Coarse-graining the state space of a spin glass

Stefan Schnabel and Wolfhard Janke

CompPhys 17

Edwards-Anderson model

- Hamiltonian : $\mathcal{H}(s_1, \cdots, s_N) = -\sum_{\langle ij \rangle} J_{ij} s_i s_j, \quad s \in \{-1, 1\}$
- Gaussian disorder : $P(J) = \frac{1}{\sqrt{2\pi}} e^{-\frac{J^2}{2}}$
- Overlap of two configurations $Q(\mathbf{S}^\alpha, \mathbf{S}^\beta) = \frac{1}{N} \sum_i s_i^\alpha s_i^\beta$
- 3d – simple cubic lattice

Edwards-Anderson model

- Hamiltonian : $\mathcal{H}(s_1, \cdots, s_N) = -\sum_{\langle ij \rangle} J_{ij} s_i s_j, \quad s \in \{-1, 1\}$
- Gaussian disorder : $P(J) = \frac{1}{\sqrt{2\pi}} e^{-\frac{J^2}{2}}$
- Overlap of two configurations $Q(\mathbf{S}^\alpha, \mathbf{S}^\beta) = \frac{1}{N} \sum_i s_i^\alpha s_i^\beta$
- 3d – simple cubic lattice

Edwards-Anderson model

- Hamiltonian : $\mathcal{H}(s_1, \cdots, s_N) = -\sum_{\langle ij \rangle} J_{ij} s_i s_j, \quad s \in \{-1, 1\}$
- Gaussian disorder : $P(J) = \frac{1}{\sqrt{2\pi}} e^{-\frac{J^2}{2}}$
- Overlap of two configurations $Q(\mathbf{S}^\alpha, \mathbf{S}^\beta) = \frac{1}{N} \sum_i s_i^\alpha s_i^\beta$
- 3d – simple cubic lattice

Edwards-Anderson model

- Hamiltonian : $\mathcal{H}(s_1, \cdots, s_N) = -\sum_{\langle ij \rangle} J_{ij} s_i s_j, \quad s \in \{-1, 1\}$
- Gaussian disorder : $P(J) = \frac{1}{\sqrt{2\pi}} e^{-\frac{J^2}{2}}$
- Overlap of two configurations $Q(\mathbf{S}^\alpha, \mathbf{S}^\beta) = \frac{1}{N} \sum_i s_i^\alpha s_i^\beta$
- 3d – simple cubic lattice

meta stable states

- Local minima in energy
- Single-flip stable states, i.e., the flip of any spin will increase energy
- All spins have negative energy: $e_k = -\sum_{\langle ij \rangle} J_{ij} s_i s_j (\delta_{ik} + \delta_{jk}) < 0$ for all k

meta stable states

- Local minima in energy
- Single-flip stable states, i.e., the flip of any spin will increase energy
- All spins have negative energy: $e_k = -\sum_{\langle ij \rangle} J_{ij} s_i s_j (\delta_{ik} + \delta_{jk}) < 0$ for all k

meta stable states

- Local minima in energy
- Single-flip stable states, i.e., the flip of any spin will increase energy
- All spins have negative energy: $e_k = -\sum_{\langle ij \rangle} J_{ij} s_i s_j (\delta_{ik} + \delta_{jk}) < 0$ for all k

An algorithm to sample stable states

- Start with spin configuration $\mathbf{S}_0$ and random numbers $\{\xi\}$
- Minimize:
  $\mu(\mathbf{S}_0, \{\xi\}) = \{\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f\}, \quad \mathcal{H}(\mathbf{S}_i) > \mathcal{H}(\mathbf{S}_{i+1})$ and $\mathcal{H}(\mathbf{S}_f)$ is meta stable
- Find a weight function $W(\mathbf{S}_0, \{\xi\})$ such that all meta stable states are equally likely
- Run a Monte Carlo simulation by varying $\mathbf{S}_0$ and $\{\xi\}$ according to $W(\mathbf{S}_0, \{\xi\})$

