Metastability in zero-temperature dynamics: some simple examples

1. Historical background on metastability

2. Glassy dynamics and metastability. Edwards ensemble

3. Some simple examples: Ising chains at zero temperature

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1. Historical background on metastability

Mean-field level (Gibbs, 1906)

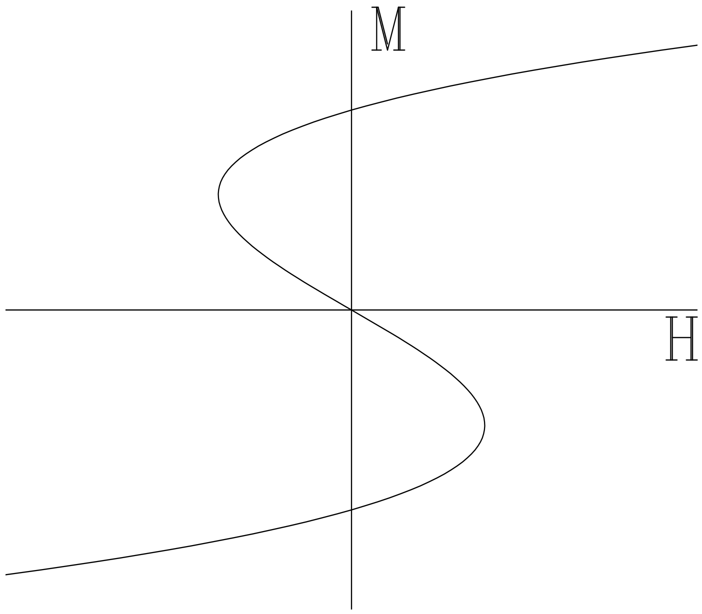
Ferromagnetic system

Landau free energy: $F(M) = (T - T_c)\frac{M^2}{2} + \frac{M^4}{4} - HM$

stationary for: $\frac{\partial F}{\partial M} = (T - T_c)M + M^3 - H = 0$

solutions $M(T,H)$ (fixed $T < T_c$):

Stable	absolute (global) minimum
Metastable	relative (local) minimum
Instable	maximum



Analytic continuation

of stable solution $M(T, H > 0)$ (+ phase)

to metastable solution $M(T, H < 0)$

Finite-dimensional case (Fisher, Langer, 1967)

Ferromagnet, finite dimension d, short-range interactions

$\star$ Free energy $F(H)$ of $+$ phase is not analytic at $H = 0$

$\star$ Metastability is an artifact of mean-field theory

Argument: critical droplet

Free energy of spherical droplet of $-$ phase, radius R:

$$f(R) = 2\,\omega R^d H M_0 + d\omega R^{d-1}\sigma_0$$

critical radius for $H < 0$: $R = R_c = \dfrac{(d-1)\sigma_0}{2\,|H|\,M_0}$

$$f_c = f(R_c) = \omega\sigma_0^d \left(\frac{d-1}{2\,|H|\,M_0}\right)^{d-1}$$

Barrier height f_c/kT similar to instanton action $S/\hbar$ in quantum theory

- Statics: $F(H)$ has imaginary part for $H < 0$:

$$\operatorname{Im} F(H) \sim \exp\left(-\frac{f_c}{kT}\right) \sim \exp\left(-\frac{\omega\sigma_0^d}{kT}\left(\frac{d-1}{2\,|H|\,M_0}\right)^{d-1}\right)$$

- Dynamics: Nucleation rate $w \sim \operatorname{Im} F(H)$

  Finite lifetime $\tau \sim 1/w$ for all $H < 0$

- True metastability

$$\frac{f_c}{kT} = \infty \Longrightarrow \begin{cases} d = \infty & \text{(mean-field)} \\ T = 0 & \text{worth a closer look} \end{cases}$$

2. Glassy dynamics and metastability. Edwards ensemble

Glasses, spin glasses, granular media, polymers, proteins, etc.

Non-stationary dynamics: aging, violation of FDT, etc.

