

# CLUSTER VARIATION METHOD: FROM STATISTICAL MECHANICS TO MESSAGE PASSING ALGORITHMS

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- Variational free energy
- Exactness, realizability, convexity, bounds
- Message-passing algorithms
- Double-loop algorithms
- Applications to disordered systems

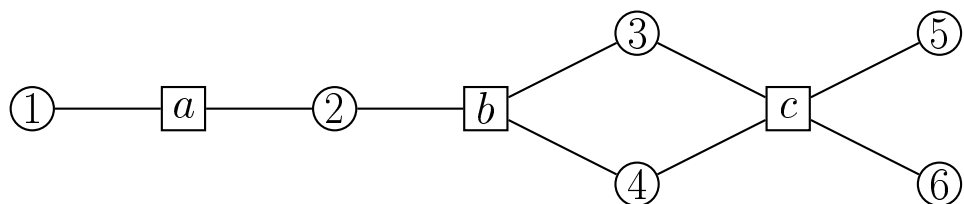
# Probabilistic Graphical Models and Statistical Mechanics Models

**Factor graph representation** (esp. useful for non-pairwise interactions)

$$H(s_1, s_2, s_3, s_4, s_5, s_6) = H_a(s_1, s_2) + H_b(s_2, s_3, s_4) + H_c(s_3, s_4, s_5, s_6)$$

$$\phi_a = \exp(-H_a), \quad \dots$$

$$p(s_1, s_2, s_3, s_4, s_5, s_6) = \frac{1}{Z} \phi_a(s_1, s_2) \phi_b(s_2, s_3, s_4) \phi_c(s_3, s_4, s_5, s_6)$$



○ Variable node

□ Factor node

**Statistical mechanics models:**

$$H(s_1, s_2, \dots, s_N) = \sum_a H_a(s_a),$$

$$p(s_1, s_2, \dots, s_N) = \frac{1}{Z} \exp[-H(s_1, s_2, \dots, s_N)],$$

$$Z = \sum_{\{s_i\}} \exp[-H(s_1, s_2, \dots, s_N)]$$

**Probabilistic graphical models** (on an undirected graph, for simplicity)

$$p(s_1, s_2, \dots, s_N) = \frac{1}{Z} \prod_a \phi_a(s_a), \quad s_a = \{s_i, i \in a\}$$

$$Z = \sum_{\{s_i\}} \prod_a \phi_a(s_a),$$

Directed graphs: replace potentials  $\phi_a$  with conditional probabilities.

Different formulations of the same problem

One is often interested in computing **marginal distributions** and/or **configurations**.

## Cluster variation method (CVM)

- Variational principle of equilibrium statistical mechanics:

$$F = -\ln Z = \min_p \mathcal{F}(p) = \min_p \sum_s [p(s)H(s) + p(s) \ln p(s)]$$

$$\sum_s p(s) = 1$$

$$\hat{p}(s) = \frac{1}{Z} \exp[-H(s)] = \operatorname{argmin} \mathcal{F}$$

$$\mathcal{F}(p) = F + \sum_s p(s) \ln \frac{p(s)}{\hat{p}(s)}$$

- *Cluster* or *Region*: subset  $\alpha$  of the factor graph, such that if a factor belongs to  $\alpha$ , all its variable nodes belong to  $\alpha$

- Cluster probability, cluster energy, cluster entropy:

$$p_\alpha(s_\alpha) = \sum_{s \setminus s_\alpha} p(s)$$

$$H_\alpha(s_\alpha) = \sum_{a \in \alpha} H_a(s_a)$$

$$S_\alpha = - \sum_{s_\alpha} p_\alpha \ln p_\alpha$$

- Cumulant expansion of the entropy:

$$S_\alpha = \sum_{\beta \subseteq \alpha} \tilde{S}_\beta \quad \Leftrightarrow \quad \tilde{S}_\beta = \sum_{\alpha \subseteq \beta} (-1)^{n_\alpha - n_\beta} S_\alpha$$

$$\mathcal{F}(p) = \sum_s p(s) H(s) - \sum_\beta \tilde{S}_\beta$$

- Truncation of the cumulant expansion to a set  $R$  of clusters made of *maximal* clusters and all their subclusters

$$\sum_{\beta} \tilde{S}_{\beta} \simeq \sum_{\beta \in R} \tilde{S}_{\beta} = \sum_{\alpha \in R} a_{\alpha} S_{\alpha}$$

$$\mathcal{F}(\{p_{\alpha}, \alpha \in R\}) = \sum_{\alpha \in R} a_{\alpha} \mathcal{F}_{\alpha}(p_{\alpha})$$

$$\mathcal{F}_{\alpha}(p_{\alpha}) = \sum_{s_{\alpha}} [p_{\alpha}(s_{\alpha}) H_{\alpha}(s_{\alpha}) + T p_{\alpha}(s_{\alpha}) \ln p_{\alpha}(s_{\alpha})]$$

