Monte Carlo simulations of (quasi) constrained ensembles

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in collaboration with
L.A. Fernández, A. Gordillo, J.J. Ruiz-Lorenzo, B. Seoane, P. Verrochio, and D. Yllanes,

Phys. Rev. Lett. **98,** 137207, (2007)

Phys. Rev. Lett. **100,** 057201, (2008)

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Phys. Rev. E **80,** 015701(R), (2009)

Phys. Rev. E, *in press*. arXiv:0910.4924

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Outline

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- Metastability is ubiquitous in Physics. In particular, first-order phase transitions and/or glassy behaviour.

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- For metastable systems (and maybe structural glasses), Exponential Critical Slowing Down

$$\tau \propto \mathrm{e}^{\Sigma L^{D-1}}, \quad (\Sigma: \text{ surface tension, D: space dimension}).$$

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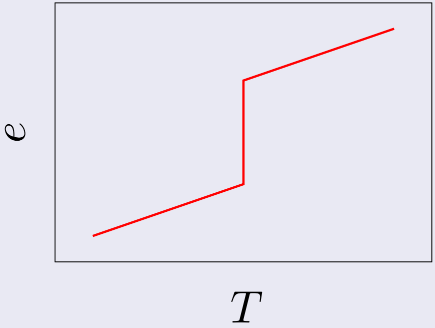
- Random-walks on reaction coordinate alleviate but do not cure. Reaction coordinate: temperature (Simulated Annealing, Parallel Tempering), energy (Wang-Landau, multicanonical), spin overlap (multioverlap), etc.

A different approach

Metastability

Discontinuity in intensive quantity (*reaction coordinate*) as a function of temperature, pressure,… in large N limit
($N = L^D$: number of degrees of freedom)



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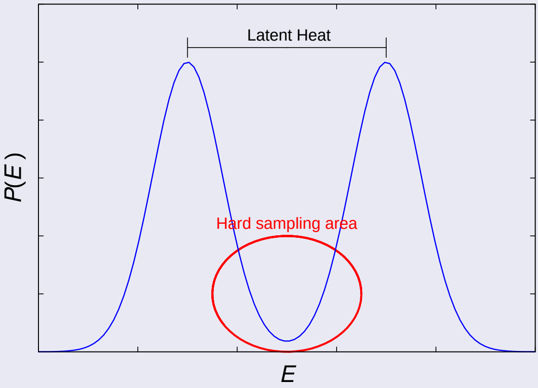
Discontinuity $\longrightarrow$ two-peaked pdf. Minimum $\sim \exp[-2\Sigma L^{D-1}]$.



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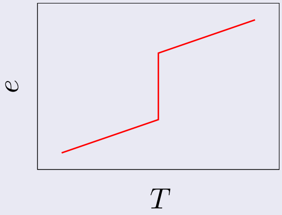
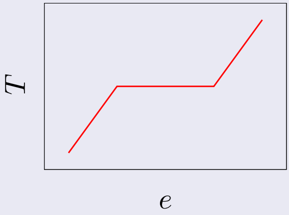
Idea: go microcanonical, and reconstruct the gentle function $\langle T \rangle_e$ from **Fluctuation-Dissipation Theorem.** Without random-walk.
Microcanonical MC: Lustig 98', FDT: Martin-Mayor 07' (see also de Pablo 03')

Advantages of micro *analysis* (even with canonical data!): Janke 98'.





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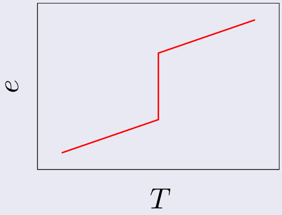

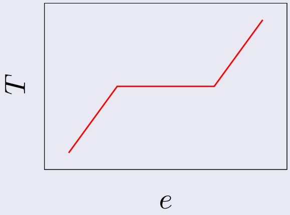

Sometimes not enough: feed extra information Tethered Monte Carlo.

