Metastable lifetimes and optimal transition paths in noisy spatially extended systems

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Seminar BINGO!

To play, simply print out this bingo sheet and attend a departmental seminar.

Mark over each square that occurs throughout the course of the lecture.

The first one to form a straight line (or all four corners) must yell out BINGO!! to win!

SEMINAR BINGO

B	I	N	G	O
Speaker bashes previous work	Repeated use of "um…"	Speaker sucks up to host professor	Host Professor falls asleep	Speaker wastes 5 minutes explaining outline
Laptop malfunction	Work ties in to Cancer/HIV or War on Terror	"…et al."	You're the only one in your lab that bothered to show up	Blatant typo
Entire slide filled with equations	"The data *clearly* shows…"	FREE Speaker runs out of time	Use of Powerpoint template with blue background	References Advisor (past or present)
There's a Grad Student wearing same clothes as yesterday	Bitter Post-doc asks question	"That's an interesting question"	"Beyond the scope of this work"	Master's student bobs head fighting sleep
Speaker forgets to thank collaborators	Cell phone goes off	You've no idea what's going on	"Future work will…"	Results conveniently show improvement

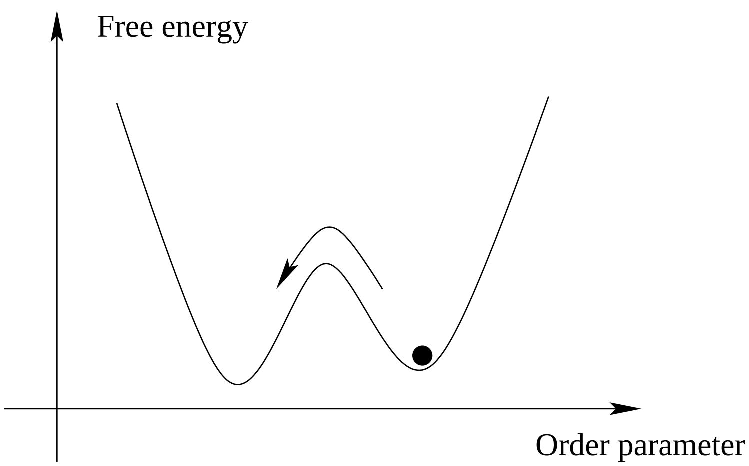
Metastability in physics

Examples:

- Supercooled liquid
- Supersaturated gas
- Wrongly magnetised ferromagnet

▷ Near first-order phase transition

▷ Nucleation implies crossing energy barrier

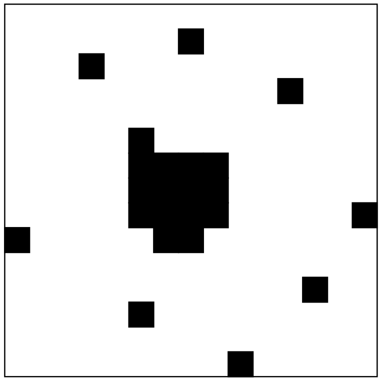


Metastability in stochastic lattice models

- ▷ 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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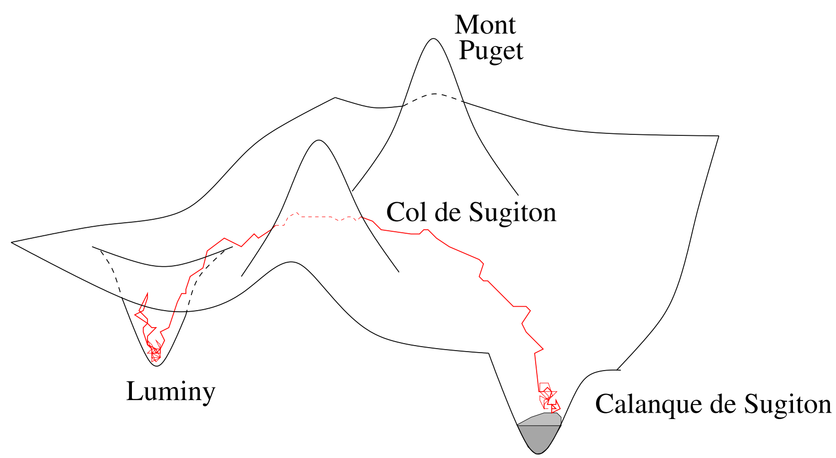

τ: transition time between potential wells (first-hitting time)

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

The model

- Lattice: $\Lambda = \mathbb{Z}/N\mathbb{Z}$, $N \geqslant 2$

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

$$\mathrm{d}x_i(t) = f(x_i(t))\,\mathrm{d}t$$

$$f(x) = -U'(x) = x - x^3 + h$$

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- Coupling between sites: discretised Laplacian, intensity γ

$$\mathrm{d}x_i(t) = f(x_i(t))\,\mathrm{d}t + \frac{\gamma}{2}\Big[x_{i+1}(t) - 2x_i(t) + x_{i-1}(t)\Big]\,\mathrm{d}t$$

