Replica Cluster Variational Method

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joint work with Tommaso Rizzo,
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arXiv:0906.2695

Bethe-Peierls approx.
Belief Propagation (BP)

random graph topologies
(i.e. locally tree-like)
replica symmetric (RS)
single state, single BP f.p.

Bethe-Peierls approx.
Belief Propagation (BP)

BEYOND BP

Kikuchi/GBP
topological structures
e.g. regular lattices

Survey Propagation (SP)
counts the number of
states (a.k.a. complexity)

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Belief Propagation (BP)

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counts the number of
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GSP?!

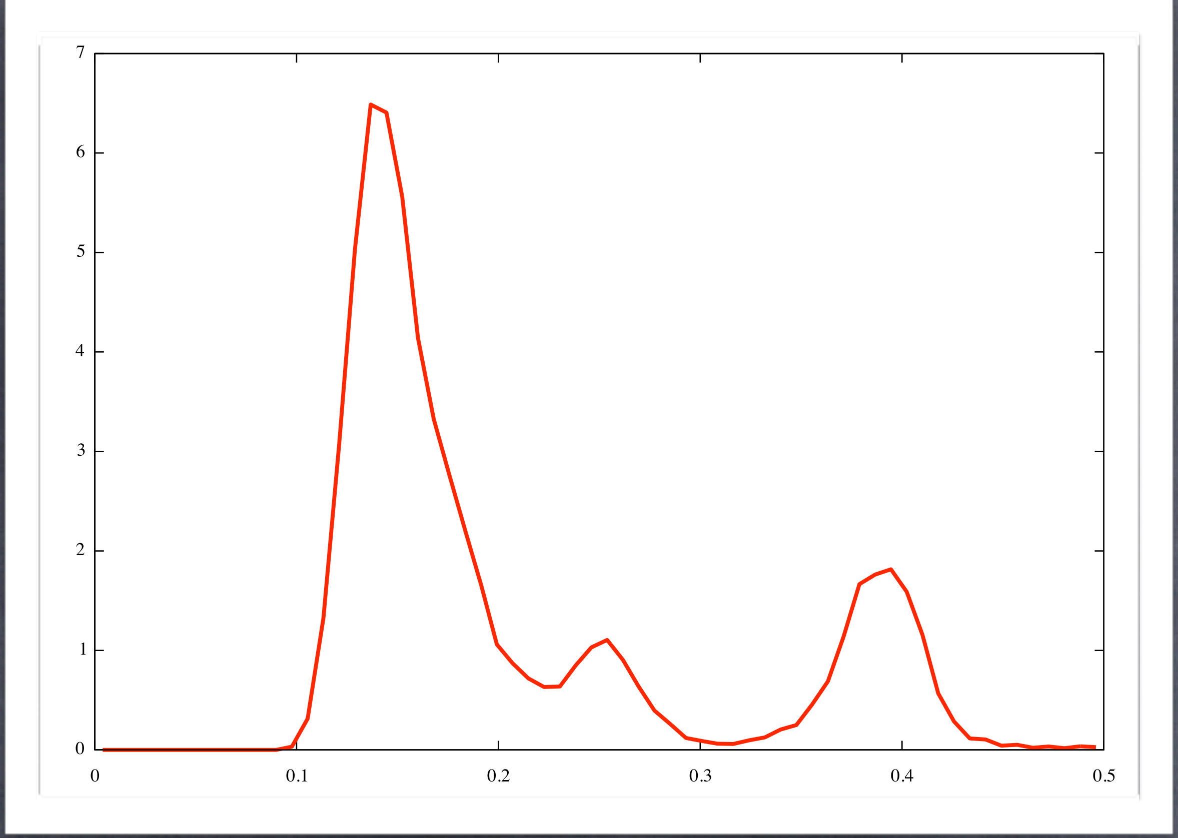
from Wikipedia: “The cluster variational method and the survey propagation algorithms are two different improvements to belief propagation. The name generalized survey propagation (GSP) is waiting to be assigned to the algorithm that merges both generalizations.”