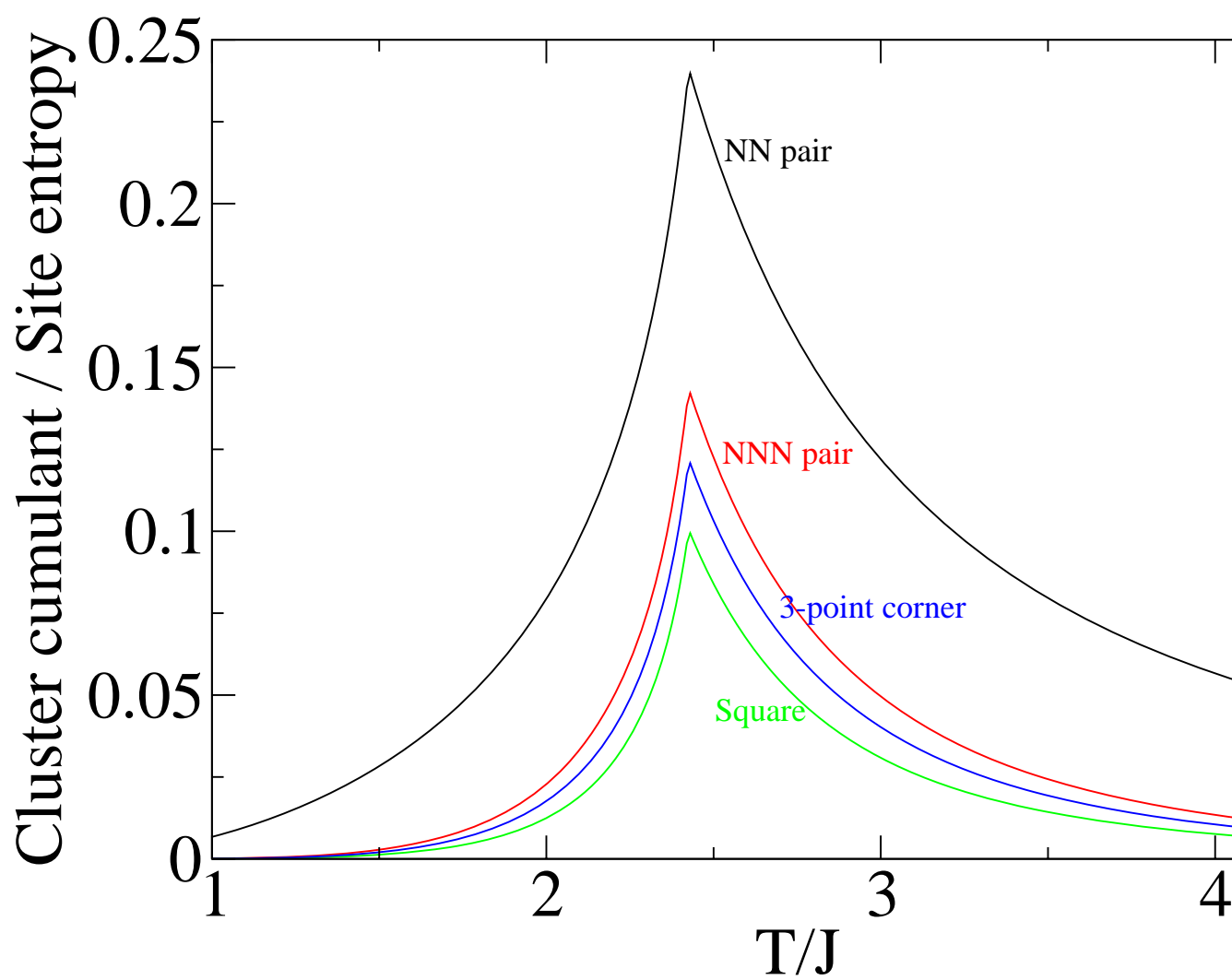
## Meaning of cumulants

Two weakly correlated variables

$$p_{12}(s_1, s_2) = p_1^{(0)}(s_1) p_2^{(0)}(s_2) [1 + \varepsilon \delta p(s_1, s_2)], \quad \varepsilon \ll 1$$

$$\tilde{S}_{12} = S_{12} - S_1 - S_2 = -\langle \ln [1 + \varepsilon \delta p(s_1, s_2)] \rangle = O(\varepsilon)$$

**Behaviour:** Ising model, square approximation



## APPLICATIONS TO LATTICE MODELS, CRITICAL

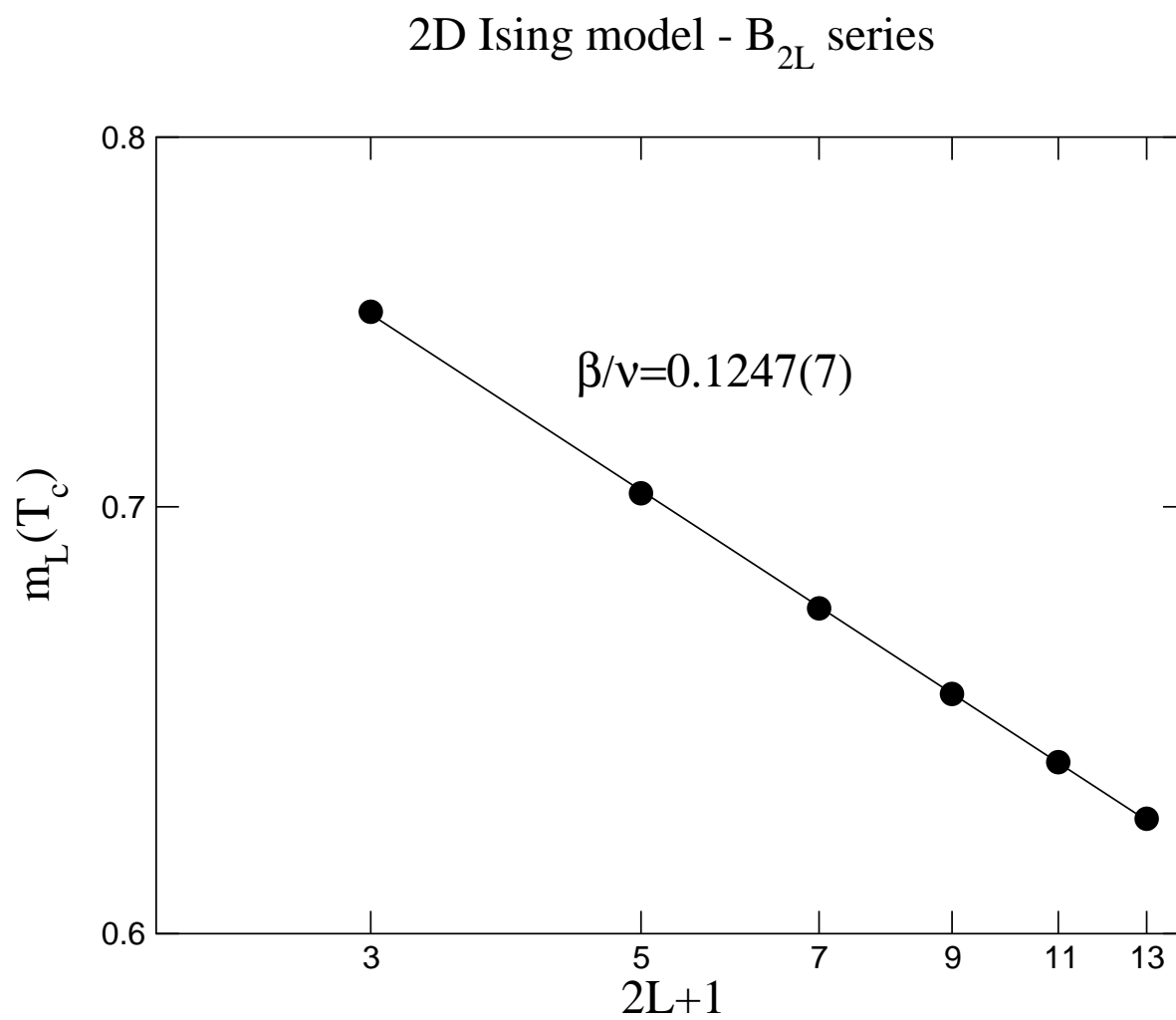
Simple cubic Ising model in zero field, magnetization vs temperat