Motion in complex energy landscape (Goldstein, 1969)

Landscape height is energy, free energy...

Valleys or metastable states separated by barriers

What are the valleys?

- TAP states (Thouless, Anderson, Palmer, 1978)
- Inherent structures (Stillinger, Weber, 1982)
- Pure states (Kirkpatrick, Thirumalai, Wolynes, 1987)
- Quasi-states (Franz, Virasoro, 2000)

Common characteristic feature

Typical number of valleys with given energy density E:

$\mathcal{N} \sim \exp(NS(E))$

$S(E)$: complexity or configurational entropy

Edwards ensemble (Edwards, 1994)

Granular system

⋆ Large (extensive) number of grains $\Longrightarrow$ thermodynamics

⋆ Solid (nonlinear) friction between grains $\Longrightarrow$ metastable configurations

Edwards ensemble:

A priori (microcanonical) ensemble of all the metastable configurations

given compacity $c = N/V \equiv -E$

uniform weight

number $\mathcal{N} \sim \exp(NS(E))$

Edwards flatness hypothesis

• A priori ensemble allows to use equilibrium techniques

spatial correlations, transport coefficients, etc.

• Thermodynamical meaning

$\frac{1}{T_{\text{eff}}} = \frac{\partial S}{\partial E}$ is an effective temperature

Validity

⋆ Mean-field level: yes

T_{eff} through dynamics (violation of FD) (Franz, Virasoro, 2000)

⋆ Finite-dimensional systems: ?!

Matter of time scales (Gaveau, Schulman; Kurchan, Biroli, Monasson)

Let us have a closer look at $T = 0$

3. Some simple examples:
Ising chains at zero temperature

Ferromagnetic Ising chain

• Equilibrium properties: Hamiltonian $\mathcal{H} = -\sum_n \sigma_n \sigma_{n+1}$

• Dynamics: Monte-Carlo

Single-spin move	(Glauber)	$+ \leftrightarrow -$
Spin-exchange move	(Kawasaki)	$+- \leftrightarrow -+$

⋆ Move performed with probability $W(\delta\mathcal{H})$:

in both cases, energy difference $\delta\mathcal{H} = \begin{cases} +4 \\ 0 \\ -4 \end{cases}$

⋆ Detailed balance

1 equation for 3 unknowns: $\dfrac{W(+4)}{W(-4)} = \exp(-4/kT)$

Zero-temperature dynamics

$W(+4) = 0$

$W(-4) = 1$ sets time unit

$W(0)$ remains a free parameter

describes diffusive moves at constant energy

4 cases

FG (full Glauber)	$(W(0) > 0)$	coarsening	(Glauber, 1963)
FK (full Kawasaki)	$(W(0) > 0)$	metastability	(Kawasaki, 1966)
RG (restricted Glauber)	$(W(0) = 0)$	metastability	(Privman, 1992)
RK (restricted Kawasaki)	$(W(0) = 0)$	metastability	(Dean et al., 2000)

Only FG is good $T = 0$ dynamics:

Coarsening: typical domain size diverges as $L(t) \sim \sqrt{t}$

Mean energy slowly converges to g.s. energy: $E(t) = -1 + 2/L(t)$

Other 3 cases: metastability

Dynamics stops after a short time $T \sim (\ln N)^{\alpha}$

Final configuration thus reached

mean energy $E(\infty) \neq -1$: not equilibrated

dependent on initial state: non-ergodicity

non-trivial features (spatial correlations...)

A priori statistical description via Edwards ensemble?