Models we are interested in

Spin glasses on regular lattices
Edwards-Anderson (EA) model

$$\mathcal{H} = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j, \quad P[\vec{\sigma}] \propto e^{-\beta\mathcal{H}}, \quad \beta = \frac{1}{T}$$

Topologies with many short loops.
Quenched disorder, frustration...
J_{ij} are Gaussian or ±1 i.i.d. r.v.
Ising spins σ_i=±1

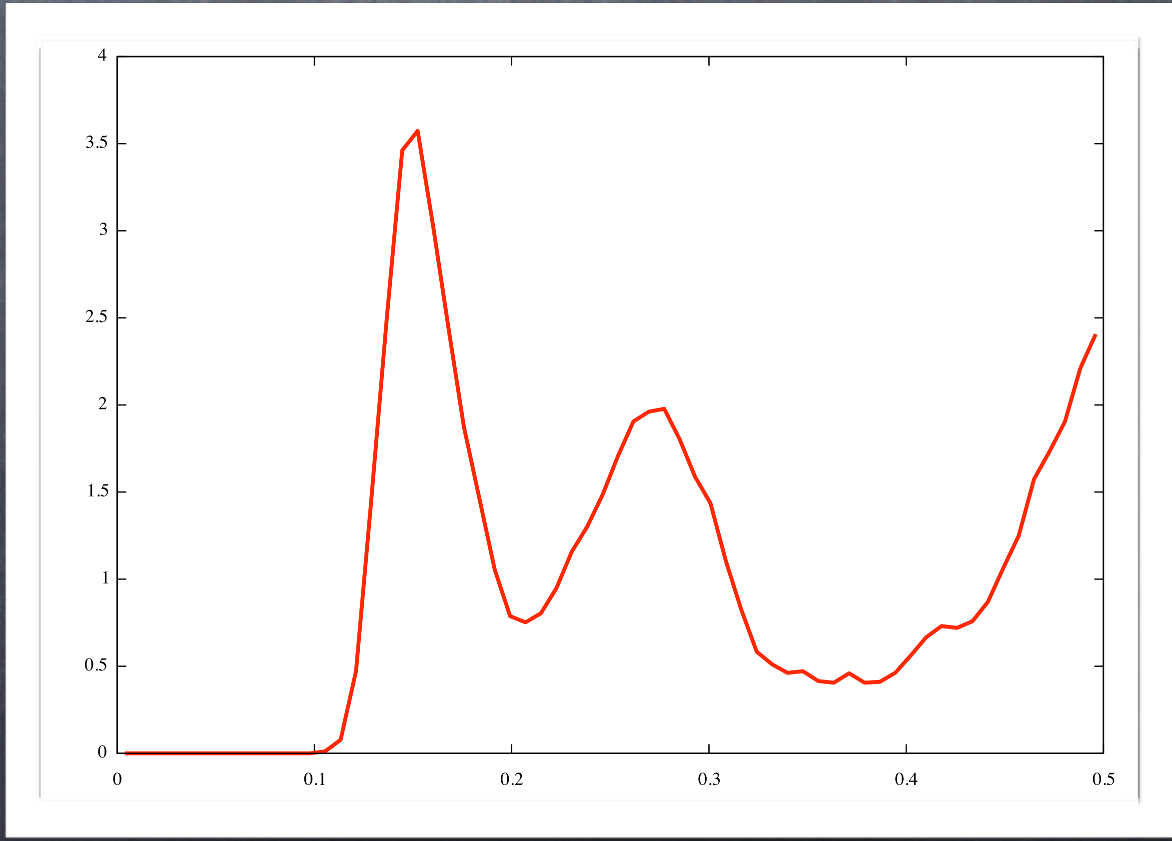


±J EA model

3D L=32

T=0.7

Complex systems at low temprature with many state and metastable states



Two type of questions

- Average over the ensemble
  - mean free-energy, energy and entropy dominated by typical samples
- Properties of a given sample
  - free-energy, energy, entropy and marginal probabilities

Two kind of results

- Analytic results for quantities averaged over the ensemble
- An algorithm for computing marginals on a given sample

Many links between the two...