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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

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

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

The model

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

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Notations

- $\mathcal{S}$ = set of stationary points of potential V_γ
- $\mathcal{S}_0$ = set of local minima of potential V_γ
- $\mathcal{S}_k$ = set of saddles of index k (k unstable directions)
- graph $\mathcal{G} = (\mathcal{S}_0, \mathcal{E})$: local minima connected by 1-saddles

▷ x_t resembles Markovian jump process on $\mathcal{G}$
▷ Mean transition times of order $\mathrm{e}^{2(V_\gamma(\text{1-saddle})-V_\gamma(\text{minimum}))/\sigma^2}$

Symmetric local dynamics: Assume $h = 0$

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Weak coupling

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

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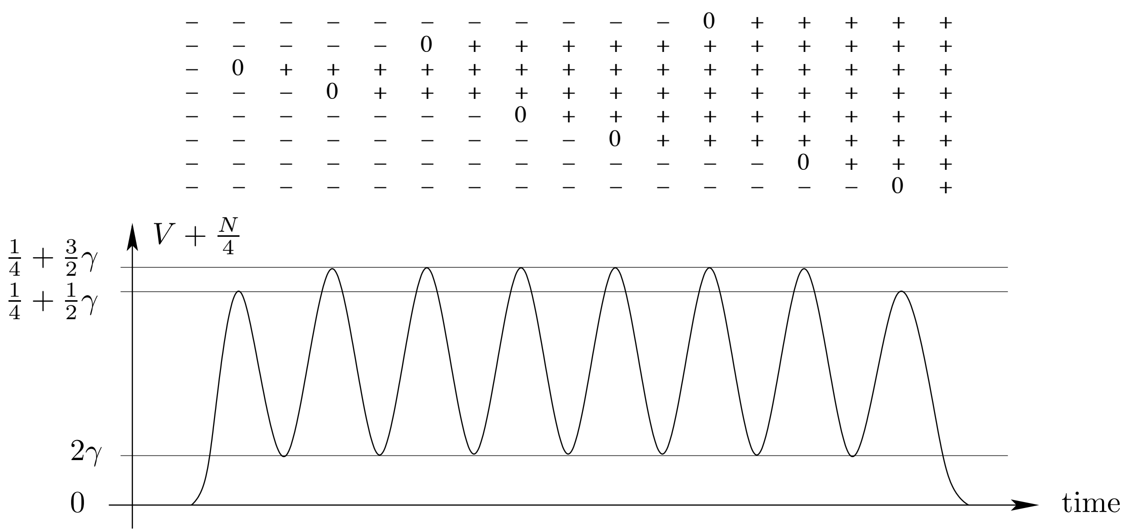
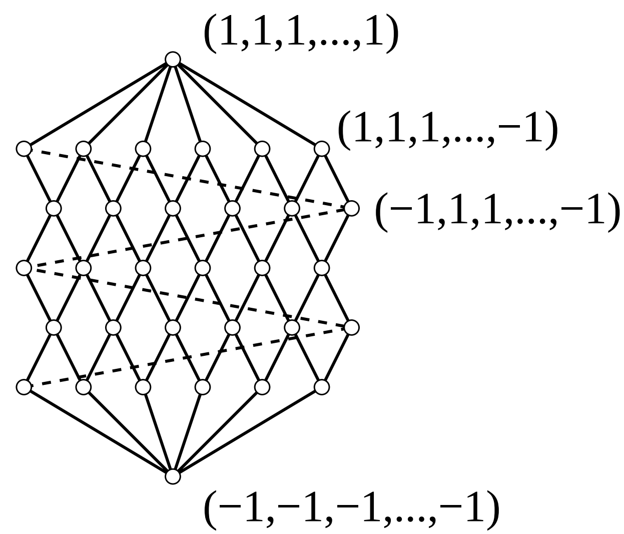
Theorem: $\forall N$, $\exists \gamma^{\star}(N) > 1/4$ s.t. points of each $S_k(\gamma)$ continuous in γ for $0 \leqslant \gamma < \gamma^{\star}(N)$

Ising-like dynamics





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

Theorem:

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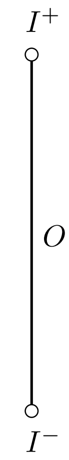

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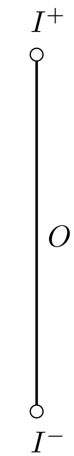

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Remark: $V_\gamma(O) - V_\gamma(I^-) = V_\gamma(O) - V_\gamma(I^+) = N/4 =: H$

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

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

$$\lim_{\sigma \to 0} \sigma^2 \log \mathbb{E}^{x_0}\{\tau_+\} = 2H = \frac{N}{2} \qquad \Rightarrow \qquad \mathbb{E}^{x_0}\{\tau_+\} \simeq e^{N/2\sigma^2}$$

