Taming large fluctuations in disordered systems

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work in collaboration with
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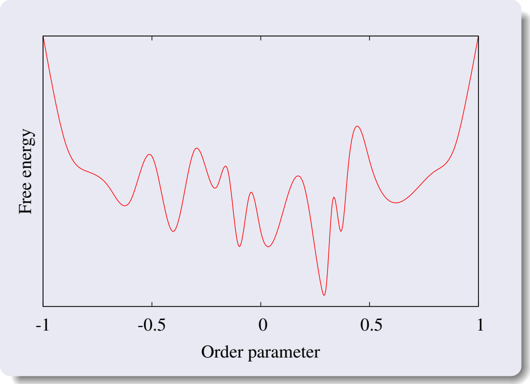
Seoul, July 2013

Foreword: from cartoons to actual computations



First picture in many talks on complex behaviour: Cartoon of a free energy profile with several, almost degenerate minima.

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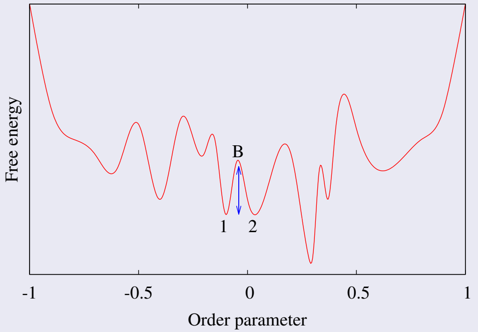
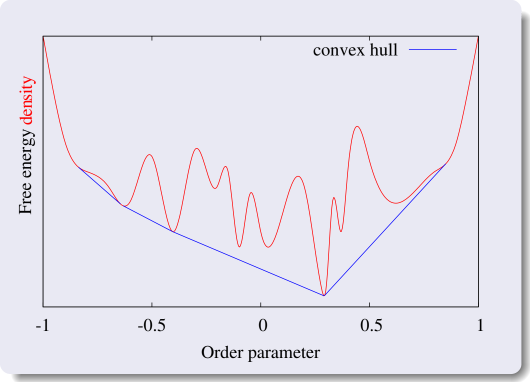


Slow dynamics (both experiment and numerics)
$\tau_{1,2} \propto \exp[\Delta F_B / k_B T]$

Typical experimental setting: non-equilibrium.

Foreword: from cartoons to actual computations



Thermodynamic limit $\longrightarrow$ convex free-energy density: throwing out the baby with the bath water.

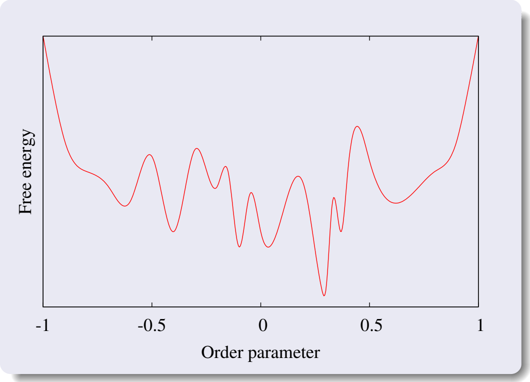
Message from spin-glasses (Franz et al. 98', Barrat & Berthier 01',

Janus collaboration 10')

time-length dictionaries:

Non-eq. finite time/ Eq. finite size

Foreword: from cartoons to actual computations



Our goal here:

Compute real free-energy profiles on complex, finite systems. Use them to

1. Overcome barriers
2. Tame huge fluctuations.

Plan of the talk

1. Some (avoidable!) huge fluctuations in disordered systems, and their cure. See also next talk by A. Gordillo-Guerrero.
2. How to compute free-energy profiles: tethered Monte Carlo.
3. A working example without quenched disorder: hard-spheres crystallization.
4. Taming large fluctuations in disordered systems:
   - RFIM-like models: the Diluted Anti-Ferromagnet in a Field (DAFF).
   - First success in a still untamed problem: temperature-chaos in spin-glasses (see poster by Beatriz Seoane).