$$T_c \simeq 4.512 \div 4.515$$

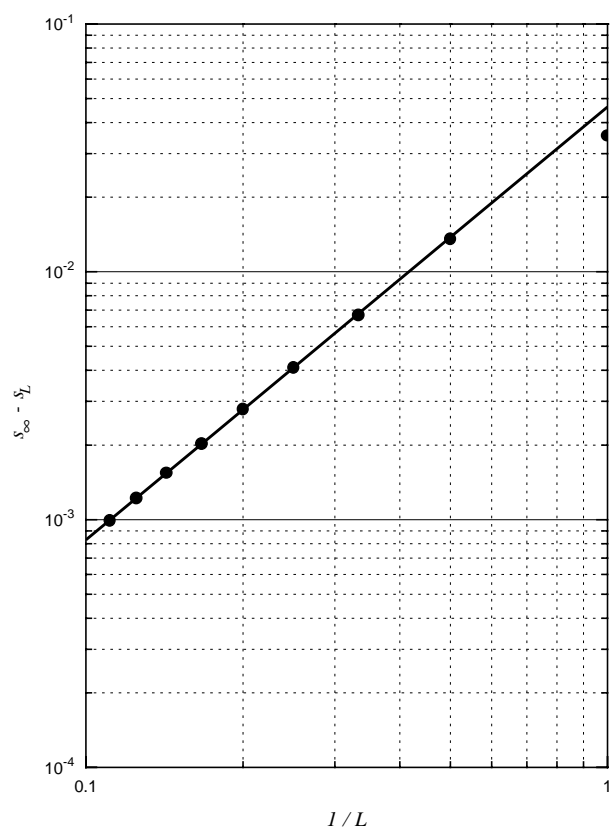
$T$	$m$ (18 site CVM)	$m$ (MCRG by Talapov and Blöte)
3.4	0.8972562	0.8972440
3.5	0.8806417	0.8806366
3.6	0.8616750	0.8616735
3.7	0.8399256	0.8399255
3.8	0.8148173	0.8148161
3.9	0.7855490	0.7855416
4.0	0.7509519	0.7509251
4.1	0.7092094	0.7091249
4.2	0.6572414	0.6569722
4.3	0.5891051	0.5881361
4.4	0.4905811	0.4859045
4.5	0.3067063	0.2378014



Critical magnetization of the square Ising ferromagnet,  $B_{2L}$  approxim



Entropy of the triangular Ising antiferromagnet,  $B_{2L}$  approximation



## Region-based free energy approximations

Given a set  $R$  of regions, assign *counting numbers*  $a_\alpha$  to regions, such that (*counting* of nodes) every factor node and every variable node is counted

$$\sum_{\alpha \in R, a \in \alpha} a_\alpha = 1 \quad \forall a$$
$$\sum_{\alpha \in R, i \in \alpha} a_\alpha = 1 \quad \forall i$$

**Junction graph:**  $R$  contains two types of regions, *large regions* and *small regions*, organized in a directed graph, with edges from large to small such that: (i) every edge connects a large region with a small region which is a subset of the former; (ii) the subgraph of the regions containing a given factor node is a connected tree

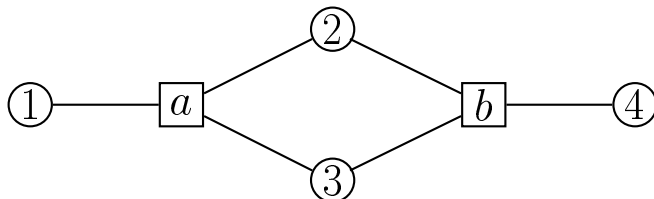
**Bethe:** large regions are made of a factor node and its variable nodes; small regions are variable nodes.

**CVM:**  $R$  is closed under intersection, which satisfies the additional c  
(single counting of every subcluster)

$$\sum_{\alpha \in R, \beta \subseteq \alpha} a_{\alpha} = 1 \quad \forall \beta \in R$$

*Bethe is a special case of CVM only if no factor node shares more variable node with another factor node.*

Be careful when applying Bethe to non-pairwise interactions, e.g.



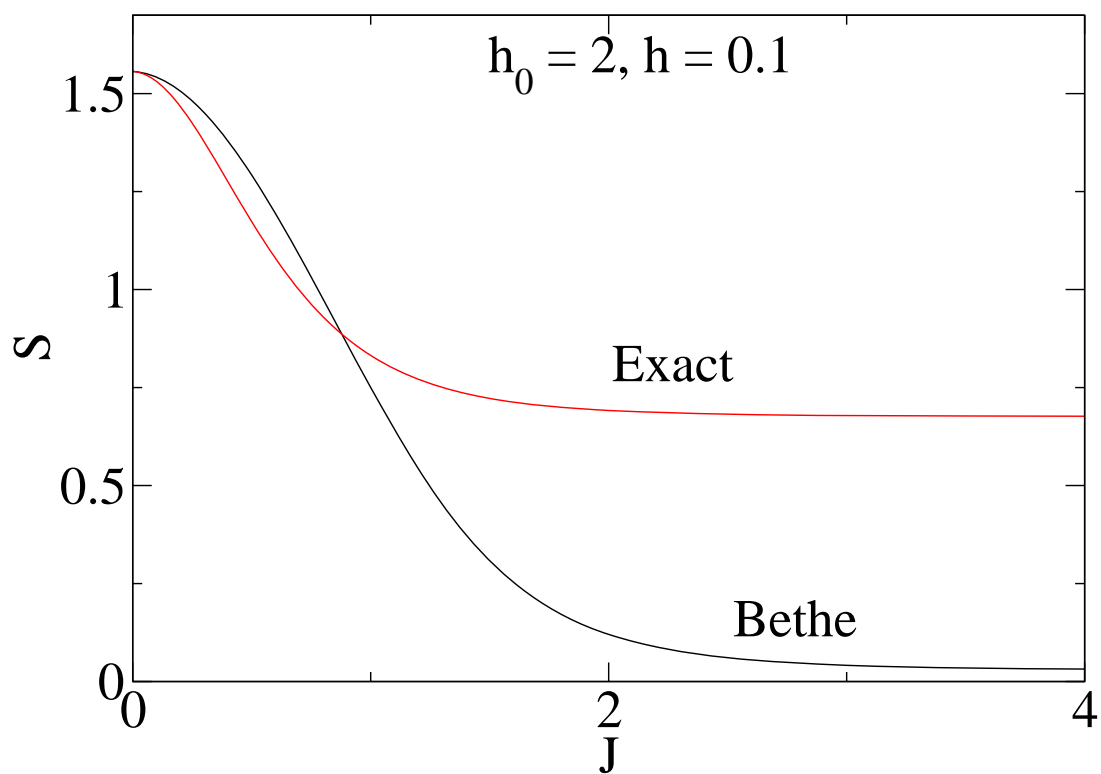
$$s_i = \pm 1, \quad i = 1, 2, 3, 4$$

$$H_a(s_1, s_2, s_3) = -h_0 s_1 - \frac{h}{2}(s_2 + s_3) - J s_1 s_2 s_3$$

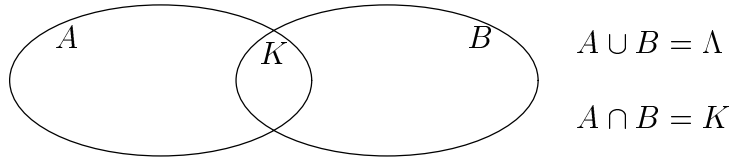
$$H_b(s_2, s_3, s_4) = -h_0 s_4 - \frac{h}{2}(s_2 + s_3) - J s_2 s_3 s_4$$

$$S = S(a123) + S(b234) - S(23)$$

$$S_{\text{Bethe}} = S(a123) + S(b234) - S(2) - S(3)$$



## THE SIMPLEST EXAMPLE



- No interactions between  $A' = A \setminus K$  and  $B' = B \setminus K$ :  $H = H_A(s_A) + H_B(s_B) + H_K(s_K)$
- The probability factors:  $p_\Lambda = \frac{p_A p_B}{p_K}$

$$p_\Lambda = \frac{e^{-H}}{\text{Tr} e^{-H}} = \frac{1}{Z} e^{-H}$$

$$p_A = \sum_{\Lambda \setminus A} p_\Lambda = \frac{1}{Z} e^{-H_A} \sum_{B'} e^{-H_B}$$

$$p_B = \sum_{\Lambda \setminus B} p_\Lambda = \frac{1}{Z} e^{-H_B} \sum_{A'} e^{-H_A}$$