An algorithm to sample stable states

- Start with spin configuration $\mathbf{S}_0$ and random numbers $\{\xi\}$
- Minimize:
  $\mu(\mathbf{S}_0, \{\xi\}) = \{\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f\}, \quad \mathcal{H}(\mathbf{S}_i) > \mathcal{H}(\mathbf{S}_{i+1})$ and $\mathcal{H}(\mathbf{S}_f)$ is meta stable
- Find a weight function $W(\mathbf{S}_0, \{\xi\})$ such that all meta stable states are equally likely
- Run a Monte Carlo simulation by varying $\mathbf{S}_0$ and $\{\xi\}$ according to $W(\mathbf{S}_0, \{\xi\})$

An algorithm to sample stable states

- Start with spin configuration $\mathbf{S}_0$ and random numbers $\{\xi\}$
- Minimize:
  $\mu(\mathbf{S}_0, \{\xi\}) = \{\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f\}, \quad \mathcal{H}(\mathbf{S}_i) > \mathcal{H}(\mathbf{S}_{i+1})$ and $\mathcal{H}(\mathbf{S}_f)$ is meta stable
- Find a weight function $W(\mathbf{S}_0, \{\xi\})$ such that all meta stable states are equally likely
- Run a Monte Carlo simulation by varying $\mathbf{S}_0$ and $\{\xi\}$ according to $W(\mathbf{S}_0, \{\xi\})$

An algorithm to sample stable states

- Start with spin configuration $\mathbf{S}_0$ and random numbers $\{\xi\}$
- Minimize:
  $\mu(\mathbf{S}_0, \{\xi\}) = \{\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f\}, \quad \mathcal{H}(\mathbf{S}_i) > \mathcal{H}(\mathbf{S}_{i+1})$ and $\mathcal{H}(\mathbf{S}_f)$ is meta stable
- Find a weight function $W(\mathbf{S}_0, \{\xi\})$ such that all meta stable states are equally likely
- Run a Monte Carlo simulation by varying $\mathbf{S}_0$ and $\{\xi\}$ according to $W(\mathbf{S}_0, \{\xi\})$

Minimization

- Chose random spin with positive energy from $\mathbf{S}_i$ and flip it $\rightarrow \mathbf{S}_{i+1}$
- Repeat until stable state is reached
- Base selection on local properties: Flip the spin with the largest random number

Minimization

- Chose random spin with positive energy from $\mathbf{S}_i$ and flip it $\rightarrow \mathbf{S}_{i+1}$
- Repeat until stable state is reached
- Base selection on local properties: Flip the spin with the largest random number

Weight function

- We use the number of spins with positive $n_{\mathrm{p}}(\mathbf{S})$ and negative $n_{\mathrm{n}}(\mathbf{S})$ energy of a spin configuration $\mathbf{S}$
- Probability of a particular sequence given $\mathbf{S}_0$:

  $$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0) = \prod_{i=0}^{f-1} \frac{1}{n_{\mathrm{p}}(\mathbf{S}_i)}$$

- Probability of a particular sequence given $\mathbf{S}_f$:

  $$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f) = \prod_{i=1}^{f} \frac{1}{n_{\mathrm{n}}(\mathbf{S}_i)}$$

- Bayes: $P(\mathbf{S}_f) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)} P(\mathbf{S}_0)$
- $W(\mathbf{S}_0, \{\xi\}) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}$

Weight function

- We use the number of spins with positive $n_{\mathrm{p}}(\mathbf{S})$ and negative $n_{\mathrm{n}}(\mathbf{S})$ energy of a spin configuration $\mathbf{S}$
- Probability of a particular sequence given $\mathbf{S}_0$:

$$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0) = \prod_{i=0}^{f-1} \frac{1}{n_{\mathrm{p}}(\mathbf{S}_i)}$$

- Probability of a particular sequence given $\mathbf{S}_f$:

$$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f) = \prod_{i=1}^{f} \frac{1}{n_{\mathrm{n}}(\mathbf{S}_i)}$$

- Bayes: $P(\mathbf{S}_f) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)} P(\mathbf{S}_0)$
- $W(\mathbf{S}_0, \{\xi\}) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}$

Weight function

- We use the number of spins with positive $n_{\mathrm{p}}(\mathbf{S})$ and negative $n_{\mathrm{n}}(\mathbf{S})$ energy of a spin configuration $\mathbf{S}$
- Probability of a particular sequence given $\mathbf{S}_0$:

$$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0) = \prod_{i=0}^{f-1} \frac{1}{n_{\mathrm{p}}(\mathbf{S}_i)}$$

