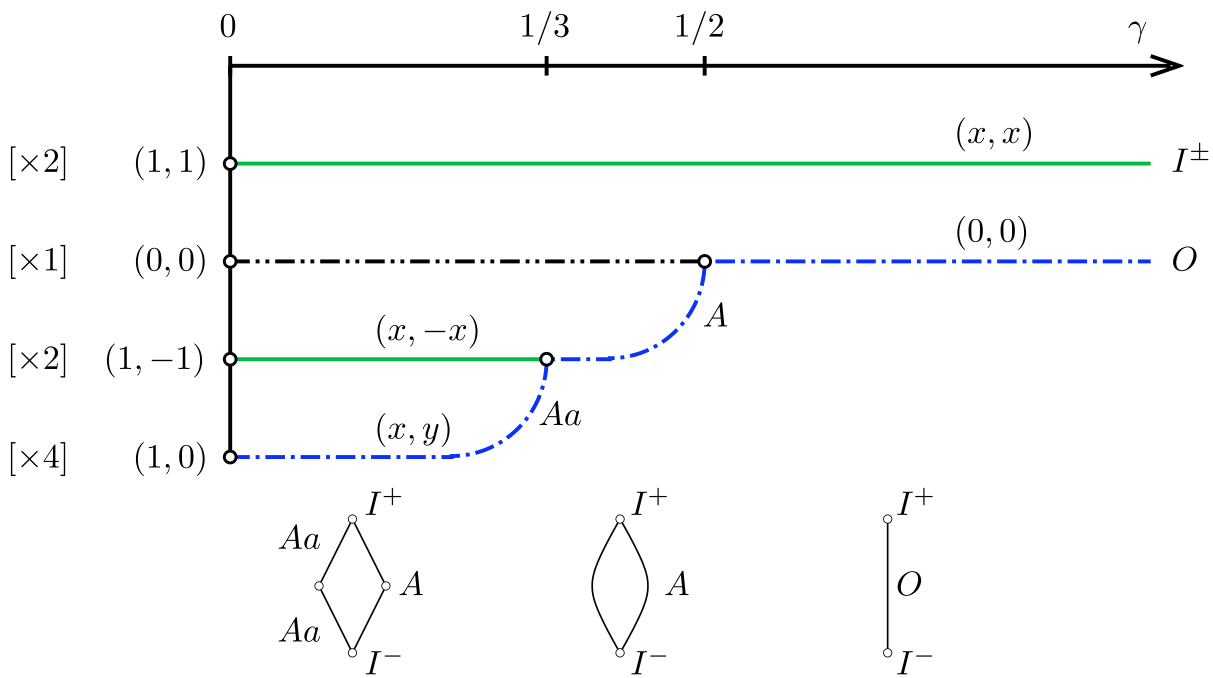
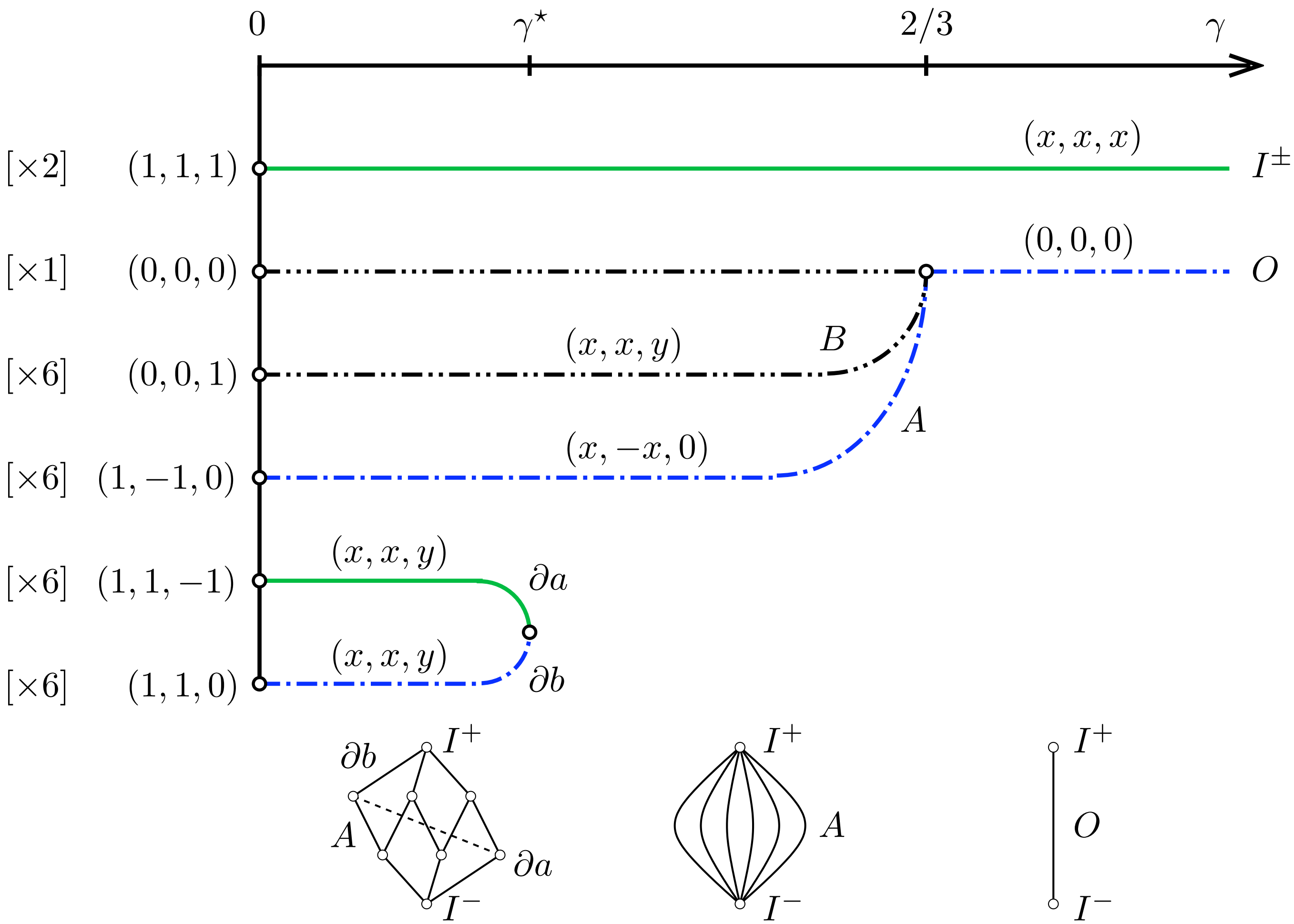