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This talk' toy models

Ising and Potts models

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

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

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

- We denote canonical averages by $\langle \cdots \rangle_\beta$:

$$C = N\left[\langle u^2\rangle_\beta - \langle u\rangle_\beta^2\right], \qquad \chi = N\left[\langle m^2\rangle_\beta - \langle m\rangle_\beta^2\right].$$

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- Variation: Q-states Potts model, $\sigma_{\boldsymbol{x}} = 1, 2, \ldots, Q$.

Effective potentials

The problem

- Standard thermodynamic hand-waving:

$$Z(\beta) = \int \mathrm{d}u\, \mathrm{e}^{N[s(u)-\beta u]} \approx \mathrm{e}^{N[s(u^*)-\beta u^*]} \quad , \quad \beta = \left.\frac{\mathrm{d}s}{\mathrm{d}u}\right|_{u=u^*}$$

$$Z(\beta, h) = \int \mathrm{d}m\, \mathrm{e}^{N[\Omega_\beta(m)-hm]} \approx \mathrm{e}^{N[\Omega_\beta(m^*)-hm^*]} \quad , \quad h = \left.\frac{\partial \Omega_\beta}{\partial m}\right|_{m=m^*}$$

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- Yet, m and u discretized variables for finite N:

$$\Delta m, \Delta u \sim \frac{1}{N}\,.$$

$s(u), \Omega_\beta(m)$: comb-like sums of Dirac's delta functions.
Smooth effective potentials require coarse-graining.

The construction of the entropy density $s(e)$

- Artificially add conjugate momenta $\{\sigma_{\boldsymbol{x}}\} \longrightarrow \{\sigma_{\boldsymbol{x}}, \pi_{\boldsymbol{x}}\}$
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- $p_\beta(e)$ is a convolution (κ and u independent!):

$$p_\beta(e) = \int\int \mathrm{d}\kappa \mathrm{d}u\; p_{\beta,u}(u) p_{\beta,\kappa}(\kappa)\, \delta(e - u - \kappa)\,.$$

  $\kappa = \frac{1}{2\beta}\left[1 + \zeta\sqrt{\frac{2}{N}}\right]$, $\zeta \sim 1$ and (almost) Gaussian distributed.
  $p_{\beta,u}(u)$ gets shifted by $\frac{1}{2\beta}$ and smoothed.

Effective potentials

Tethered effective potential $\Omega_N(\hat{m}, \beta)$, analogue to $s(e, N)$

- Conjugate momenta now leave unchanged $Z(\beta)$

$$Z(\beta) = \sum_{\{\sigma_{\boldsymbol{x}}\}} \int \prod_{\boldsymbol{x}} \frac{\mathrm{d}\pi_{\boldsymbol{x}}}{\sqrt{2\pi}} \mathrm{e}^{-\beta U \, - \, \sum_{\boldsymbol{x}} \frac{\pi_{\boldsymbol{x}}^2}{2}} \, .$$

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- We couple $\pi_{\boldsymbol{x}}$ with order parameter:

$$p_\beta(\hat{m}) = \frac{1}{Z} \sum_{\{\sigma_{\boldsymbol{x}}\}} \int \prod_{\boldsymbol{x}} \frac{\mathrm{d}\pi_{\boldsymbol{x}}}{\sqrt{2\pi}} \mathrm{e}^{-\beta U} \delta(N\hat{m} - Nm - \sum_{\boldsymbol{x}} \frac{\pi_{\boldsymbol{x}}^2}{2}) = \mathrm{e}^{N\Omega_N(\hat{m},\beta)}$$

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- $\hat{m} \approx m + \frac{1}{2}$: $p_\beta(\hat{m})$ is a convolution of $p_{\beta,m}$ and $p_{\beta,r}$.