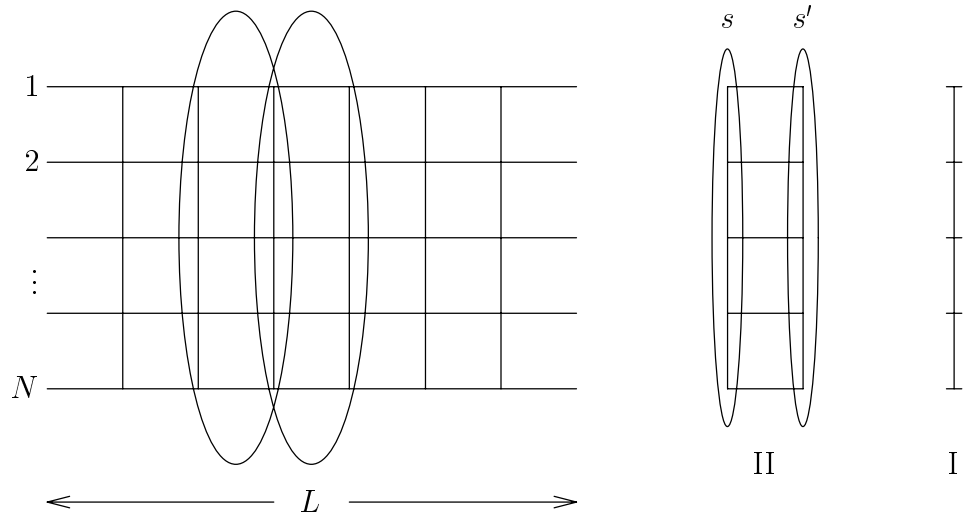
$$p_K = \sum_{A'} p_A = \sum_{B'} p_B = \frac{1}{Z} \sum_{A'} e^{-H_A} \sum_{B'} e^{-H_B}$$

- The cluster variation method with  $R = A, B, K$  is exact, since:

$$S_\Lambda = S_A + S_B - S_K$$

## ONE DIMENSIONAL SYSTEMS

- Strip of width  $N$ :



$$p_{\Lambda} = \frac{\prod_{\alpha \in \text{II}} p_{\alpha}}{\prod_{\alpha \in \text{I}} p_{\alpha}} \quad \Rightarrow \quad S_{\Lambda} = \sum_{\alpha \in \text{II}} S_{\alpha} - \sum_{\alpha \in \text{I}} S_{\alpha}$$

The cluster variation method with  $R = \text{II} \cup \text{I}$  is exact ( $L = 1$ : the Bethe approximation is exact for the chain).

- In the thermodynamic limit  $L \rightarrow \infty$  (open boundary conditions) translational invariance is recovered:

$$\frac{F}{L} = \min_{\Lambda} \sum (p_{\text{II}} H_{\text{II}} + p_{\text{II}} \ln p_{\text{II}} - p_{\text{I}} \ln p_{\text{I}})$$

Solving for  $p_{\text{II}}$  we recover the transfer matrix formalism:

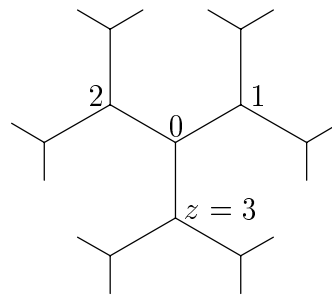
$$\frac{F}{L} = -\ln \max \left\{ \sum_{s,s'} p_{\text{I}}^{1/2}(s) \exp [-H_{\text{II}}(s, s')] p_{\text{I}}^{1/2}(s') \right\}$$

$$\sum_s p_{\text{I}}(s) = 1$$



## TREE-LIKE LATTICES (when Bethe $\equiv$ CVM)

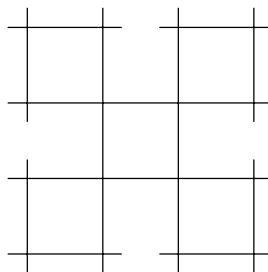
- Bethe lattice (interior of a Cayley tree), NO LOOPS:



$$p_{\Lambda} = \frac{\prod_{\alpha \in \text{LINKS}} p_{\alpha}}{\prod_{\alpha \in \text{SITES}} p_{\alpha}^{z_{\alpha}-1}} \quad \Rightarrow \quad S_{\Lambda} = \sum_{\alpha \in \text{LINKS}} S_{\alpha} - \sum_{\alpha \in \text{SITES}} (z_{\alpha} - 1) S_{\alpha}$$

The cluster variation method with  $R = \text{LINKS} \cup \text{SITES}$  is exact ( $z=2$  Bethe-Peierls approximation is exact for the simple chain).

- Cactus lattice (interior of a Husimi tree):



$$p_{\Lambda} = \frac{\prod_{\alpha \in \text{PLAQS}} p_{\alpha}}{\prod_{\alpha \in \text{SITES}} p_{\alpha}} \quad \Rightarrow \quad S_{\Lambda} = \sum_{\alpha \in \text{PLAQS}} S_{\alpha} - \sum_{\alpha \in \text{SITES}} S_{\alpha}$$

The cluster variation method with  $R = \text{PLAQS} \cup \text{SITES}$  is exact.

## REALIZABILITY

$$s_i = \pm 1, \quad i = 1, 2, 3$$

$$\begin{aligned} p_i(s_i) &= 1/2 & i &= 1, 2, 3 \\ p_{ij}(s_i, s_j) &= \frac{1 + cs_i s_j}{4} & i &< j \end{aligned}$$

**Q.** Is there a global  $p(s_1, s_2, s_3)$  marginalizing to the above probabilities

**A.** Only for  $-1/3 \leq c \leq 1$

**Q.** Is this global  $p$  given by

$$\frac{p_{12}(s_1, s_2)p_{13}(s_1, s_3)p_{23}(s_2, s_3)}{p_1(s_1)p_2(s_2)p_3(s_3)} \quad ?$$

**A.** Only for  $c = 0$

Extending local thermodynamic states on a *square lattice*:

$$S \simeq \sum_{[ijkl]} S_{[ijkl]} - \sum_{\langle ij \rangle} S_{ij} + \sum_i S_i$$

does not mean that

$$\prod_{[ijkl]} p_{[ijkl]}(s_i, s_j, s_k, s_l) \prod_{\langle ij \rangle} p_{ij}^{-1}(s_i, s_j) \prod_i p_i(s_i)$$

is a good approximation to the true equilibrium distribution.

In general such a global  $p$  does not marginalize to  $p_{[ijkl]}$ ,  $p_{ij}$ ,  $p_i$  and is not normalized  $\Rightarrow$  CVM free energy is not, in general, an upper bound.