⋆ Restricted dynamics (RG and RK) relatively simple

Descent dynamics: $\delta\mathcal{H} < 0$ only

Fully irreversible: every spin flips at most once

examples of kinetically constrained systems (Sollich, Ritort, 2002)

⋆ Full Kawasaki dynamics is more complex

Restricted Glauber dynamics

Mapping onto random sequential addition (RSA) problem

satisfied bond	$\sigma_n\sigma_{n+1} = +1$	$\bullet$
unsatisfied bond	$\sigma_n\sigma_{n+1} = -1$	$\circ$

- Spin move: reaction $\circ\circ \to \bullet\bullet$

  RSA of dimers (Flory, 1939)

- Jamming time $T \approx \ln(aN) + \xi$

  ξ follows Gumbel's law

- Final state

  $\circ$ are isolated $\circ\bullet\bullet\circ\bullet\bullet\bullet\circ\bullet\circ\bullet\bullet\circ\bullet$

  domain sizes are ≥ 2 $---++++--+++--$

Goal (EPJB **27** (2002) 363)

⋆ Quantitative characterization of final states

⋆ Quantitative comparison between

$$\begin{cases} \text{Edwards ensemble predictions} \\ \text{exact dynamical results} \end{cases}$$

Edwards ensemble

A priori combinatorics of all metastable configurations

Energy density: $E = -1 + 2\,\mathrm{Prob}(\circ)$

2×2 transfer-matrix formalism

- Entropy

$$S(E) = E\ln(-2E) - \frac{1+E}{2}\ln(1+E) + \frac{1-E}{2}\ln(1-E)$$

$\star$ $S > 0$ for $-1 < E < 0$

$$\star \text{ Maximum} : S_{\max} = \ln\frac{\sqrt{5}+1}{2} = 0.481212$$

$$E_{\max} = -\frac{1}{\sqrt{5}} = -0.447214$$

- Correlation functions

spin (site) correlations	$C_n = \langle \sigma_0 \sigma_n \rangle$
energy (bond) correlations	$\Gamma_n = \langle \sigma_0 \sigma_1 \sigma_n \sigma_{n+1} \rangle$

$$\Gamma_n = E^2 + (1-E^2)\left(-\frac{1+E}{1-E}\right)^{|n|}$$

Exact dynamical results

Initial condition $\begin{cases} \circ & \text{with prob.} \quad p \\ \bullet & \text{with prob.} \quad 1-p \end{cases}$

Initial energy: $E(0) = -1 + 2p$

Size distribution of active domains

$$p_\ell(t) = \mathrm{Prob}_t(\bullet\underbrace{\circ\cdots\circ}_{\ell}\bullet)$$

$$\frac{\mathrm{d}p_\ell(t)}{\mathrm{d}t} = -(\ell-1)p_\ell(t) + 2\sum_{k\geq\ell+2} p_k(t)$$

$$p_\ell(0) = (1-p)^2 p^\ell \quad \Longrightarrow \quad p_\ell(\infty) = p\,\mathrm{e}^{-2p}\,\delta_{\ell,1}$$

Final energy: $E(\infty) = -1 + 2p\,\mathrm{e}^{-2p}$

Random initial state: $p = 1/2 \Longrightarrow E(\infty) = -1 + \mathrm{e}^{-1} = -0.632121$