Avoidable huge fluctuations in Disordered systems

Canonical ensemble + metastability + quenched disorder = disaster

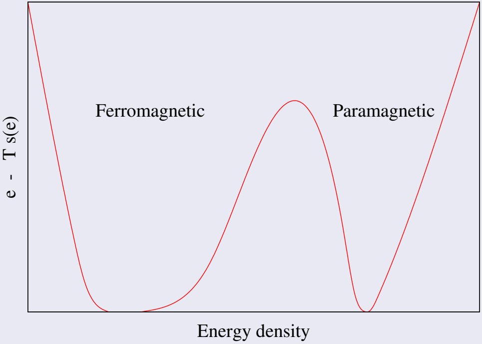
Complex systems: we can only dispense with Canonical ensemble

Avoidable huge fluctuations in Disordered systems

Canonical ensemble + metastability + quenched disorder = disaster

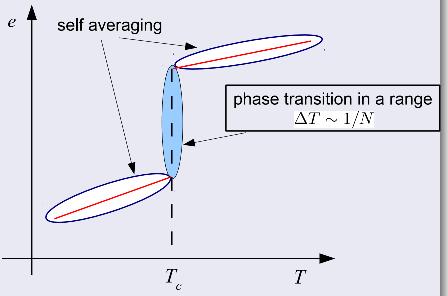
Take simple problem: site-diluted ferromagnetic Potts model.

Unfrustrated, but disordered. First-order transition with temperature, from paramagnetic to ferromagnetic state.



Avoidable huge fluctuations in Disordered systems

Rare events dominate disorder average (Berche et al. 2005)



- Phase-coexistance: specific heat is $C \sim L^D \propto N$

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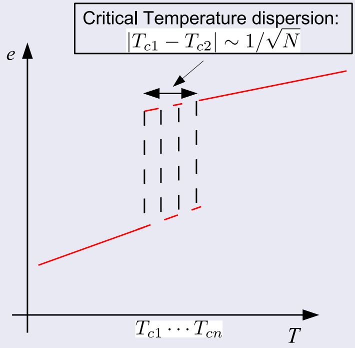

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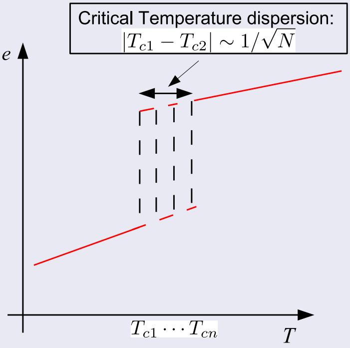
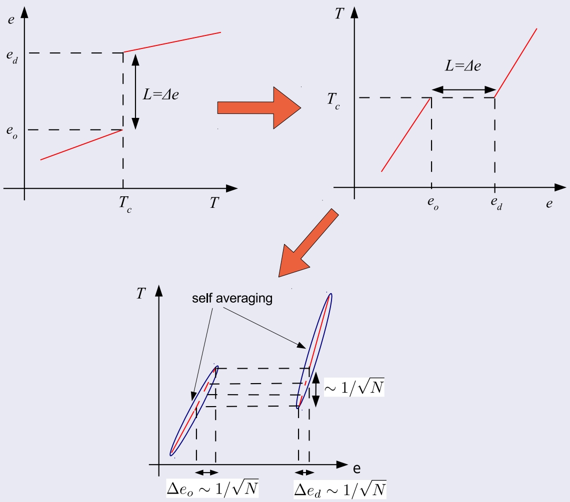


- Phase-coexistance: specific heat is $C \sim L^D \propto N$
- Fixed T: fraction of samples at phase coexistance $\sim \frac{1}{\sqrt{N}}$
- Rare-events dominance: $\overline{C} \propto N \times \frac{1}{\sqrt{N}} = \sqrt{N}$.

Avoidable huge fluctuations in Disordered systems

Self-averageness in the microcanonical ensemble (crucial in next talk!)