The above is well defined only if

- odd correlations vanish
- $\langle s_i s_k \rangle_{\langle \langle ik \rangle \rangle} = \langle s_i s_j \rangle_{\langle \langle ij \rangle \rangle}^2$

## DISORDER POINTS

- Ising model with competitive interactions: for instance, on the square

$$H = -K_1 \sum_{\langle ij \rangle} s_i s_j - K_2 \sum_{\langle\langle ij \rangle\rangle} s_i s_j - K_4 \sum_{[ijkl]} s_i s_j s_k s_l,$$

with  $K_1$  (nearest neighbour coupling)  $> 0$ ,  $K_2$  (next nearest neighbour coupling)  $< 0$ ,  $K_4$  (plaquette coupling).

- Integrable case:

$$\cosh(2K_1) = \frac{e^{4K_2+2K_4} + e^{-4K_2+2K_4} + 2e^{-2K_2}}{2(e^{2K_2} + e^{2K_4})}$$

Free energy:

$$F = -\ln [\exp(-K_4) + \exp(K_4 - 2K_2)]$$

- The cluster variation method with  $R = \{\text{plaquettes and their subclusters with maximal clusters larger than the plaquette}\}$  is exact in the i.c. case.

The probability factors:

$$p_\Lambda = \prod_{\alpha \in \text{PLAQS}} p_\alpha \left( \prod_{\alpha \in \text{LINKS}} p_\alpha \right)^{-1} \prod_{\alpha \in \text{SITES}} p_\alpha \quad \Rightarrow$$

$$S_\Lambda = \sum_{\alpha \in \text{PLAQS}} S_\alpha - \sum_{\alpha \in \text{LINKS}} S_\alpha + \sum_{\alpha \in \text{SITES}} S_\alpha$$

- Correlation function  $\Gamma(x, y) = \langle s(x_0, y_0) s(x_0 + x, y_0 + y) \rangle$ :

$$\Gamma(x, y) = g^{|x|+|y|}, \quad g = \frac{\exp(-4K_2) - \cosh(2K_1)}{\sinh(2K_1)}$$

- Many-site correlation functions can be calculated, e.g.

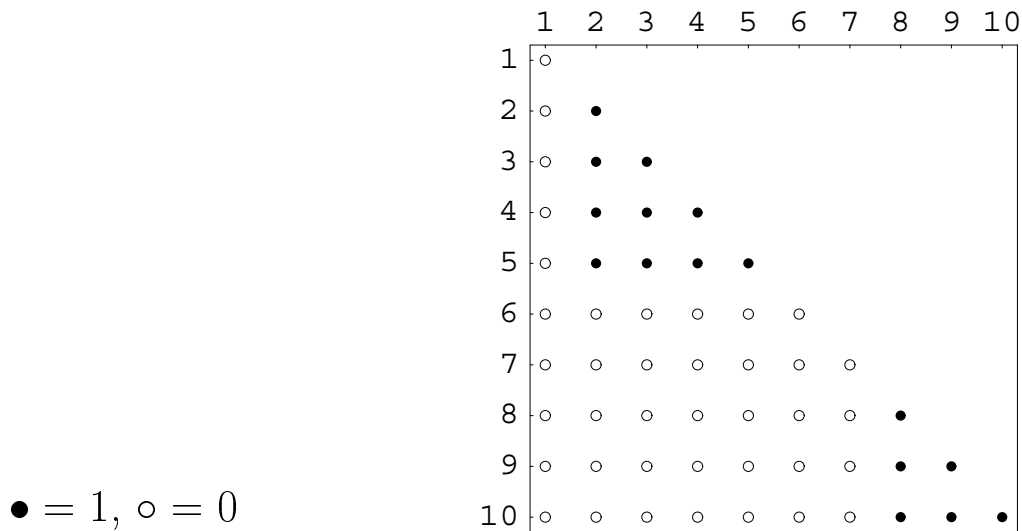
$$q = \langle s_i s_j s_k s_l \rangle_{[ijkl]}$$

$$q = \frac{e^{4K_4} (1 - e^{8K_2}) + 4e^{2K_2} (e^{2K_4} - e^{2K_2})}{e^{4K_4} (1 - e^{8K_2}) + 4e^{2K_2} (e^{2K_4} + e^{2K_2})}$$

- Similar results can be derived for other two-dimensional models.

# EATON MODEL of PROTEIN FOLDING

$$H = \sum_{i=1}^L \sum_{j=i}^L h_{i,j} x_{i,j}, \quad x_{i,j} = \prod_{k=i}^j x_k, \quad x_k = 0, 1$$



Constraints:  $x_{i,j} = x_{i+1,j} x_{i,j-1}$

Probability factors in a CVM-like way due to constraints and locality of interactions

Local interactions  $\Rightarrow$

$$p(\{x_{i,j}\}) = \frac{p^{(1,2)}p^{(2,3)} \dots p^{(L-1,L)}}{p^{(2)} \dots p^{(L-1)}}$$

$$\begin{cases} p^{(j)} = & \text{prob of row } j \\ p^{(j,j+1)} = & \text{joint prob of rows } j \text{ and } j+1 \end{cases}$$

Constraints  $\Rightarrow$  (for instance)

$$\begin{aligned} p^{(j)}(0, \dots 0_i, 1_{i+1}, \dots 1) &= p_{i,i+1}^{(j)}(0, 1) = \\ &= \frac{p_{1,2}^{(j)}(0, 0) \dots p_{i,i+1}^{(j)}(0, 1) \dots p_{L-1,L}^{(j)}(1, 1)}{p_2^{(j)}(0) \dots p_i^{(j)}(0)p_{i+1}^{(j)}(1) \dots p_{L-1}^{(j)}(1)} \end{aligned}$$

and similarly for  $p^{(j,j+1)}$ .

It follows

$$p(\{x_{i,j}\}) = \prod_{\alpha \in R} p_{\alpha}(x_{\alpha})^{a_{\alpha}},$$

where  $R = \{\text{square plaquettes, corners (on the diagonal), and their sub}$



## CVM as an APPROXIMATION

- Leaving apart exactly solvable cases,

$$S \simeq \sum_{\alpha \in R} a_{\alpha} S_{\alpha}$$

can be a reasonable approximation, but

$$\prod_{\alpha \in R} p_{\alpha}^{a_{\alpha}}$$

**is not a probability.**

- **Upper bound:** the CVM free energy is not an upper bound of the exact free energy (contrast with mean field)
- **Convexity:** due to negative  $a_{\alpha}$  coefficients, convexity is no more guaranteed (and hence multiple minima can appear), unless

$$\forall S \subseteq R \quad \sum_{\alpha \in R_S} a_{\alpha} \geq 0 \quad R_S = \{\alpha \in R \mid \exists \beta \subseteq \alpha, \beta \in S\}$$

- Anyway, we are left with the problem of finding minima of  $\mathcal{F}$  with norm and compatibility constraints on probabilities:

$$\sum_{s_\alpha} p_\alpha(s_\alpha) = 1 \quad \forall \alpha \in R,$$

$$p_\alpha(s_\alpha) = \sum_{s_\beta \setminus s_\alpha} p_\beta(s_\beta) \quad \forall \alpha \subset \beta \in R.$$

## Algorithms to find min in $F_{\text{CVM}}$

**Constraints** are always implemented through

- Lagrange multipliers, *or*
- effective/cavity fields, *or*
- messages,

equivalently.