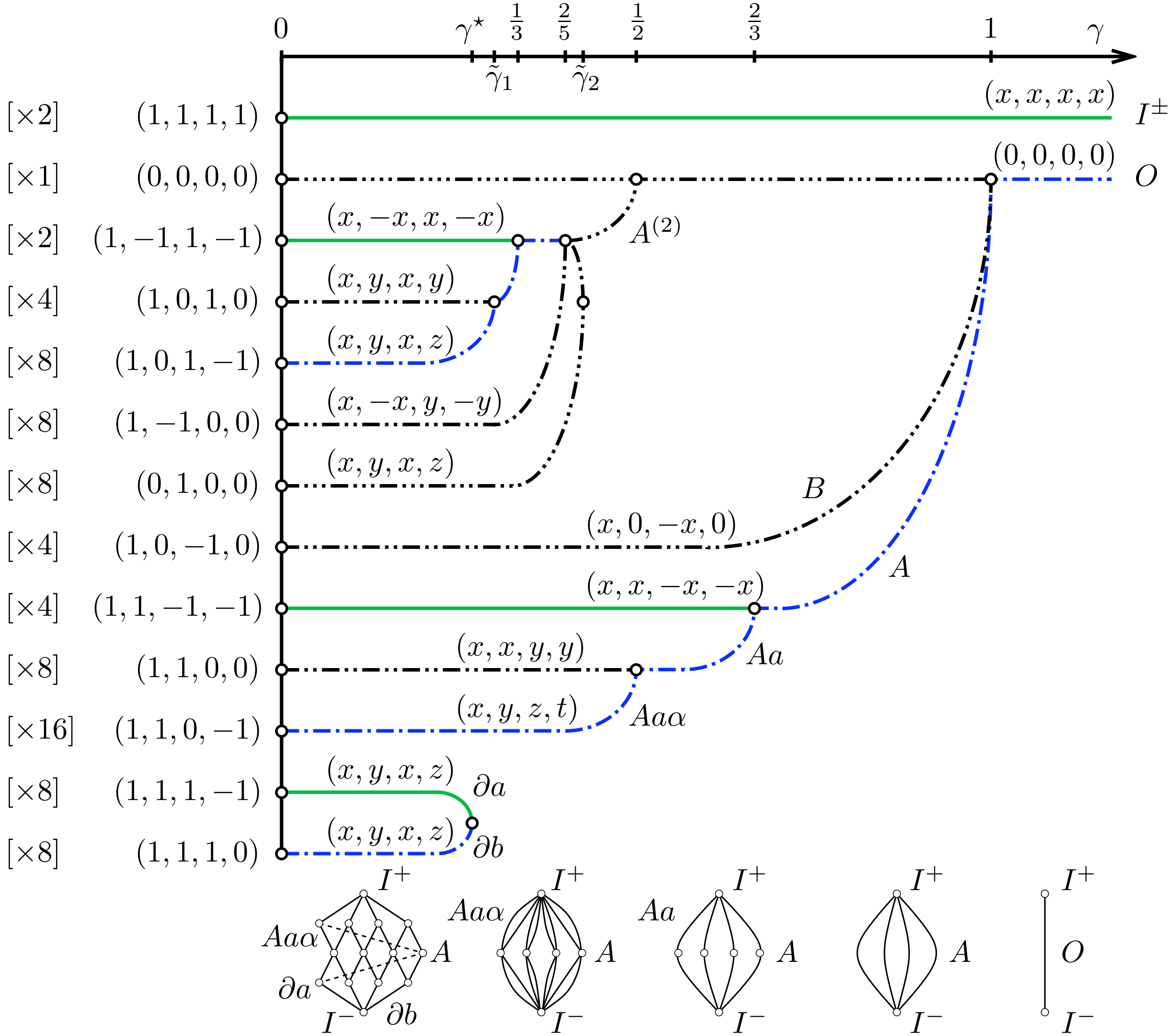