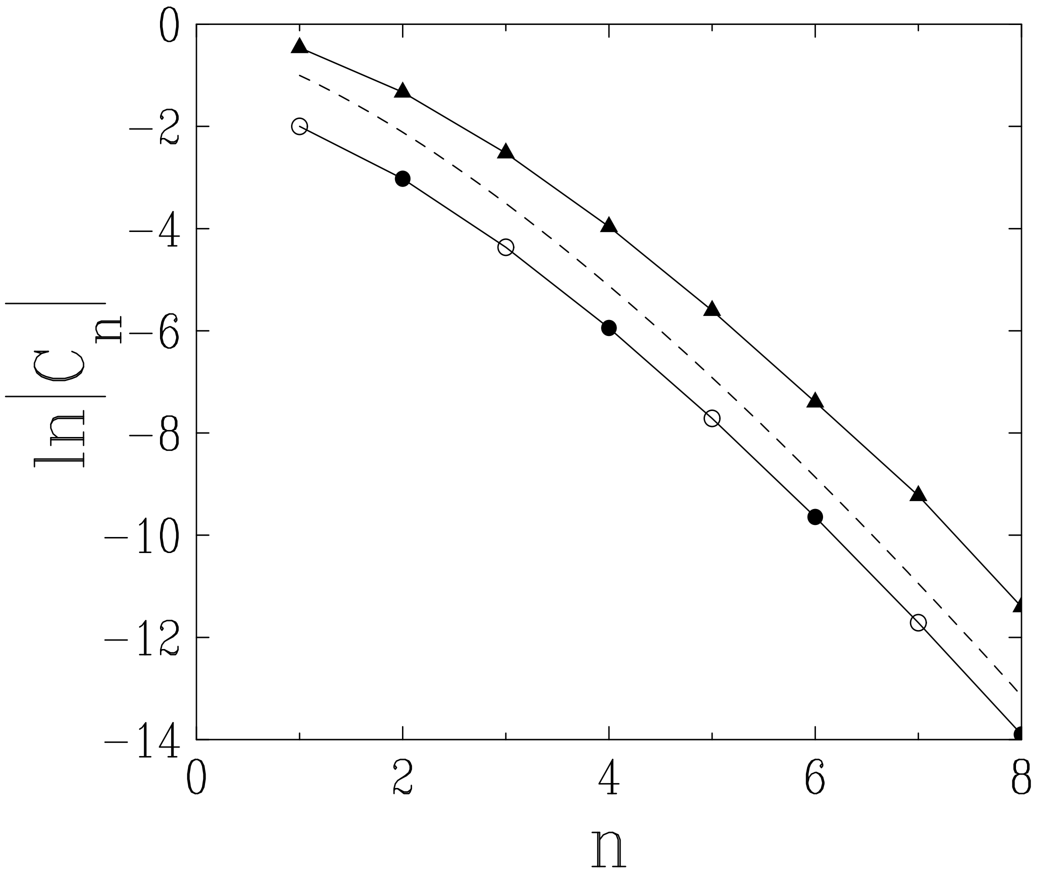
Energy (bond) correlations

$$\Gamma_n(\infty) - E(\infty)^2 = 2p\,\mathrm{e}^{-2p}\left((1-2p)\frac{(-2p)^n}{n!} - 2p\sum_{m\geq n+1}\frac{(-2p)^m}{m!}\right)$$

$\star$ super-exponential fall-off in en $\dfrac{(-2p)^n}{n!}$: characteristic of lattice RSA

$\star$ also observed (numerical simulation) for spin (site) correlations

qualitative difference with a priori approach based on Edwards ensemble



Random initial state ($p = 1/2$)

Full (open) symbols show positive (negative) correlations

Circles: $(-1)^n$ times connected energy correlation (analytical)

Triangles: full spin correlation function (simulation)

Dashed line: $1/(n+1)!$

Dynamical vs. Edwards entropy

$\star$ Single domain of $\ell \geq 2$ sites, initially empty

Number ν_ℓ of $\bullet$ in final configuration:

$\nu_\ell = 2 + \nu_{\ell_1} + \nu_{\ell_2} \qquad \ell_1 + \ell_2 = \ell - 2$

$\phi_\ell(\lambda) = \langle \exp(\lambda \nu_\ell) \rangle$ explicitly known:

$$\sum_{\ell \geq 0} \phi_\ell(\lambda)\, x^\ell = \frac{(e^\lambda + 1)\exp(2xe^\lambda) + e^\lambda - 1}{(e^\lambda + 1)(1 - xe^\lambda)\exp(2xe^\lambda) + (e^\lambda - 1)(1 + xe^\lambda)}$$

$\star$ General initial state (p)