### **(G)BP: (generalized) belief propagation**

1. Solve analytically w.r.t. the  $p_\alpha$ 's and
2. solve constraints w.r.t. messages by iteration.

Very *fast, single loop* algorithm, often *not convergent*.

**NIM: natural iteration method**

**CCCP: concave–convex procedure**

**HAK: class of algorithms by Heskes, Albers and Kappen**

1. Outer loop: update probabilities
2. Inner loop: update multipliers, or messages, to solve constraints

*Slower, double loop algorithms, proof of convergence exists (except in a few cases).*

## Details: Bethe approximation (Ising example)

$$\begin{aligned}
\mathcal{F} = & - \sum_i h_i \sum_{s_i} s_i p_i(s_i) - \sum_{\langle ij \rangle} J_{ij} \sum_{s_i, s_j} s_i s_j p_{ij}(s_i, s_j) \\
& + \sum_{\langle ij \rangle} \sum_{s_i, s_j} p_{ij} \ln p_{ij} - \sum_i (z_i - 1) \sum_{s_i} p_i \ln p_i \\
& + \sum_i \lambda_i \left( \sum_{s_i} p_i - 1 \right) + \sum_{\langle ij \rangle} \lambda_{ij} \left( \sum_{s_i, s_j} p_{ij} - 1 \right) \\
& + \sum_{\langle ij \rangle} \left[ \sum_{s_i} \mu_{i,j}(s_i) (p_i - \sum_{s_j} p_{ij}) + \sum_{s_j} \mu_{j,i}(s_j) (p_j - \sum_{s_i} p_{ij}) \right]
\end{aligned}$$

## Thouless–Anderson–Palmer (TAP)

To obtain the corresponding free energy from the Bethe free energy use

$$p_i(s_i) = \frac{1 + s_i m_i}{2} \quad p_{ij}(s_i, s_j) = \frac{1 + s_i m_i + s_j m_j + s_i s_j c_{ij}}{4},$$

then solve analytically for the  $c_{ij}$ 's and expand to second order in  $\beta$ .

## Natural Iteration Method (NIM)

Define site probs as *marginals* of pair probs

$$p_i = \frac{1}{z_i} \sum_{j \in \text{NN } i} \sum_{s_j} p_{ij},$$

then solve stationarity w.r.t. pair probs to get the basic iterative eqs.

$$\begin{aligned} p_{ij}(s_i, s_j) = & \exp \left[ -1 - \lambda_{ij} + \frac{1}{z_i} h_i s_i + \frac{1}{z_j} h_j s_j + J_{ij} s_i s_j \right. \\ & + \mu_{i,j}(s_i) + \mu_{j,i}(s_j) - \frac{1}{z_i} \sum_{k \in \text{NN } i} \mu_{i,k}(s_i) - \frac{1}{z_j} \sum_{k \in \text{NN } j} \mu_{j,k}(s_j) \\ & \left. \times [p_i(s_i)]^{1-1/z_i} [p_j(s_j)]^{1-1/z_j} \right] \end{aligned}$$

At each iteration, find Lagrange mults, e.g. by iteration:

$$\mu_{i,j}(s_i) = \hat{\mu}_{i,j}(s_i) + b \ln \frac{p_i(s_i)}{\sum_{s_j} p_{i,j}(s_i, s_j)}$$

## Effective fields

Stationarity is solved by

$$p_i(s_i) = \exp \left[ F_i + \left( h_i + \sum_{k \in \text{NN } i} h_{i,k} \right) s_i \right]$$

$$p_{ij}(s_i, s_j) = \exp \left[ F_{ij} + \left( h_i + \sum_{\substack{k \neq j \\ k \in \text{NN } i}} h_{i,k} \right) s_i + \left( h_j + \sum_{k \in \text{NN } j}^{\substack{k \neq i}} h_{j,k} \right) s_j + \right]$$

and compatibility leads to

$$h_{i,j} = \tanh^{-1} \left[ \tanh \left( h_j + \sum_{k \in \text{NN } j}^{\substack{k \neq i}} h_{j,k} \right) \tanh J_{ij} \right] .$$

The corresponding iterative algorithm is nothing but **Belief propagation**

## Cavity fields

Cavity bias (factor  $\rightarrow$  variable):  $= h_{i,j}$

Cavity field (variable  $\rightarrow$  factor):  $= \sum_{k \in \text{NN } i}^{\substack{k \neq j}} h_{i,k}$

## Belief propagation (BP)

Pair and site probs are rewritten in terms of messages:

$$\begin{aligned} p_i(s_i) &= \exp(h_i s_i) \prod_{j \in \text{NN}i} m_{j \rightarrow i}(s_i) \\ p_{ij}(s_i, s_j) &= \exp(-\lambda + h_i s_i + h_j s_j + J_{ij} s_i s_j) \times \\ &\times \prod_{k \in \text{NN}i, k \neq j} m_{k \rightarrow i}(s_i) \prod_{k \in \text{NN}j, k \neq i} m_{k \rightarrow j}(s_j). \end{aligned}$$

The messages are related to Lagrange mults by

$$\exp[\mu_{i,j}(s_i)] = \exp(h_i s_i) \prod_{k \in \text{NN}i, k \neq j} m_{k \rightarrow i}(s_i).$$

As the effective fields, messages can be determined iteratively by imposing compatibility

$$m_{j \rightarrow i}(s_i) \propto \sum_{s_j} \exp(h_j s_j + J_{ij} s_i s_j) \prod_{k \in \text{NN}j, k \neq i} m_{k \rightarrow j}(s_j).$$

When convergent, fixed point is a minimum of the Bethe free energy.



## Generalized belief propagation (GBP)

$$p_\alpha(s_\alpha) \propto \left[ \exp \left( - \sum_{a \in \alpha} H_a(s_a) \right) \right] \prod_{\beta \subseteq \alpha} \prod_{\gamma \notin \alpha} m_{\gamma \rightarrow \beta}(s_\beta)$$

where

$$m_{\gamma \rightarrow \beta}(s_\beta) = \exp(\mu_{\gamma \rightarrow \beta}(s_\beta))$$

and  $\mu_{\gamma \rightarrow \beta}(s_\beta)$  is the Lagrange multiplier for the constraint

$$\sum_{\beta \subseteq \alpha \in R} a_\alpha p_\alpha(s_\beta) = \sum_{\gamma \subseteq \alpha \in R} a_\alpha p_\alpha(s_\beta).$$

## Concave convex procedure (CCCP)

The free energy is split into concave + convex:

$$\mathcal{F}[\{p_\alpha\}] = \mathcal{F}_{\text{vex}}[\{p_\alpha\}] + \mathcal{F}_{\text{cave}}[\{p_\alpha\}].$$

Iterative equations are derived from:

$$\nabla \mathcal{F}_{\text{vex}}[\{p_\alpha^{(t+1)}\}] = -\nabla \mathcal{F}_{\text{cave}}[\{p_\alpha^{(t)}\}].$$