$N = 3$



0
$\gamma^\star$
2/3
γ
$[\times 2]$ $(1,1,1)$
$[\times 1]$ $(0,0,0)$
$[\times 6]$ $(0,0,1)$
$[\times 6]$ $(1,-1,0)$
$[\times 6]$ $(1,1,-1)$
$[\times 6]$ $(1,1,0)$
(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)
(x, x, −x, −x)
A
(x, x, y, y)
Aa
(x, y, z, t)
Aaα
(x, y, x, z)
∂a
(x, y, x, z)
∂b
I^+
Aaα
A
∂a
I^-
∂b
I^+
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I^-
I^+
Aa
A
I^-
I^+
A
I^-
I^+
O
I^-

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

$$
\begin{aligned}
\mathcal{S}_0 &= O_{I^+} = \{I^+, I^-\} \\
\mathcal{S}_1 &= O_A = \{A, RA, \dots, R^{N-1}A\} \\
\mathcal{S}_2 &= O_B = \{B, RB, \dots, R^{N-1}B\} \\
\mathcal{S}_3 &= O_O = \{O\}
\end{aligned}
$$

with

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

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

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$$\begin{aligned}
\mathcal{S}_0 &= O_{I^+} = \{I^+, I^-\} \\
\mathcal{S}_1 &= O_A = \{A, RA, \dots, R^{N-1}A\} \\
\mathcal{S}_2 &= O_B = \{B, RB, \dots, R^{N-1}B\} \\
\mathcal{S}_3 &= O_O = \{O\}
\end{aligned}$$