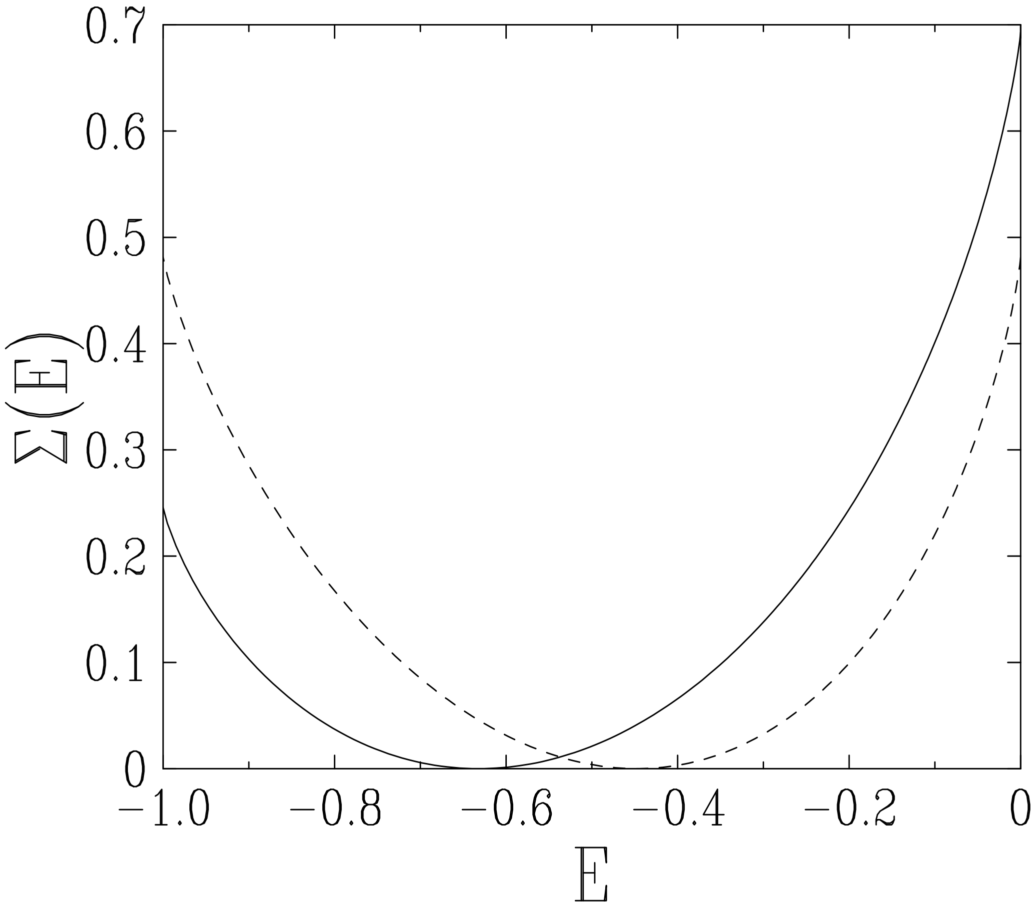
Distribution of final energy E has large-deviation form:

$P_N(E) \sim \exp(-N\Sigma_p(E))$

$$\Sigma_p = \ln z - \frac{(1+(2p-1)z)^2 - (z-1)^2 e^{4pz}}{4pz^2\, e^{2pz}(2(1-p)+(2p-1)z)} \ln \frac{1+(2p-1)z+(1-z)e^{2pz}}{1+(2p-1)z-(1-z)e^{2pz}}$$

$$E = -1 + \frac{(1+(2p-1)z)^2 - (z-1)^2\, e^{4pz}}{2pz^2\, e^{2pz}(2(1-p)+(2p-1)z)}$$

quantitative difference between $\Sigma_{1/2}(E)$ and $\Sigma(E) = S_{\max} - S(E)$



Random initial state $(p = 1/2)$

Full line: dynamical entropy $\Sigma_{1/2}(E)$ against energy E

Dashed line: prediction $\Sigma(E) = S_{\max} - S(E)$ of Edwards a priori approach

Full Kawasaki dynamics (preprint to appear soon)