Tethering (I): computing the free-energy profile

(Martin-Mayor 07'; Fernandez, Martin-Mayor, Yllanes 09', Martin-Mayor, Yllanes, Seoane 11')

Take, for instance, Ising model

- Square or cubic lattice, periodic boundary conditions.
- Partition function and main observables ($N = L^D$):

$$Z = \sum_{\{\sigma_{\boldsymbol{x}}\}} \exp\left[\beta \sum_{\langle \boldsymbol{x},\boldsymbol{y}\rangle} \sigma_{\boldsymbol{x}}\sigma_{\boldsymbol{y}} + h \sum_{\boldsymbol{x}} \sigma_{\boldsymbol{x}}\right], \qquad \sigma_{\boldsymbol{x}} = \pm 1,$$

$$U = Nu = -\sum_{\langle \boldsymbol{x},\boldsymbol{y}\rangle} \sigma_{\boldsymbol{x}}\sigma_{\boldsymbol{y}}, \qquad M = Nm = \sum_{\boldsymbol{x}} \sigma_{\boldsymbol{x}}.$$

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Take, for instance, Ising model

Trivial bath of decoupled daemons (Gaussian, Poissonian,etc.); we have α daemons per spin:

$$\hat{Z}_{\text{bath}} = \int_{-\infty}^{\infty} \prod_{a=1}^{\alpha N} \frac{\mathrm{d}\eta_a}{\sqrt{2\pi}} \, \mathrm{e}^{-\frac{1}{2}\sum_a \eta_a^2} = 1$$

Artificially couple spins to daemons

$$\hat{M} = N\hat{m} = Nm + \frac{1}{2\alpha}\sum_a \eta_a^2 \quad \longrightarrow \text{Lustig's microcanonic Monte Carlo}$$

$$\hat{M} = N\hat{m} = Nm + \frac{1}{\alpha}\sum_a \eta_a \quad \longrightarrow \text{Umbrella sampling}$$

Tethering (II): computing the free-energy profile

Study constrained ensemble: fixed $\hat{m}$

For instance, linear daemon-spins coupling

$$\mathrm{e}^{-N\Omega_N(\beta,\hat{m})} = \sum_{\{\sigma_{\boldsymbol{x}}\}} \int_{-\infty}^{\infty} \prod_{a=1}^{\alpha N} \frac{\mathrm{d}\eta_a}{\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}\sum_a \eta_a^2}\, \mathrm{e}^{-\beta U}\, \delta\left[\hat{M} - Nm - \frac{1}{\alpha}\sum_a \eta_a\right]$$

Tethering (II): computing the free-energy profile

Study constrained ensemble: fixed $\hat{m}$

$\Omega_N(\beta, \hat{m})$: Helmholtz free-energy density for N spins,

$$Z(\beta, h) = \text{“trivial factor”} \times \int \mathrm{d}\hat{m}\, \mathrm{e}^{-N[\Omega_N(\beta,\hat{m}) - h\hat{m}]}$$

Integrate-out daemons $\to$ tethered weight: dog-leash of length $\sqrt{\frac{1}{\alpha N}}$

$$\mathrm{e}^{-N\Omega_N(\beta,\hat{m})} = \sqrt{\frac{\alpha}{2\pi N}} \sum_{\{\sigma_{\boldsymbol{x}}\}} \mathrm{e}^{-\beta U} \exp\left[-\frac{N\alpha}{2}(\hat{m} - m)^2\right]$$

Tethering (III): computing the free-energy profile

- Local Monte Carlo (e.g. Metropolis) simulation at fixed $\hat{m}$, β is simple. Also cluster methods available (Martin-Mayor 07'; Martin-Mayor, Yllanes 09').
- Reconstruction of Helmholthz free-energy from fluctuation-dissipation

$$\frac{\partial \Omega_N}{\partial \hat{m}} = \langle \hat{h} \rangle_{\beta,\hat{m}}\,, \quad \hat{h} = \alpha(\hat{m} - m)$$

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Compute $\langle \hat{h} \rangle_{\beta,\hat{m}}$ in a $\hat{m}$-mesh, then compute a line integral. Generalization to several order parameters straighforward (virtually imposible with multi-histogram methods).