The microcanonical ensemble

(β and e reverse their roles)

- Integrate-out $\{\pi_{\boldsymbol{x}}\}$: microcanonical mean value at fixed e! (Lustig 98')

$$\exp\left[N\, s(e,N)\right] = \sum_{\{\sigma_{\boldsymbol{x}}\}} \int \prod_{\boldsymbol{x}} \mathrm{d}\pi_{\boldsymbol{x}}\, \delta\Big(\frac{1}{2}\sum_{\{\sigma_{\boldsymbol{x}}\}} \pi_{\boldsymbol{x}}^2 + uN - eN\Big)\,,$$

$$= \textit{constant} \times \sum_{\{\sigma_{\boldsymbol{x}}\}} (e-u)^{\frac{N-2}{2}}\, \theta(e-u).$$

$$\langle O\rangle_e = \frac{\sum_{\{\sigma_{\boldsymbol{x}}\}} O(e;\{\sigma\})\,\omega^{\mathrm{mic}}(\{\sigma\})}{\sum_{\{\sigma_{\boldsymbol{x}}\}} \omega^{\mathrm{mic}}(\{\sigma\})}\,, \qquad \omega^{\mathrm{mic}} = (e-u)^{\frac{N-2}{2}}\,\theta(e-u)\,.$$

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  - We have an extensive number of daemons.
  - Daemons are continuous variables.
  - We integrate them out.

The tethered ensemble

- Integrating demons out in the *constrained* (fixed $\hat{m}$) partition function $\rightarrow$ tethered expectation values:

$$\langle O \rangle_{\hat{m},\beta} = \frac{\sum_{\{\sigma_{\boldsymbol{x}}\}} O(\hat{m}; \{\sigma_{\boldsymbol{x}}\}) \omega^{\text{teth}}(\beta, \hat{m}, N; \{\sigma_{\boldsymbol{x}}\})}{\sum_{\{\sigma_{\boldsymbol{x}}\}} \omega^{\text{teth}}(\beta, \hat{m}, N; \{\sigma_{\boldsymbol{x}}\})},$$

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$$\hat{h}(\hat{m};\{\sigma_{\boldsymbol{x}}\}) = -1 + \frac{N/2-1}{\hat{M}-M} \quad \Longrightarrow \quad \langle \hat{h} \rangle_{\hat{m},\beta} = \frac{\partial \Omega_N(\hat{m},\beta)}{\partial \hat{m}}.$$

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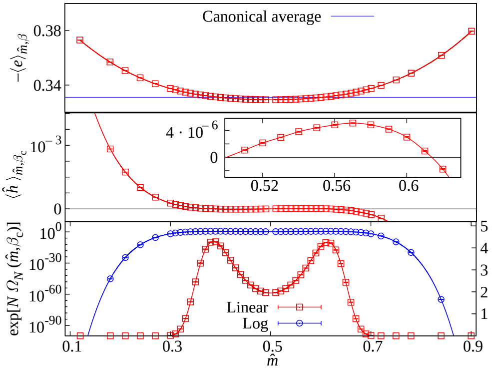
- Tethered mean values $\langle O \rangle_{\hat{m},\beta}$ ↔ canonical mean values $\langle O \rangle_{\beta}(h)$, for any external field h:

$$\langle O \rangle_{\beta}(h) = \int \mathrm{d}\hat{m}\ \langle O \rangle_{\hat{m},\beta} \exp[N(\Omega_N(\hat{m},\beta) + h\hat{m})].$$

A prototypical tethered computation



Result: $\langle u\rangle_{\beta_c} = -0.330\,983\,1(15)$

(Ising, $L = 128$, $D = 3$)

Steps

1. Select a mesh of $\hat{m}$ values.

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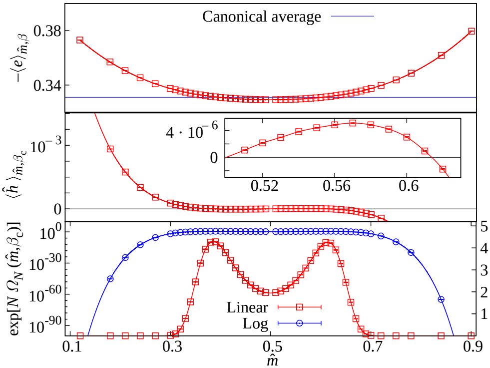