- Probability of a particular sequence given $\mathbf{S}_f$:

$$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f) = \prod_{i=1}^{f} \frac{1}{n_{\mathrm{n}}(\mathbf{S}_i)}$$

- Bayes: $P(\mathbf{S}_f) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)} P(\mathbf{S}_0)$
- $W(\mathbf{S}_0, \{\xi\}) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}$

Weight function

- We use the number of spins with positive $n_{\mathrm{p}}(\mathbf{S})$ and negative $n_{\mathrm{n}}(\mathbf{S})$ energy of a spin configuration $\mathbf{S}$
- Probability of a particular sequence given $\mathbf{S}_0$:

$$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0) = \prod_{i=0}^{f-1} \frac{1}{n_{\mathrm{p}}(\mathbf{S}_i)}$$

- Probability of a particular sequence given $\mathbf{S}_f$:

$$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f) = \prod_{i=1}^{f} \frac{1}{n_{\mathrm{n}}(\mathbf{S}_i)}$$

- Bayes: $P(\mathbf{S}_f) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)} P(\mathbf{S}_0)$
- $W(\mathbf{S}_0, \{\xi\}) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}$

Weight function

- We use the number of spins with positive $n_{\mathrm{p}}(\mathbf{S})$ and negative $n_{\mathrm{n}}(\mathbf{S})$ energy of a spin configuration $\mathbf{S}$
- Probability of a particular sequence given $\mathbf{S}_0$:

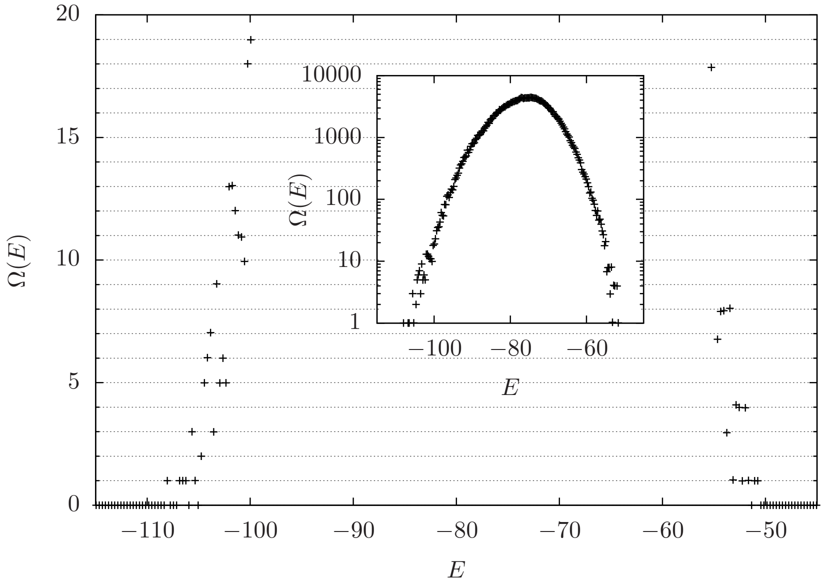
$$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0) = \prod_{i=0}^{f-1} \frac{1}{n_{\mathrm{p}}(\mathbf{S}_i)}$$

- Probability of a particular sequence given $\mathbf{S}_f$:

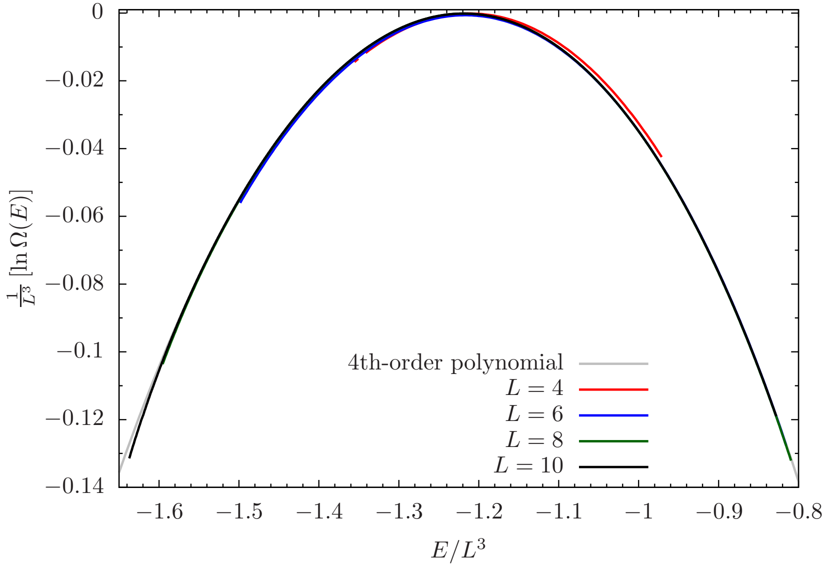
$$P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f) = \prod_{i=1}^{f} \frac{1}{n_{\mathrm{n}}(\mathbf{S}_i)}$$