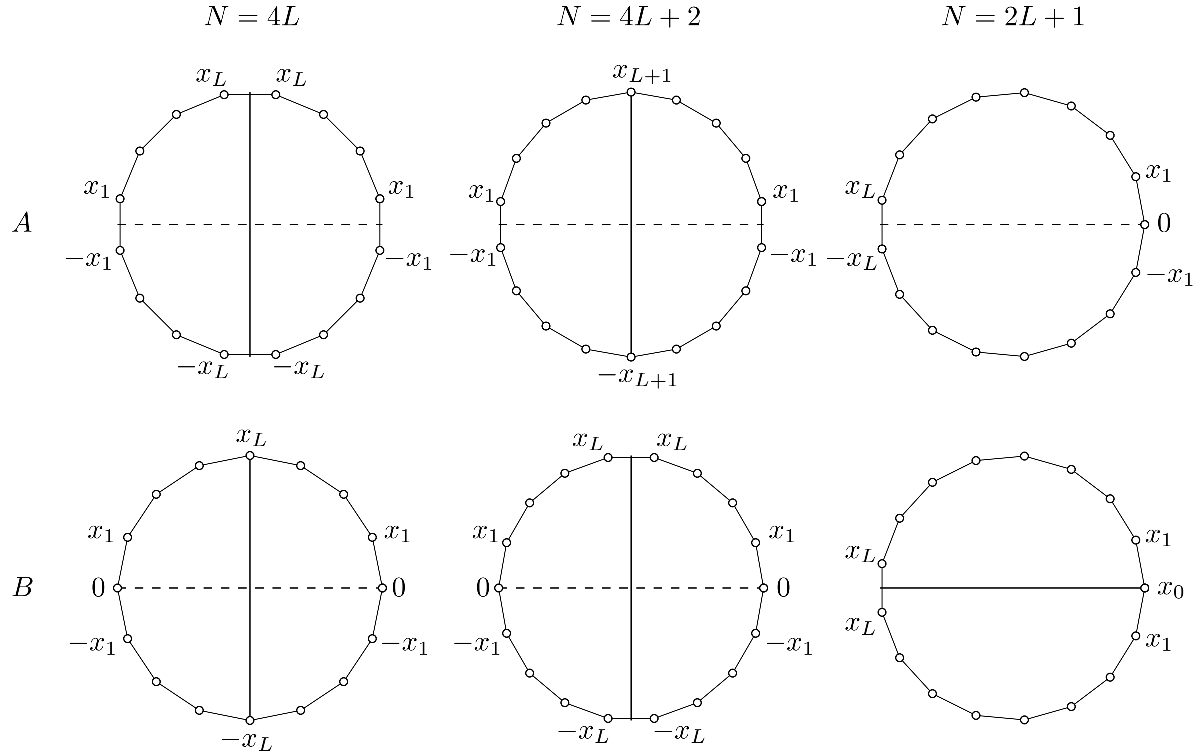
with

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

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

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

Symmetries



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

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

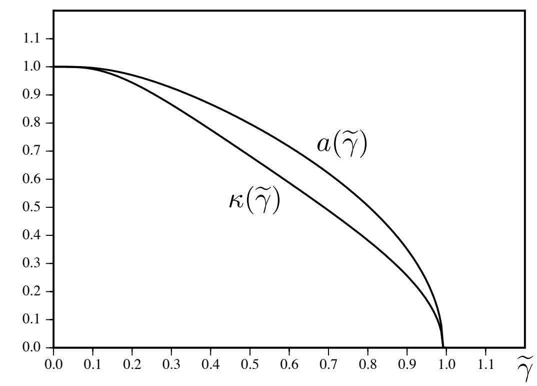
$$\begin{aligned} \mathcal{S}_0 &= O_{I^+} = \{I^+, I^-\} \\ \mathcal{S}_{2m-1} &= O_{A^{(m)}} & m = 1, \dots, M \\ \mathcal{S}_{2m} &= O_{B^{(m)}} & m = 1, \dots, M \ , \\ \mathcal{S}_{2M+1} &= O_O = \{O\} \end{aligned}$$