- During a transition, paths are likely to pass close to O

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

$N = 2$

$z^\star$	$O_{z^\star}$	$C_{z^\star}$	$\mathsf{Fix}(C_{z^\star})$
$(0,0)$	$\{(0,0)\}$	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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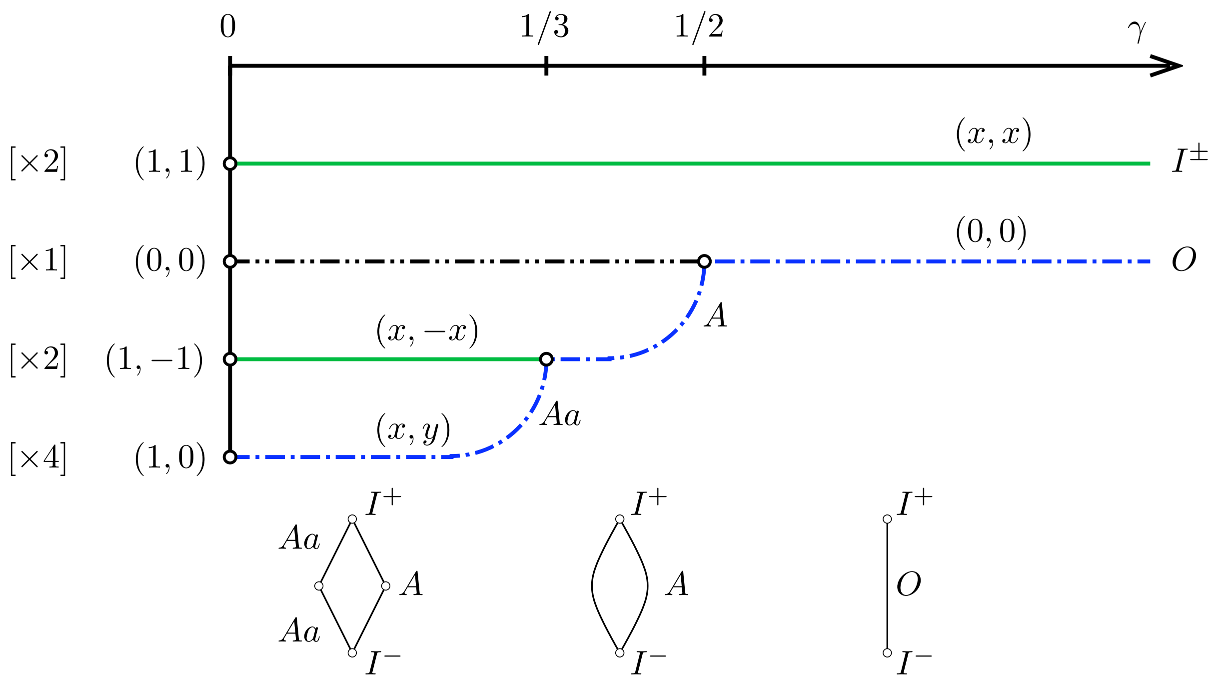
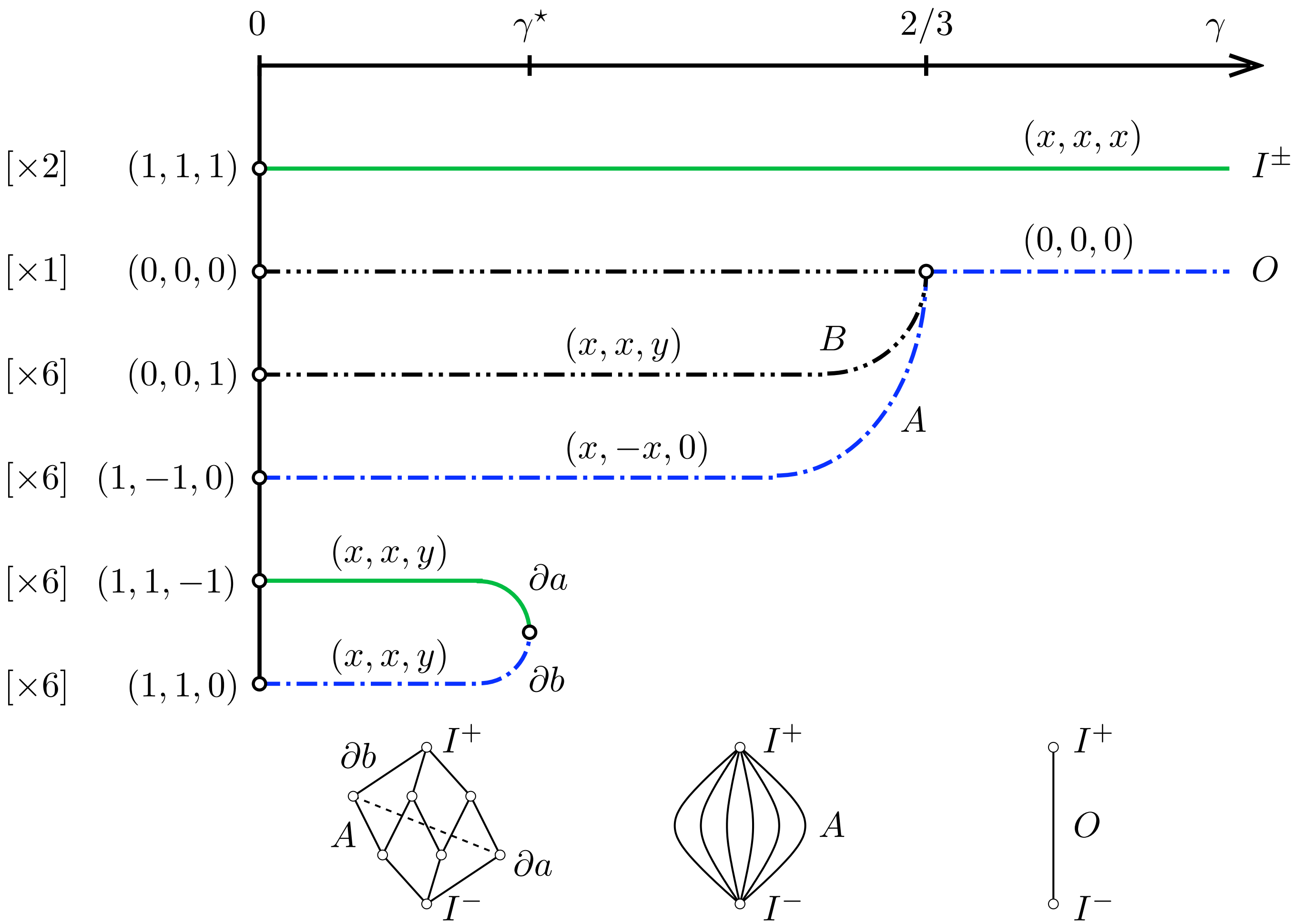
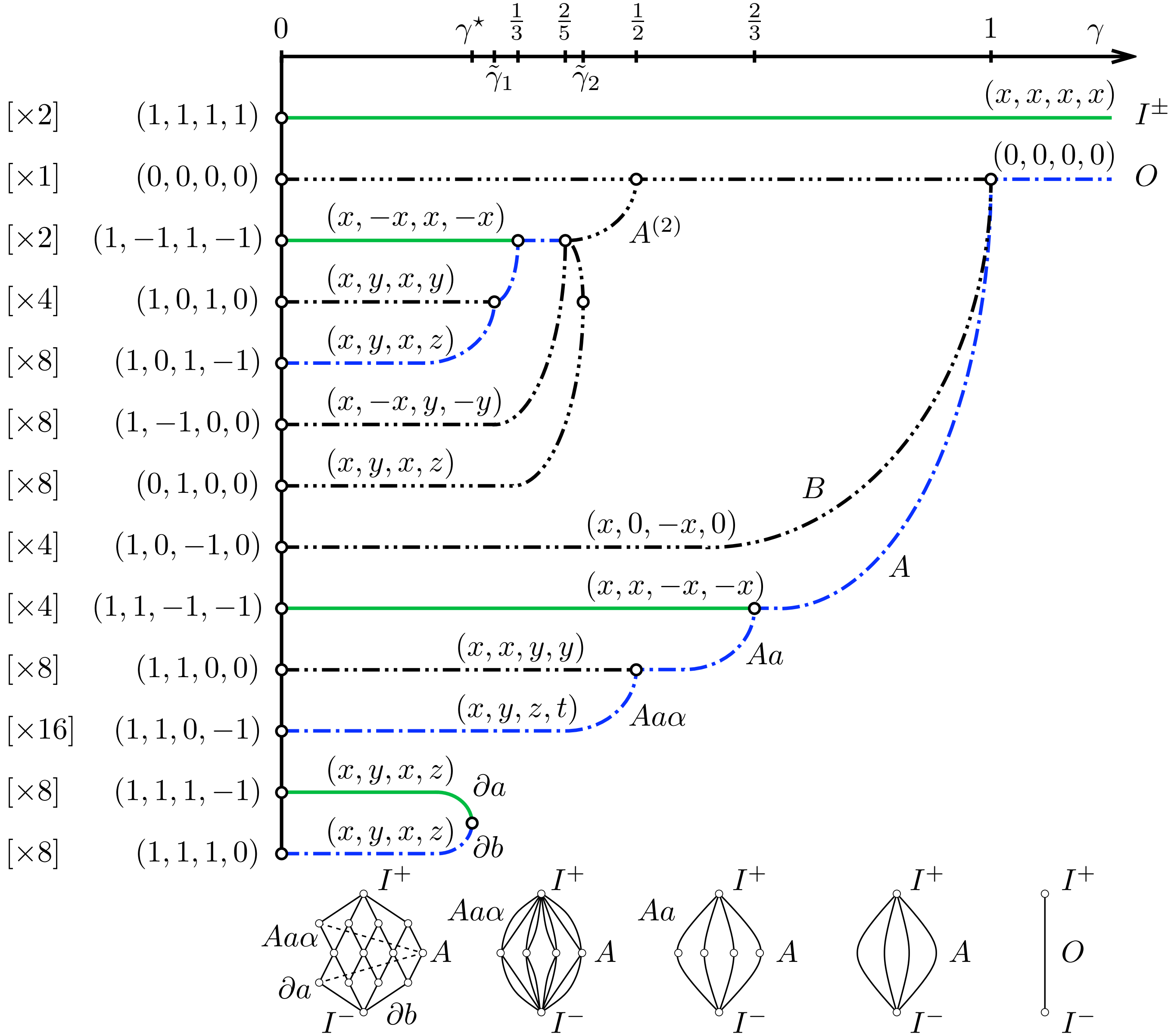