- Bayes: $P(\mathbf{S}_f) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)} P(\mathbf{S}_0)$
- $W(\mathbf{S}_0, \{\xi\}) = \frac{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_f)}{P(\mathbf{S}_0, \mathbf{S}_1, \ldots, \mathbf{S}_f | \mathbf{S}_0)}$

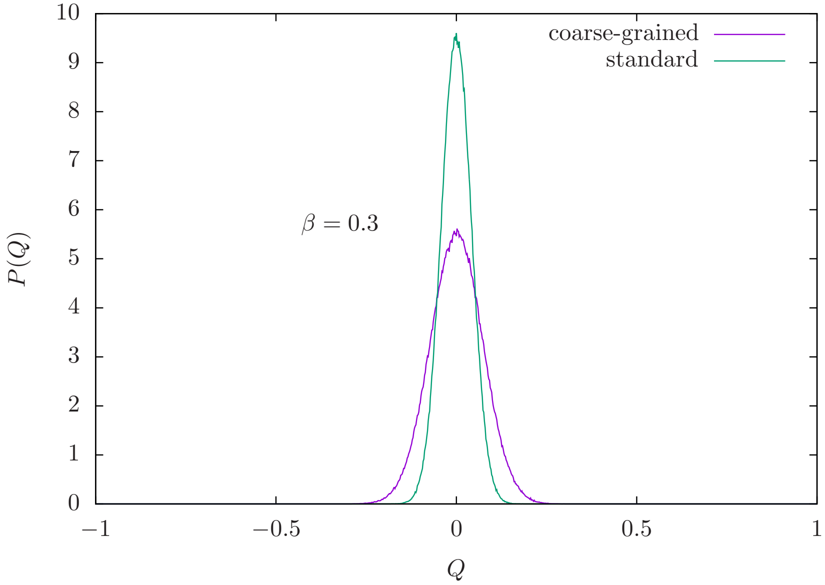
Distribution, single sample $L = 4$