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

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

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

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



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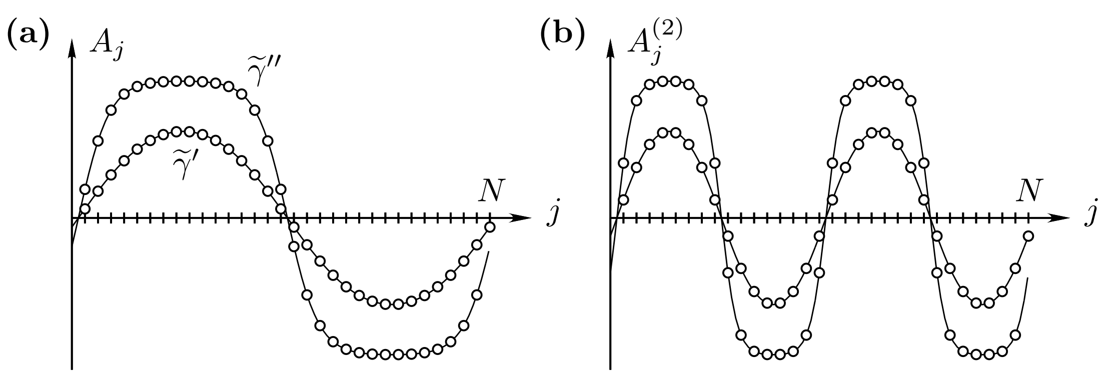
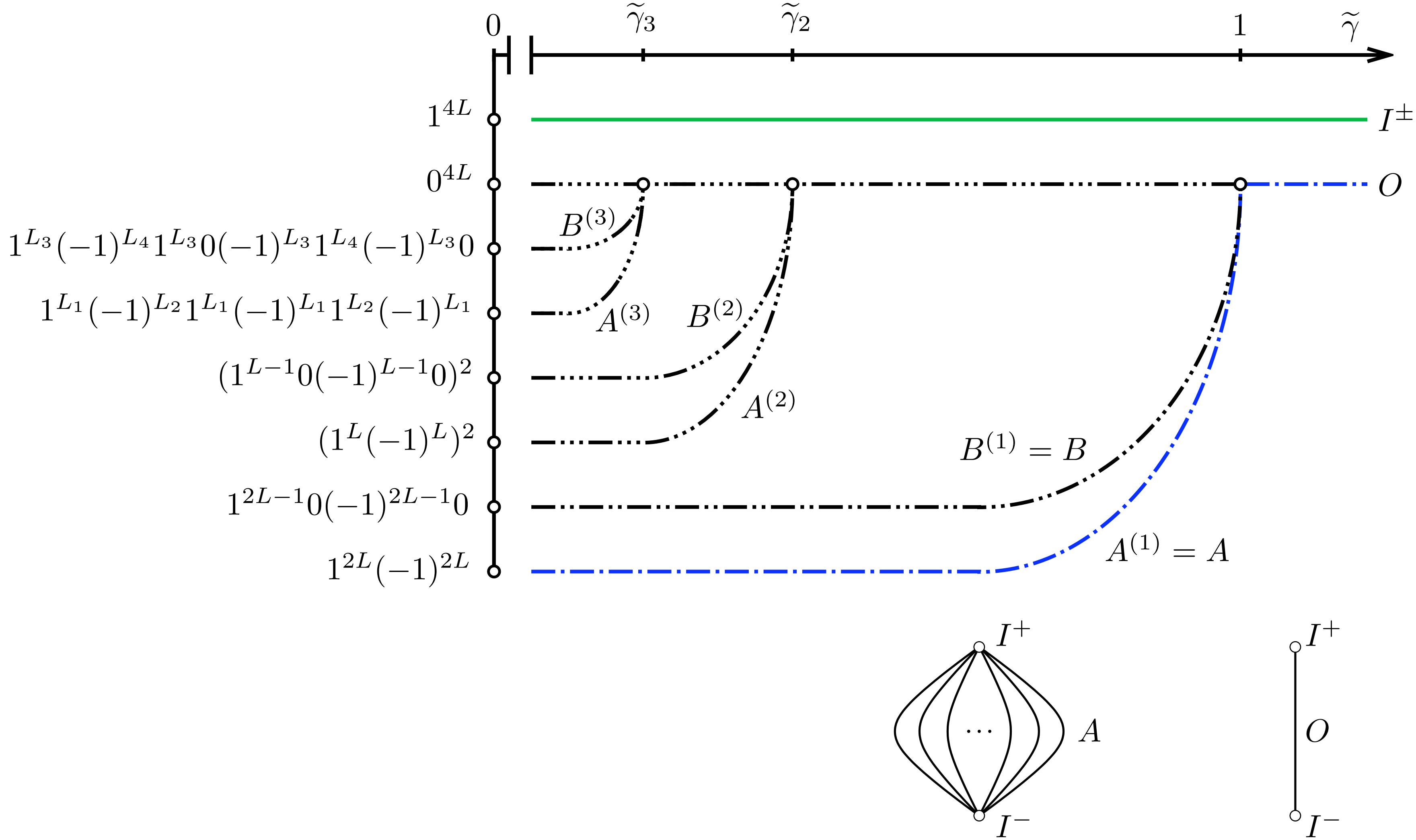