$N = 3$


0
$\gamma^\star$
2/3
γ
[×2] (1, 1, 1)
(x, x, x)
$I^\pm$
[×1] (0, 0, 0)
(0, 0, 0)
O
[×6] (0, 0, 1)
(x, x, y)
B
[×6] (1, −1, 0)
$(x, -x, 0)$
A
[×6] (1, 1, −1)
(x, x, y)
∂a
[×6] (1, 1, 0)
(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)
(x, x, y, y)
Aa
(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, $\exists \delta(N) > 0$ s.t. for $\gamma_1 - \delta(N) < \gamma < \gamma_1$, $|\mathcal{S}| = 2N + 3$, and can be decomposed as

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

with

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

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

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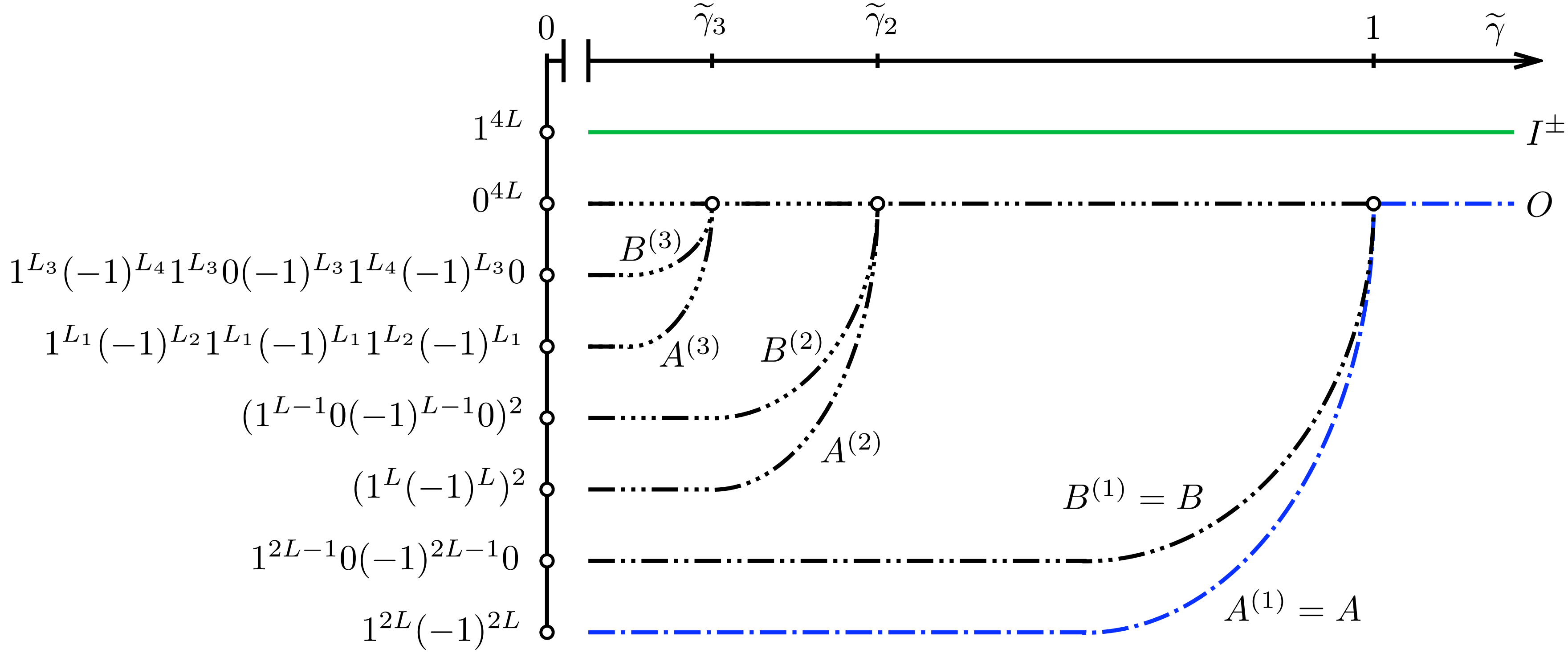
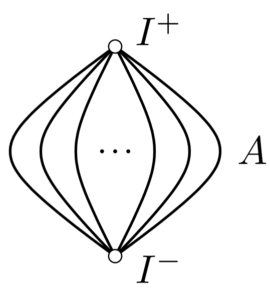
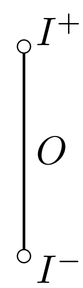
$$\begin{aligned} x \in \mathcal{S} \quad &\Leftrightarrow \quad f(x_n) + \tfrac{\gamma}{2}\Big[x_{n+1} - 2x_n + x_{n-1}\Big] = 0 \\ &\Leftrightarrow \quad \begin{cases} x_{n+1} = x_n + \varepsilon w_n - \frac{1}{2}\varepsilon^2 f(x_n) \\ w_{n+1} = w_n - \frac{1}{2}\varepsilon\Big[f(x_n) + f(x_{n+1})\Big]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