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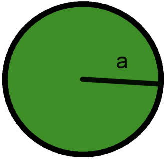
Think large:
Fluids: $m \sim$ particle-number density, $\hat{h} \sim$ pressure
Thermal systems: $m \sim$ internal energy, $\hat{h} \sim$ temperature
Antiferromagnets: $m \sim$ staggered magnetization, $\hat{h} \sim$ stagg. field
…

HS: spheres that do not overlap

$$V(r) = \begin{cases} \infty & r < \sigma \\ 0 & r > \sigma \end{cases}$$



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A working example: hard-spheres cristallization

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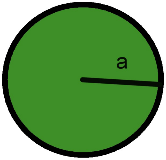

- All allowed configurations, same energy. Entropy rules.
- At high-density, crystalline solid has larger entropy than fluid.
  - Experimentally achieved 30 years later (Pusey and van Megen 86', Pusey et al. 89') than numerical prediction (Alder and Wainwright 57'; Wood and Jacobson 57') .
  - Face-Centered Cubic (FCC) crystal (Bolhuis et al. 97'; Mau, Huse 99')
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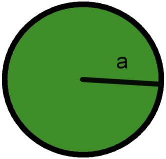

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  - Crystallization transition, a major challenge to computational physics:
    - Free-energy barriers: equilibrium simulation up to $N = 500$ HS only.
    - One needs to place by hand HS in FCC crystal positions. Good crystals do not form spontaneously in the simulation.

HS crystallization (II): which order parameter?

Goal: label unambiguously fluid $\longrightarrow$ crystal intermediate states.

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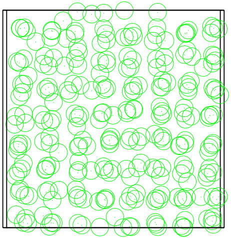
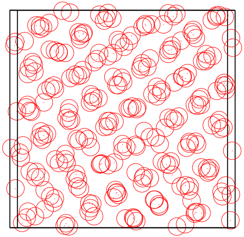
  The standard Q_6 is rotationally invariant (Steinhartdt et al. 83',ten Wolde et al., 95')

  Tethering large Q_6 ⟶ strong dependency on initial conditions

FCC start



Random start



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- But, for intermediate C, two compiting states:
  - Helicoidal, missaligned crystals: large Q_6.
  - Phase-separated liquid/solid mixture: small Q_6.

We need both Q_6 and C.

HS (III): The coexistence pressure (Fernandez, VMM,Seoane, Verrocchio 12')

- Fixed-pressure gradient of Helmholtz potential:

$$\nabla \Omega_N(\hat{Q}_6, \hat{C}) = \alpha\big(\hat{Q}_6 - \langle Q_6(\{\boldsymbol{r}\})\rangle_{\hat{Q}_6,\hat{C}}\,,\ \hat{C} - \langle C(\{\boldsymbol{r}\})\rangle_{\hat{Q}_6,\hat{C}}\big)\,.$$

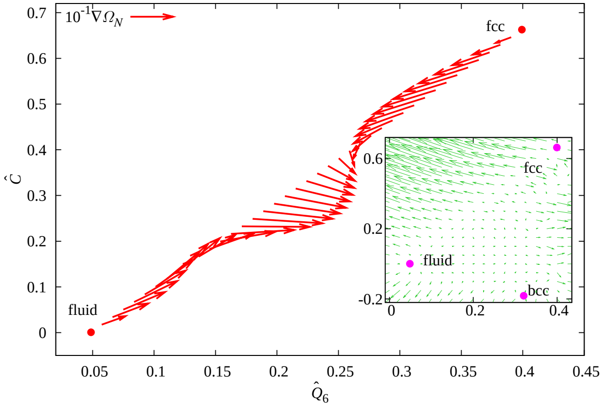
- Large N expansion: dominated by minimum at $(\hat{Q}_6^*, \hat{C}^*)$