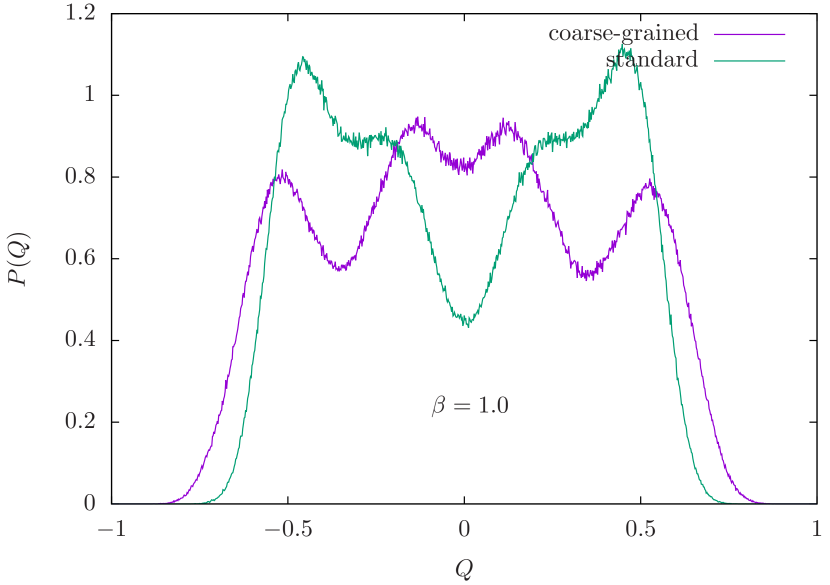
Distribution of meta stable states



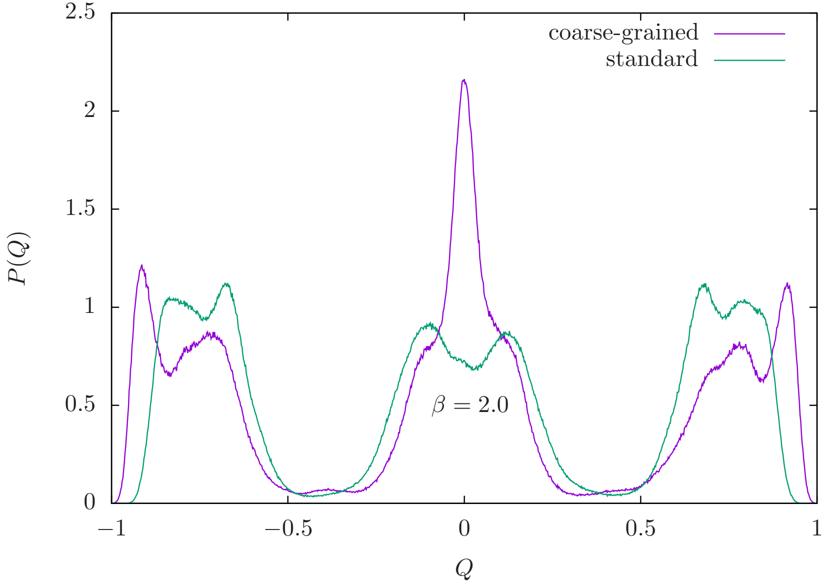
Overlap distributions single sample $L = 10$



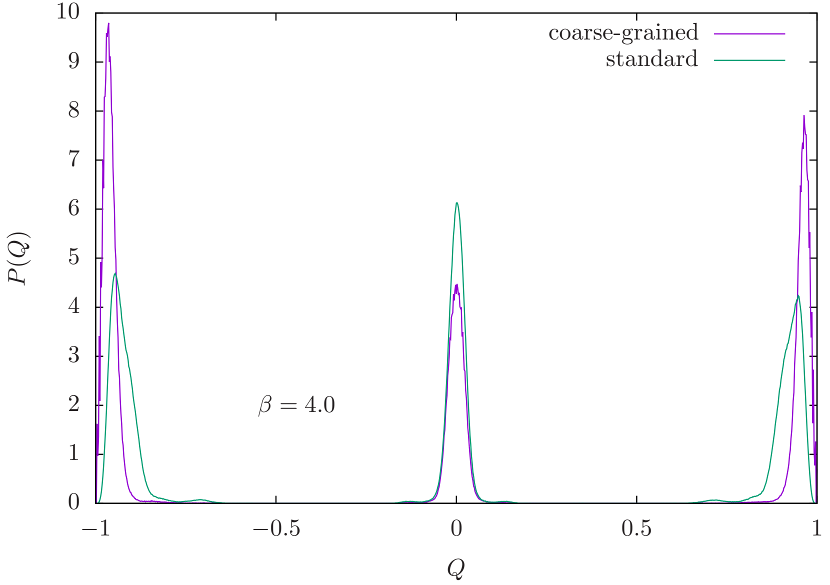
Overlap distributions single sample $L = 10$



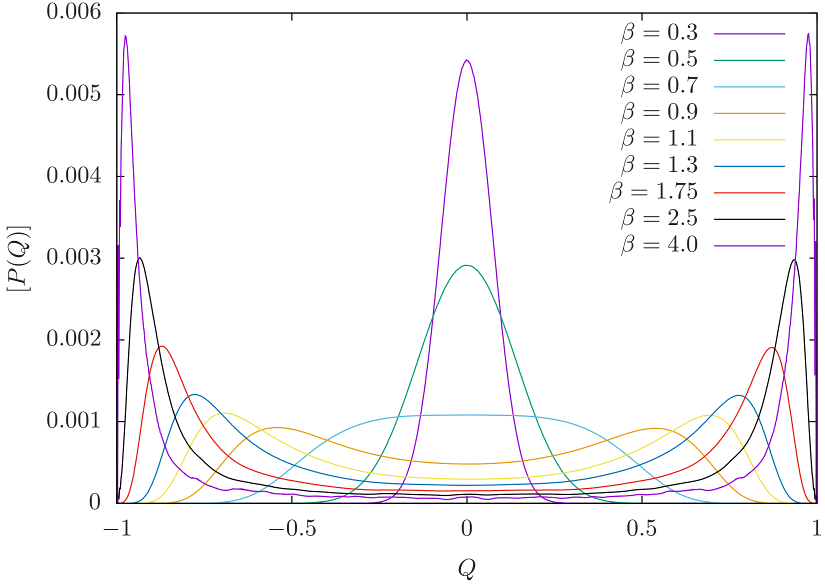
Overlap distributions single sample $L = 10$