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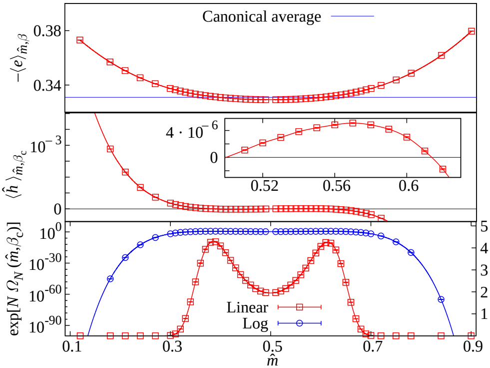

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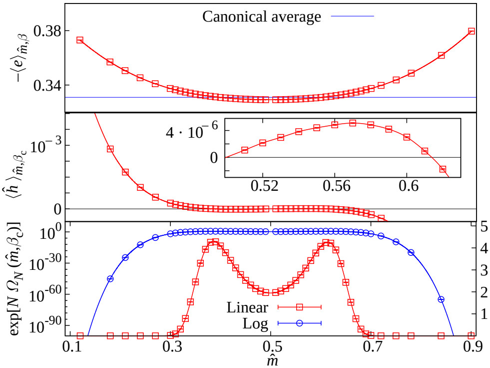

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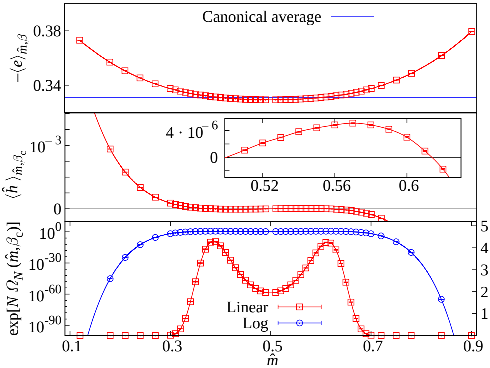

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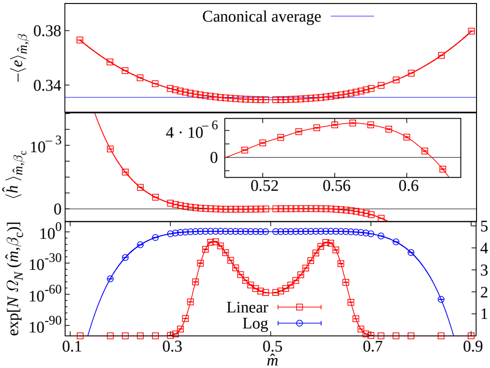

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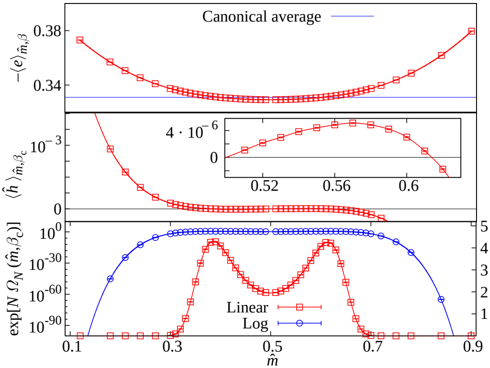

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Outline

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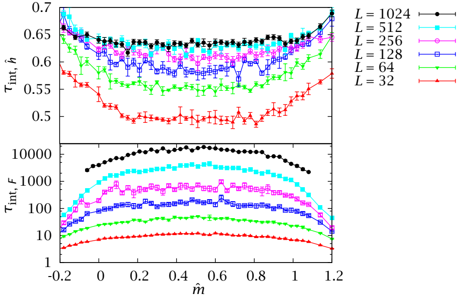
- Discrete spin sistems: p_{accept} takes a finite number of values $\Longrightarrow$ Look-up-table provide significant speed-up.

Autocorrelation times for Metropolis



- τ_{int}: dramatic dependence on observable, and on $\hat{m}$.
- Functions of m (e.g. $\hat{h}$): no measurable critical slowing down.
- Energy or propagator's Fourier transform ($\vec{k} \neq 0$) $\tau_{\mathrm{int}}(\hat{m} = 0.5) \approx L^2$
  Worst case: $m \sim 0$ or $\hat{m} = \frac{1}{2}$.