$$\mathrm{e}^{-N\beta g(p,T)} = \int \mathrm{d}\hat{C}\hat{Q}_6\,\mathrm{e}^{-N\Omega_N(\hat{Q}_6,\hat{C})}\,,\ g(p,T) = \Omega_N(\hat{Q}_6^*, \hat{C}^*) + \mathcal{O}(1/N)\,.$$

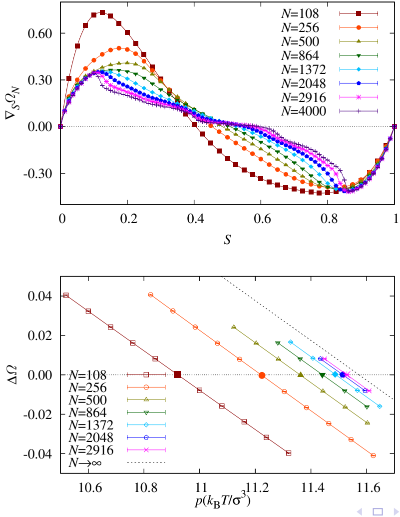
- Locate minimum: $\nabla \Omega_N(\hat{Q}_6^*, \hat{C}^*) = 0$
- If several local minima are relevant, compute line-integral to get relative weight.

HS (III): The coexistence pressure (Fernandez, VMM,Seoane, Verrocchio 12')

Equal chemical-potential: $\Omega_N(\hat{Q}_6^{\text{liquid}}, \hat{C}^{\text{liquid}}) = \Omega_N(\hat{Q}_6^{\text{FCC}}, \hat{C}^{\text{FCC}})$



Line parameter S: $S = 0$ fluid, $S = 1$ FCC; p: volume-histogram reweighting



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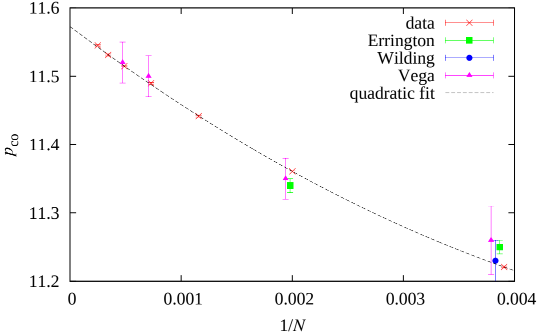
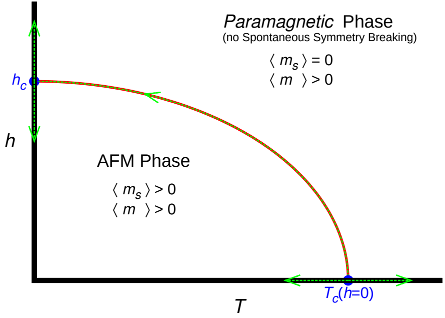


Our estimate ($k_B T/\sigma^3$ units)	$p_{co}^{N=\infty} = 11.5727(10)$
Previous equilibrium (Wilding & Bruce 2000)	$p_{co}^{N=\infty} = 11.50(9)$
Non-equilibrium ($N = 1.6 \times 10^5$, Zykova-Timan, 2010)	$p_{co}^{N=\infty} = 11.576(6)$

Disordered systems: the DAFF (and the RFIM)

- Next talk: the Cardy-Jacobsen conjecture
- Experimental RFIM: Diluted Anti-Ferromagnet in a Field.
- Two order parameters:
  - $m_s = \frac{1}{V}\sum_i (-1)^{x_i+y_i+z_i}\epsilon_i s_i$: AFM ordering.
  - $m = \frac{1}{V}\sum_i \epsilon_i s_i$: FM ordering.