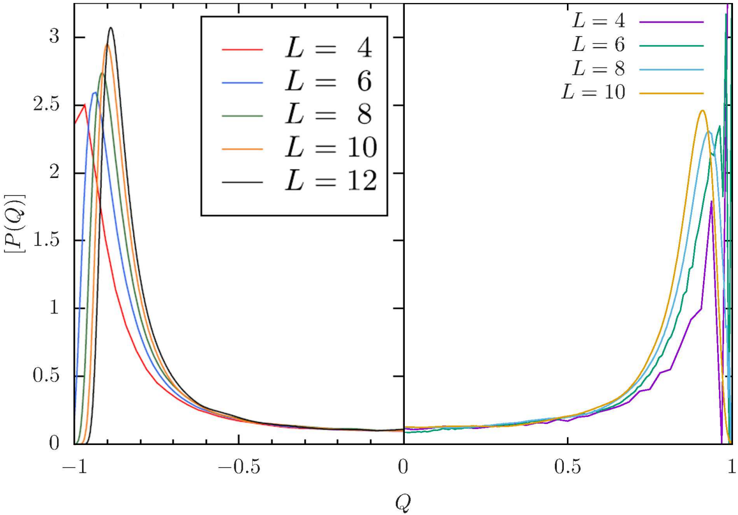
Overlap distributions single sample $L = 10$



Overlap distributions $L = 10$

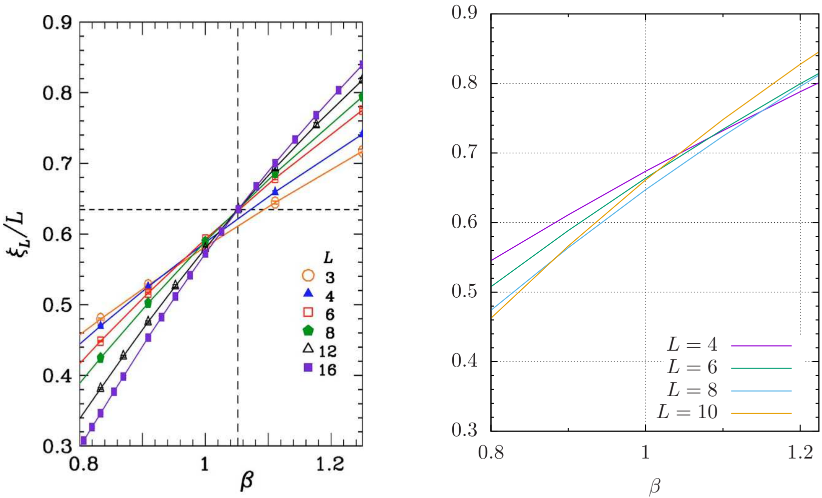


Overlap distribution T=0.42



B. Yucesoy, H. G. Katzgraber, and J. Machta, PRL **109**, 177204 (2012)

Correlation length



H. G. Katzgraber, M. Körner, and A. P. Young, Phys Rev B **73**, 224432 (2006)

Concluding remarks

- The distribution of local minima can be determined with great accuracy.
- The algorithm is more effective than standard single spin-flip dynamics.
- Overlap-distributions differ for single samples, but are similar on average.

Concluding remarks

- The distribution of local minima can be determined with great accuracy.
- The algorithm is more effective than standard single spin-flip dynamics.
- Overlap-distributions differ for single samples, but are similar on average.

Concluding remarks

- The distribution of local minima can be determined with great accuracy.
- The algorithm is more effective than standard single spin-flip dynamics.
- Overlap-distributions differ for single samples, but are similar on average.

Concluding remarks

- The distribution of local minima can be determined with great accuracy.
- The algorithm is more effective than standard single spin-flip dynamics.
- Overlap-distributions differ for single samples, but are similar on average.

Thanks for your attention