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  - $k = \langle\hat{\beta}\rangle_e \longrightarrow$ Potts model: $p^{\text{cluster}}_{\text{accept}} \approx 60\%$.

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- We can follow the Fortuin-Kasteleyn construction.
- Edwards-Sokal: introduce bond-occupation variables n_{xy} $(=0,1)$

$$\exp[\beta(\sigma_x\sigma_y-1)] = \sum_{n_{xy}=0,1} [(1-p)\delta_{n_{xy},0} + p\delta_{\sigma_x,\sigma_y}\,\delta_{n_{xy},1}], \quad p = 1-e^{-2\beta}.$$

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  - Given $\{n_{xy}\}$, the spins within cluster i are equal to $S_i = \pm 1$. Not all $\{S_i\}$ configurations have the same probability:

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b) Cluster flipping:

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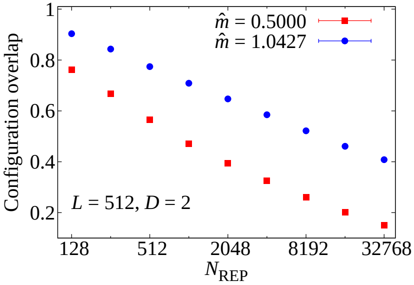

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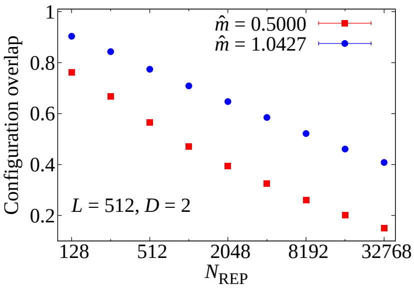

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Integrated autocorrelation times

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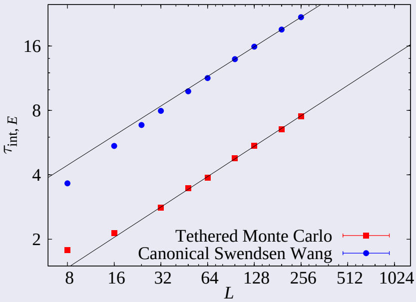

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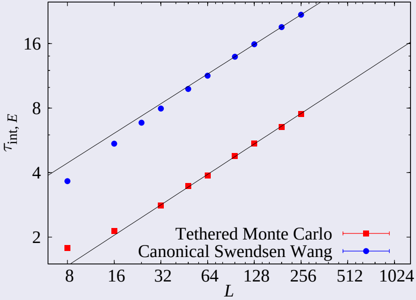

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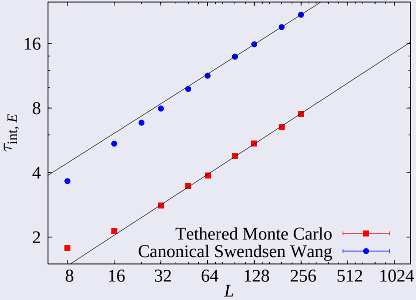

Canonical averages for $L = 128$, $D = 3$

	MCS	$-\langle e \rangle_\beta$	C	χ	ξ
SW	48×10^6	0.3309822(16)	22.155(18)	21193(13)	82.20(3)
TMC	50×10^6	0.3309831(15)	22.174(13)	21202(13)	82.20(5)

Outline

A standard example: $D = 2,\ Q = 10$, Potts model

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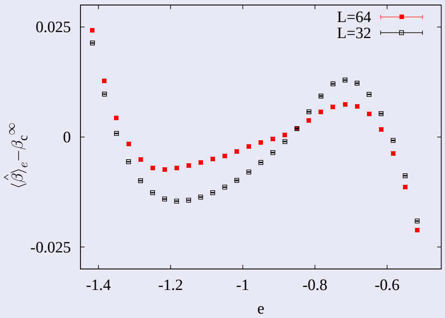

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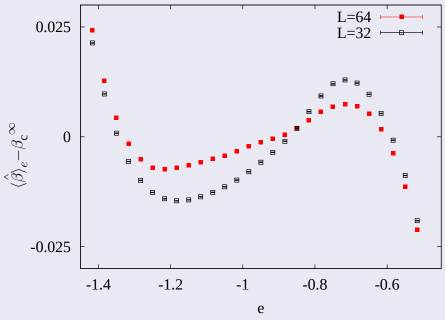