- ▷ 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

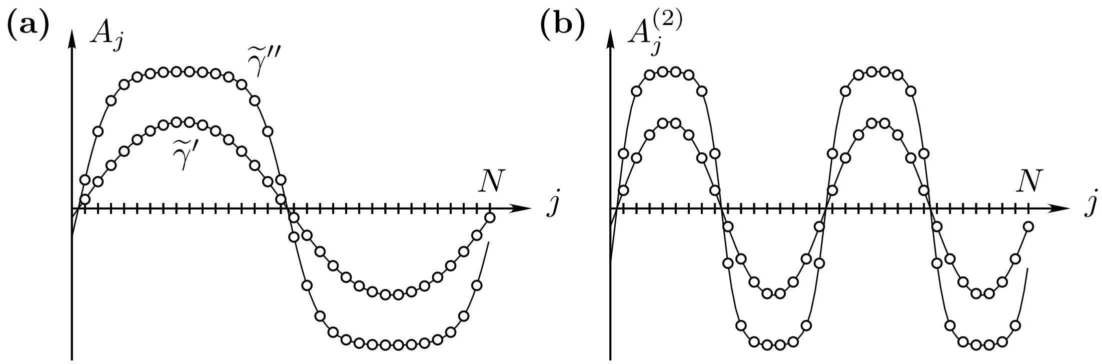
Let $\widetilde{\gamma} = \frac{\gamma}{\gamma_1} = \gamma(1 - \cos(2\pi/N))$,

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

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

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

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

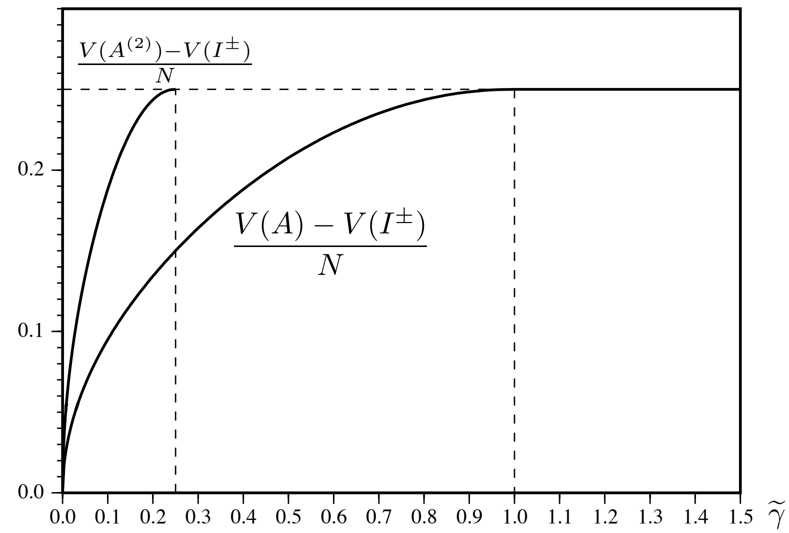


N large

Potential difference:

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

(explicit expression
in terms of elliptic integrals)



N large

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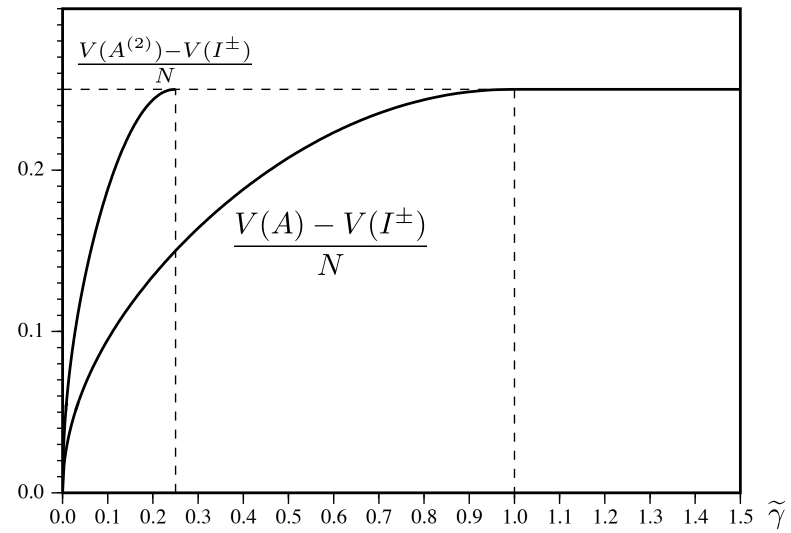