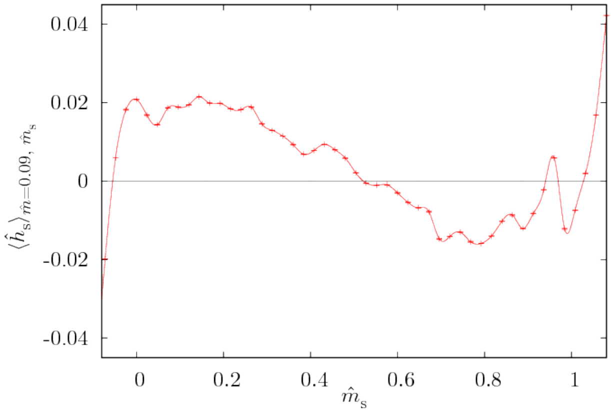
- $T = 0$ fixed-point: hyperscaling-violations exponent θ.
- θ extremely elusive.
- Dramatic self-averageness violations (Parisi and Sourlas 02')

We tether both order parameters

$$h \leftrightarrow m \text{ and } h_s \leftrightarrow m_s \;:\quad Z_N(\beta, h, h_s) \leftrightarrow \Omega_N(\beta, \hat{m}, \hat{m}_s)\,.$$

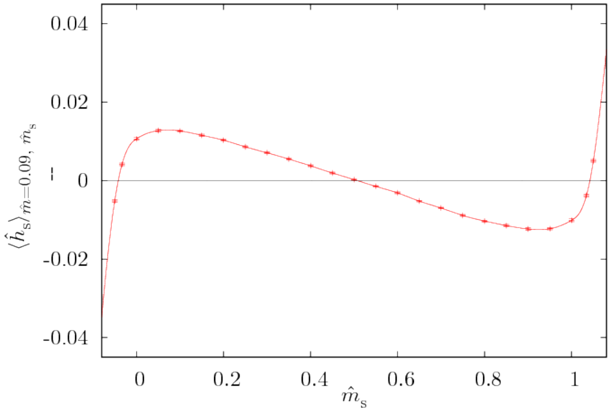
We will be looking at $h_s = 0^+$ (spontaneous symmetry breaking).

Corrugated landscape: $\langle \hat{h}_s \rangle = \frac{\partial \Omega}{\partial \hat{m}_s}$ for a single $L = 24$ sample.



Note that $\Omega(\hat{m}_s, \hat{m})$ has three minima and two maxima (at fixed $\hat{m}$).

But disorder-averaged $\overline{\langle h \rangle}$ and $\overline{\langle h_s \rangle}$ are smooth!!

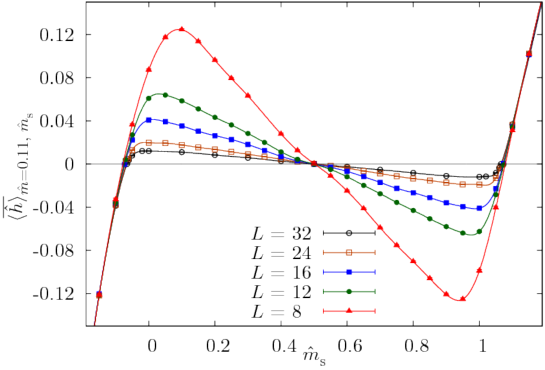


$\overline{\Omega}$ has only two symmetric minima separated by one central maximum.

Binder et al. 2010: $\overline{\Omega}_{\min} - \overline{\Omega}_{\max} \sim L^{\theta - D}$, first order transition: $\theta = D - 1 = 2$.

Tethered ($L \leq 32$, 1000 samples): $\theta = 1.469(20)$

Standard $T = 0$ ($L \leq 192$, 5×10^7 samples): $\theta = 1.4847(11)$ Fytas, VMM 13'



A yet untamed problem: spin glasses

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See poster by Beatriz Seoane

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- Caveat: finding useful order-parameters is crucial. It requires a strong physical command of the problem.