- Effects of diffusive moves

  multiple spin flips allowed

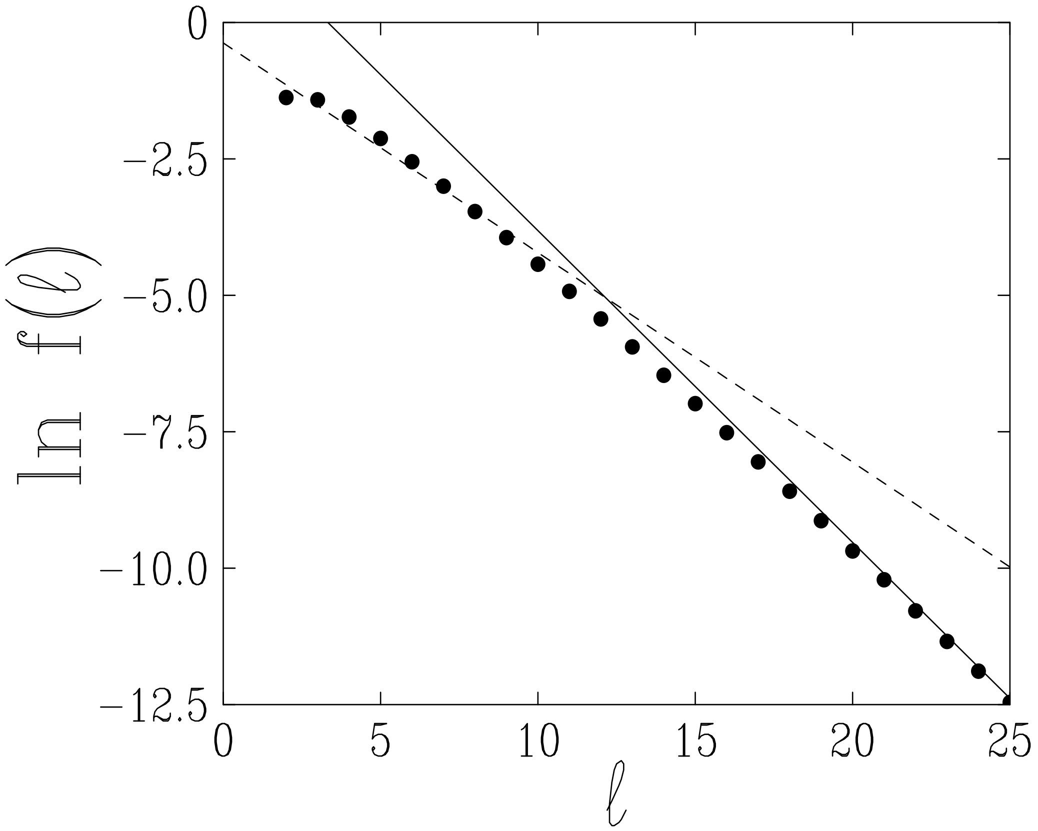
  slightly slower dynamics: jamming time $T_N \sim b(\ln N)^3$,

  Final states: those of RG (domain sizes ≥ 2)

- No analytical approach available $\Longrightarrow$ numerical simulations

One key quantity (Berg et al., 2002)

Distribution $f(\ell)$ of domain sizes in final states



Symbols: Numerical results (Metropolis: $W(0) = 1$)

Dashed line: Prediction of Edwards a priori approach:

exponential law with char. length 2.603, related to mean energy

Full line: Fitted asymptotic exponential decay (measured char. length 1.75)

Conclusions

• True metastability: mean-field or $T = 0$

• Seemingly simple example of ferromagnetic Ising chain rich enough

4 cases (order parameter conserved or not, diffusive moves allowed or not)

Only FG good $T = 0$ dynamics

Other 3 (FK, RG, RK) yield metastability

• Restricted (descent) dynamics (RG and RK)

⋆ provide interesting examples of kinetic constraints

⋆ can be mapped onto RSA problems:

RF:	dimers	○○ → ●●
RK:	hollow trimers	○○○ → ●○●

Are all the metastable states equivalent?

(Does a priori statistical description à la Edwards hold?)

No! even at qualitative level

⋆ Restricted dynamics

super-exponential fall-off of spin and energy correlations in $\dfrac{1}{n!}$ or $\dfrac{1}{\sqrt{n!}}$

⋆ Unrestricted dynamics (Full Kawasaki)

domain sizes neither exponentially distributed nor independent