Corollary: $\forall 0 < \tilde{\gamma} \leqslant 1$, $\exists N_0(\tilde{\gamma})$ s.t. $\forall N \geqslant N_0(\tilde{\gamma})$, $\forall 0 < r < \frac{1}{2}$, $\forall x_0 \in \mathcal{B}(I^-, r)$:

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

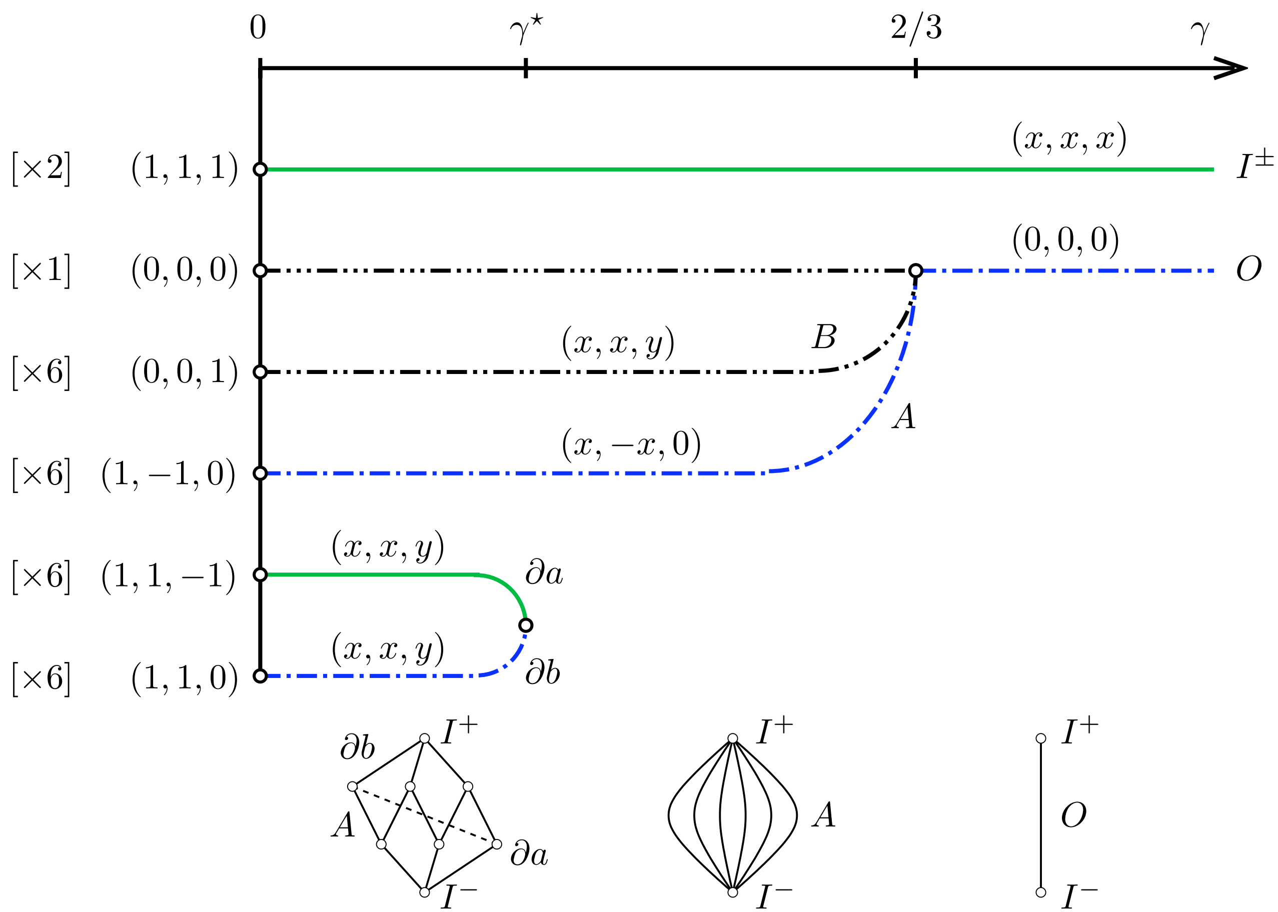
  $$\lim_{\sigma \to 0} \sigma^2 \log \mathbb{E}^{x_0}\{\tau_+\} = 2H(\tilde{\gamma}) \qquad \Rightarrow \qquad \mathbb{E}^{x_0}\{\tau_+\} \simeq \mathrm{e}^{2H(\tilde{\gamma})/\sigma^2}$$