In the Bethe case one chooses

$$\begin{aligned}\mathcal{F}_{\text{cave}}[\{p_i\}] &= -\sum_i z_i \sum_{s_i} [p_i(H_i + \ln p_i)], \\ \mathcal{F}_{\text{vex}}[\{p_i, p_{ij}\}] &= \mathcal{F} - \mathcal{F}_{\text{cave}}.\end{aligned}$$

## Algorithm by Heskes, Albers and Kappen (HAK)

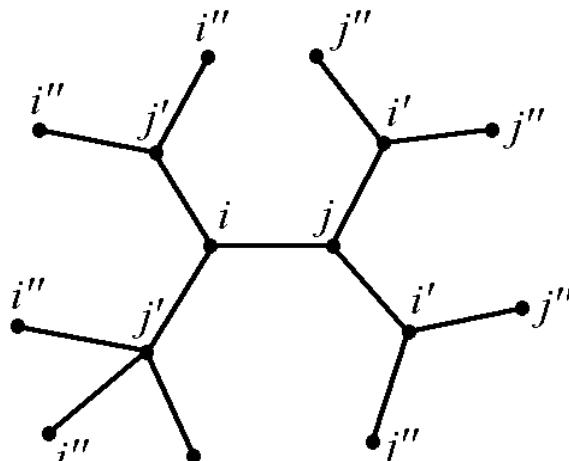
$$p^{(t+1)} = \operatorname{argmin}_p \mathcal{F}_{\text{vex}}(p, p^{(t)})$$

where  $p \equiv \{p_\alpha, \alpha \in R\}$  and  $\mathcal{F}_{\text{vex}}(p, p')$  is a *convex* function of  $p$  properties

- $\mathcal{F}_{\text{vex}}(p, p') \geq \mathcal{F}(p)$
- $\mathcal{F}_{\text{vex}}(p, p) = \mathcal{F}(p)$

The free energy *decreases* at each iteration

## CP (conditional probability) algorithm



$$p_{ij\{i'j'\}}(x_i, x_j, \{x_{i'}, x_{j'}\}) = p_{ij}(x_i, x_j) \prod_{i'} \frac{p_{ji'}(x_j, x_{i'})}{\sum_{\tilde{x}_{i'}} p_{ji'}(x_j, \tilde{x}_{i'})} \prod_{j'} \frac{p_{ij'}(x_i, x_{j'})}{\sum_{\tilde{x}_{j'}} p_{ij'}(x_i, \tilde{x}_{j'})}$$

$$p_{\{i'j'\}}(\{x_{i'}, x_{j'}\}) = \sum_{x_i, x_j} p_{ij\{i'j'\}}(x_i, x_j, \{x_{i'}, x_{j'}\})$$

$$p_{ij}(x_i, x_j) = \sum_{\{x_{i'}, x_{j'}\}} \frac{w_{ij\{i'j'\}}(x_i, x_j, \{x_{i'}, x_{j'}\})}{\sum_{\tilde{x}_i, \tilde{x}_j} w_{ij\{i'j'\}}(\tilde{x}_i, \tilde{x}_j, \{x_{i'}, x_{j'}\})} p_{\{i'j'\}}(\{x_{i'}, x_{j'}\})$$