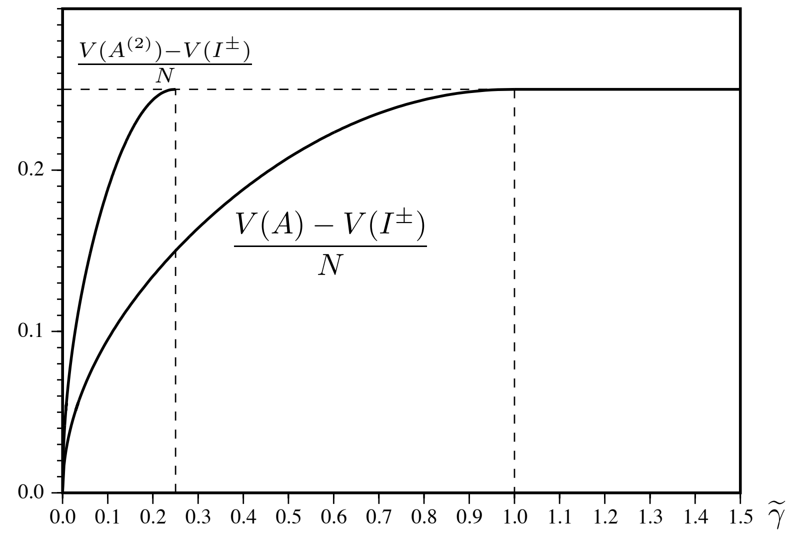
Case N large: bifurcation diagram (N=4L)



Potential difference:

$$H(\widetilde{\gamma}) = \frac{V(A)-V(I^{\pm})}{N}$$
$$= \frac{1}{4} - \frac{1}{3(1+\kappa^2)}\left[\frac{2+\kappa^2}{1+\kappa^2} - 2\frac{\mathsf{E}(\kappa)}{\mathsf{K}(\kappa)}\right]$$
$$+\,\mathcal{O}\left(\frac{\kappa^2}{N}\right)$$

$\kappa = \kappa(\widetilde{\gamma})$



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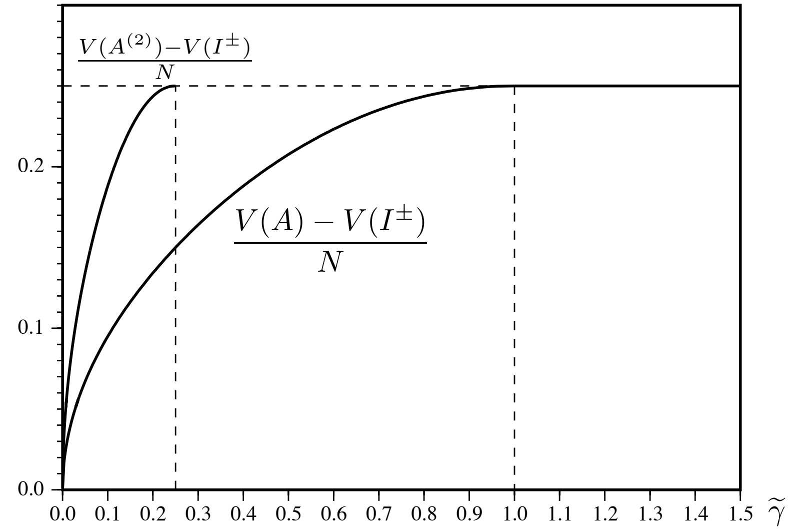

Corollary: $\forall 0 < \widetilde{\gamma} \leqslant 1$, $\exists N_0(\widetilde{\gamma})$ s.t. $\forall N \geqslant N_0(\widetilde{\gamma})$, $\forall 0 < r < R \leqslant \frac{1}{2}$, $\forall x_0 \in \mathcal{B}(I^-, r)$:

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

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

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

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

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

Ideas of the proof

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

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

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

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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):

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

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

Ideas of the proof

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$\Omega(I)$ monotonous in I $\Rightarrow$ twist map.

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▷ "$\varepsilon^3 = 0$":

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

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

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

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

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

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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,

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

- ▷ N particles "connected by springs" in a periodic ext. potential.
- ▷ Stationary pts can be analysed by Fourier transf. for $(\psi_1, \dots, \psi_n)$.