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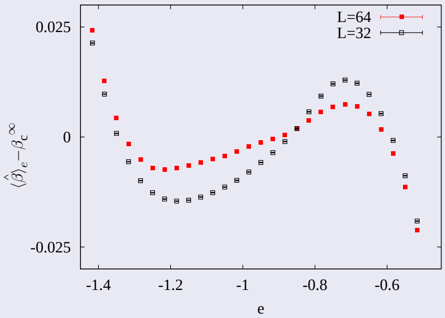

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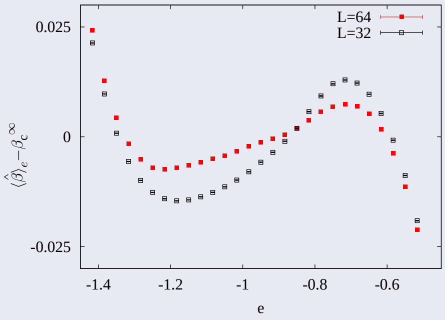

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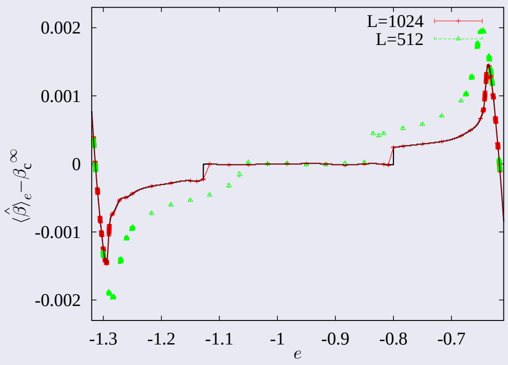
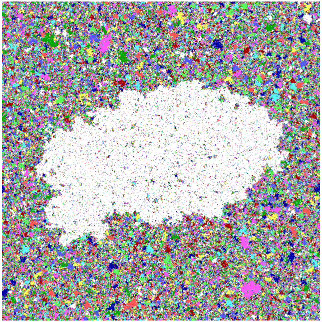
- Surface tension:

$$\Sigma_L = \frac{L}{2} \int_{e^*}^{e_d} \mathrm{d}e \, (\langle\hat{\beta}\rangle_e - \beta_c)$$

Geometric transitions





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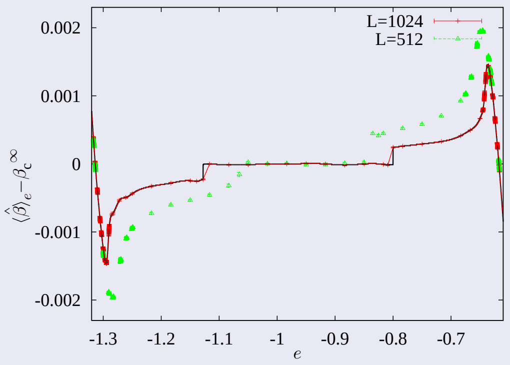

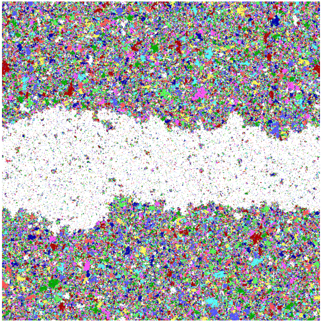

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Sample-to-sample variance of specific-heat, magnetic susceptibility, etc., expressed in natural units, is diverging in large L limit (long-tailed $P(\chi_J/\overline{\chi_J})$, Berche et al. 05)

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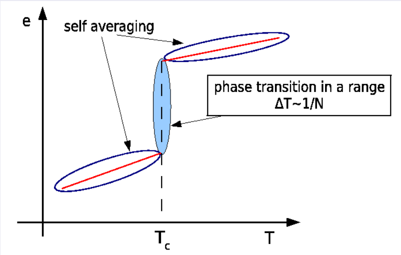
- Two types of variables, dynamical (i.e. spins) and quenched (geologically slow: atomic impurities, vacancies, etc.).
- Impurities $\longrightarrow$ random Hamiltonian H_J. Site-dependent coupling constants (sample), extracted from some pdf $P(J)$.
- Quenched approximation: fast variables (spins) allowed **no backreaction** on slow ones. In practice:
  1. Take J-dependent thermal average $\langle \ldots \rangle_J$.
  2. Average $\langle \ldots \rangle_J$ with $P(J)$.
- Metastability in single sample already bad enough, yet even worse. . .