**CP fixed points** are minima of the **Bethe** free energy

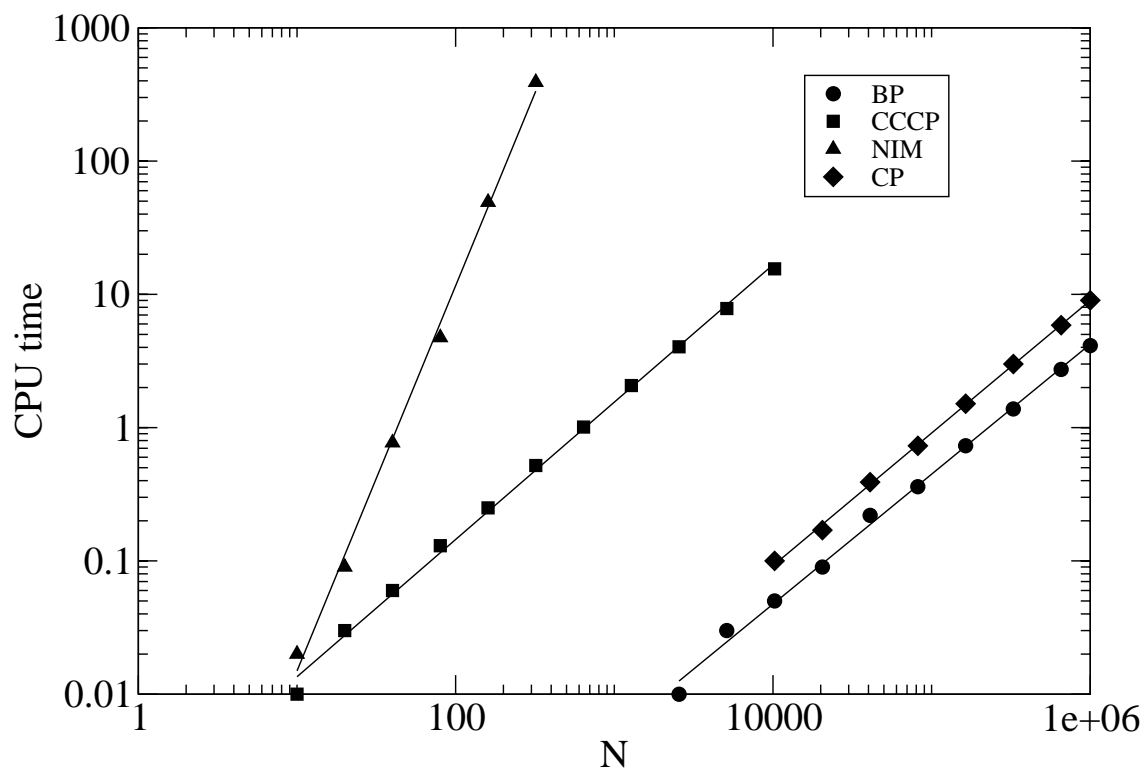
Analog to *hard-spin mean-field*

**Converges** more often than BP

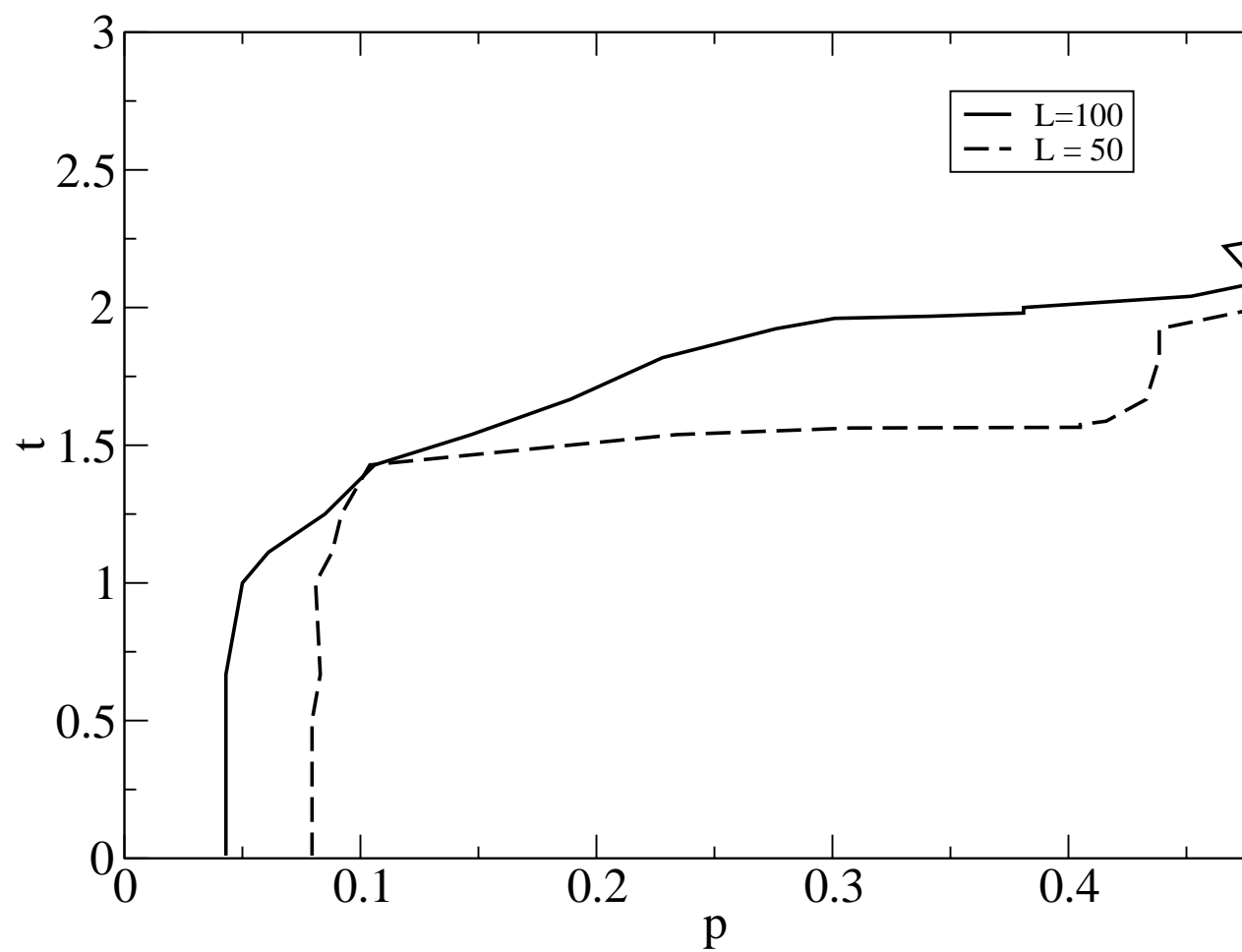
**Comparable** with best double loop algorithms, **slower** ( $\sim 1$  order of magnitude slower) than BP

## SPEED OF ALGORITHMS

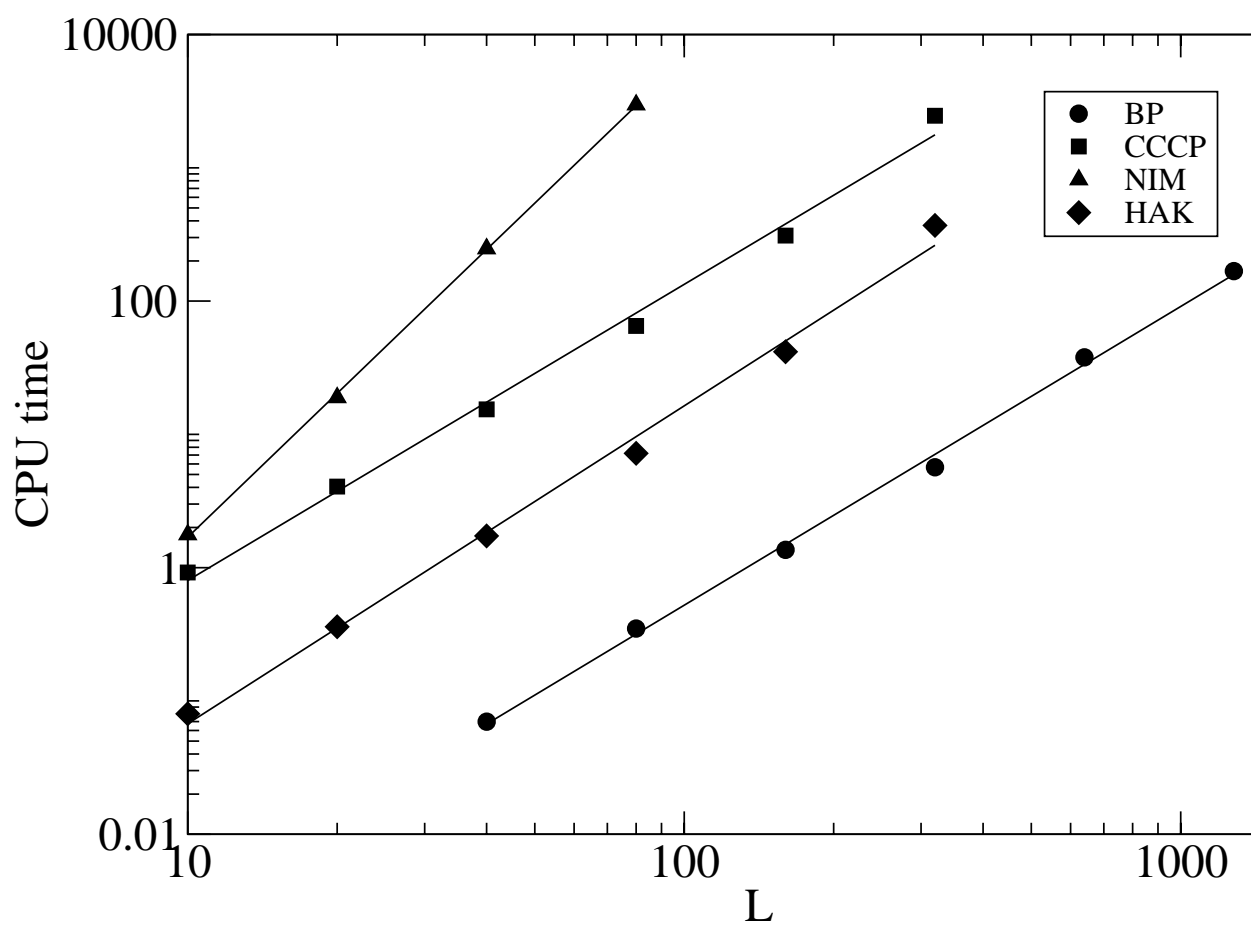
1D Ising model in random field, exact solution through Bethe approximation  
energy is *convex over the constraint set* (HAK cannot be distinguished  
on this graph)



2D Edwards–Anderson model with a fraction  $p$  of AF bonds: convergence  
for the BP algorithm with ferromagnetic initial condition



CPU times for the 2d model: paramagnetic case ( $CP \sim HAK$ )





CPU times for the 2d model: ferromagnetic case ( $CP \sim HAK$ )