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

Asymmetric case $h \neq 0$

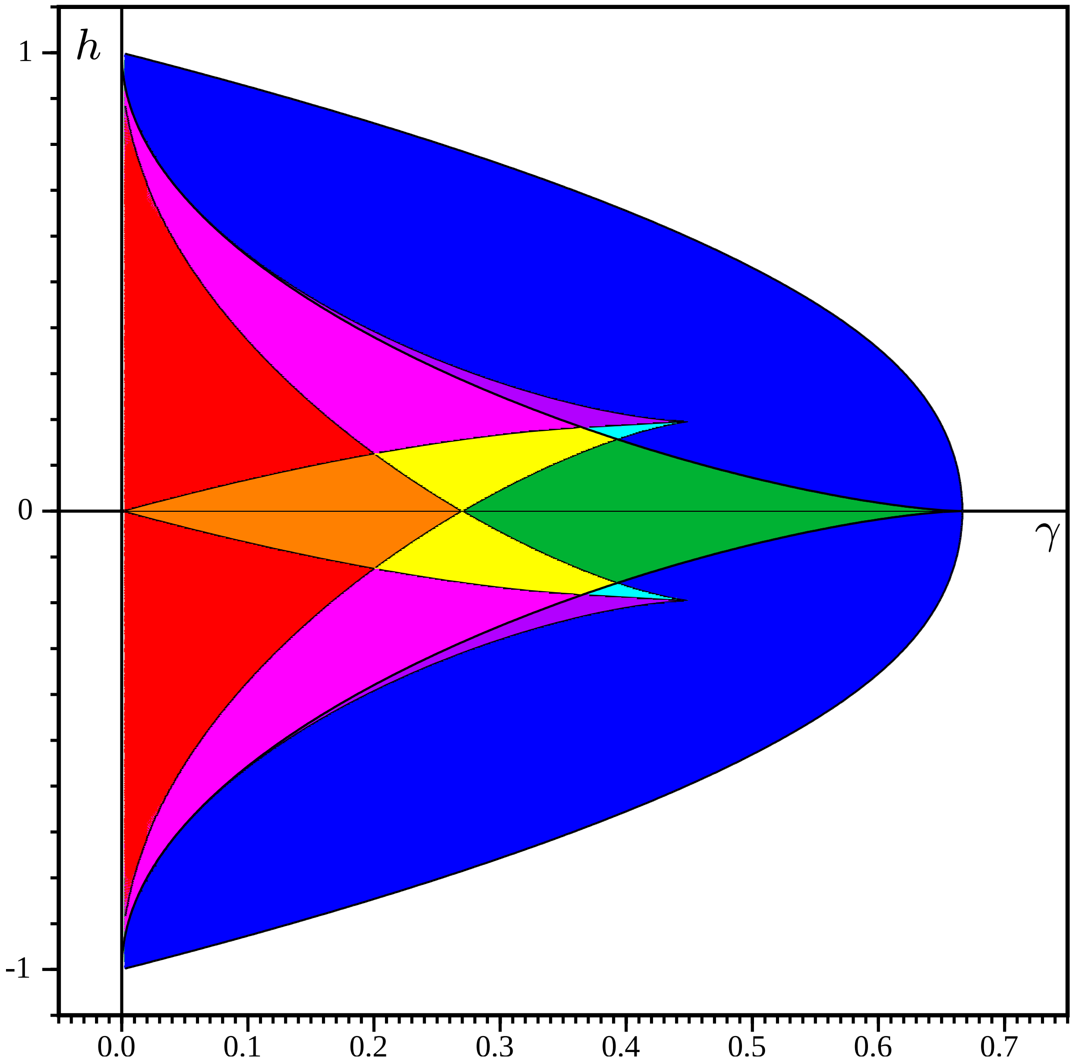
E.g. $N = 3$

Recall symmetric case:



Asymmetric case $h \neq 0$

E.g. $N = 3$



Outlook

- Asymmetric potential (magnetic field)
- Prefactors of $\mathbb{E}\{\tau\}$ (Barret & Bovier)
- Continuum limit $N \to \infty$ (SPDE)
- Inhomogeneous noise intensity (heat flow)
- Time-dependent magnetic field (hysteresis)

References

- N. B., Bastien Fernandez and Barbara Gentz, *Metastability in interacting nonlinear stochastic differential equations I: From weak coupling to synchronisation*, Nonlinearity **20**, 2551–2581 (2007)
- N. B., Bastien Fernandez and Barbara Gentz, *Metastability in interacting nonlinear stochastic differential equations II: Large-N behaviour*, Nonlinearity **20**, 2583–2614 (2007)