Sample-to-sample variance of specific-heat, magnetic susceptibility, etc., expressed in natural units, is diverging in large L limit (long-tailed $P(\chi_J/\overline{\chi_J})$, Berche et al. 05)

$\Longrightarrow$ need **huge** number of samples.

Why rare events (Berche et al' 05)?



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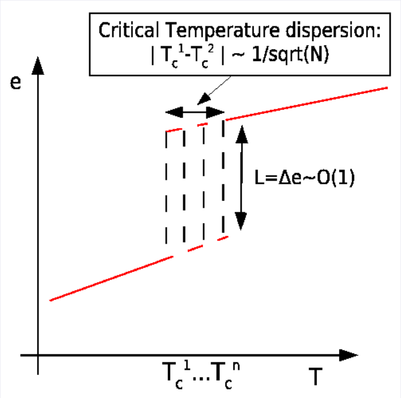

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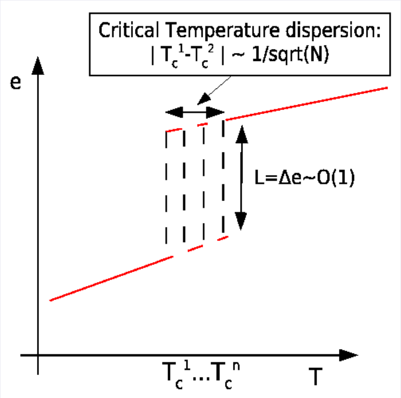

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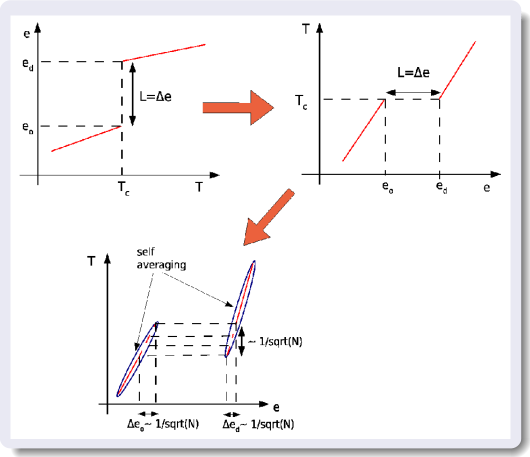
- Rare events dominated: $\overline{C} \propto N \times \frac{1}{\sqrt{N}} = \sqrt{N}$, (saturates Chayes bound)

The microcanonical cure



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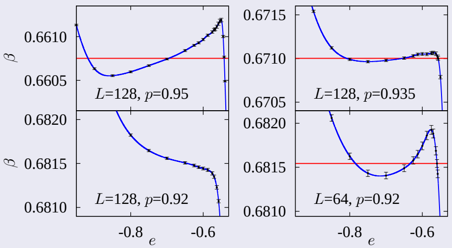

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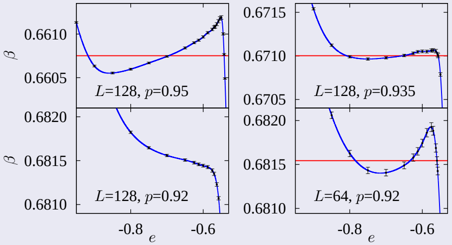

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- $\langle\hat{\beta}\rangle_e$ self-averaging
- Scaling analysis: survival of first-order transition (Gordillo et al. 08).

Outline

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- For disordered systems, these methods allow for a redefinition of the quenched averaged: we cured the rare events syndrome.