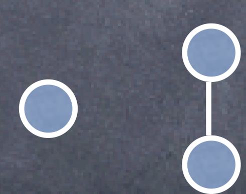
Kikuchi's CVM

$$F = \sum_{\vec{\sigma}} \mathcal{H}[\vec{\sigma}] P[\vec{\sigma}] - T \sum_{\vec{\sigma}} P[\vec{\sigma}] \log P[\vec{\sigma}]$$

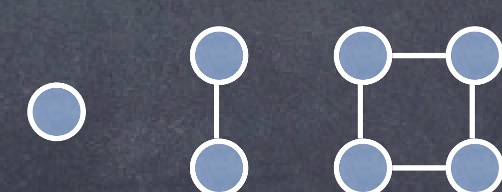
Energy: easy   Entropy: difficult

Mean field 

$$P[\vec{\sigma}] = \prod_i P_i(\sigma_i)$$

Bethe 

$$P[\vec{\sigma}] = \prod_{<ij>} \frac{P_{ij}(\sigma_i, \sigma_j)}{P_i(\sigma_i) P_j(\sigma_j)} \prod_i P_i(\sigma_i)$$

CVM (plaquette) 

Bethe free-energy

$$F = -\sum_{<ij>} J_{ij} \sum_{\sigma_i,\sigma_j} \sigma_i \sigma_j P_{ij}$$
$$+T \sum_{<ij>} \sum_{\sigma_i,\sigma_j} P_{ij} \ln P_{ij} - T \sum_i (d_i - 1) \sum_{\sigma_i} P_i \ln P_i$$

+ constraints imposing normalizations and consistency $\sum_{\sigma_j} P_{ij}(\sigma_i, \sigma_j) = P_i(\sigma_i)$

Lagrange multipliers are the messages in the MPA

Kikuchi free-energy

$$F = \sum_r c_r \left(\sum_{x_r} P_r E_r + T \sum_{x_r} P_r \ln P_r \right)$$

to be minimized under normalization and compatibility constraints

$$\sum_{x_{r \setminus s}} P_r = P_s$$

possibly with a fast MPA (GBP) sending messages = Lagrange multipliers

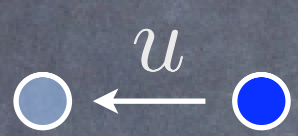
Alternative expression for the Kikuchi free-energy

$$F = -\sum_r c_r \ln \left[\sum_{x_r} \psi_r(x_r) \prod_{m_{rs} \in M(r)} m_{rs} \right]$$

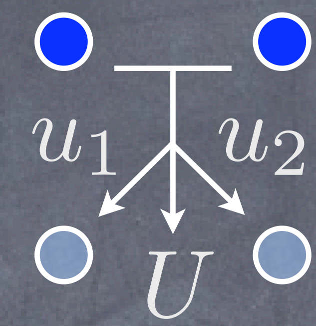
Partial derivatives w.r.t. m_{rs} -> BP/GBP eqs.
No P ln P term

Plaquette CVM

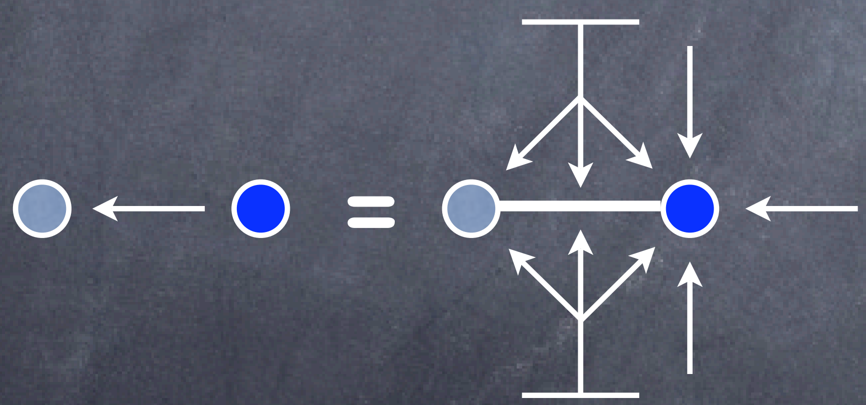
- 2 kind of messages

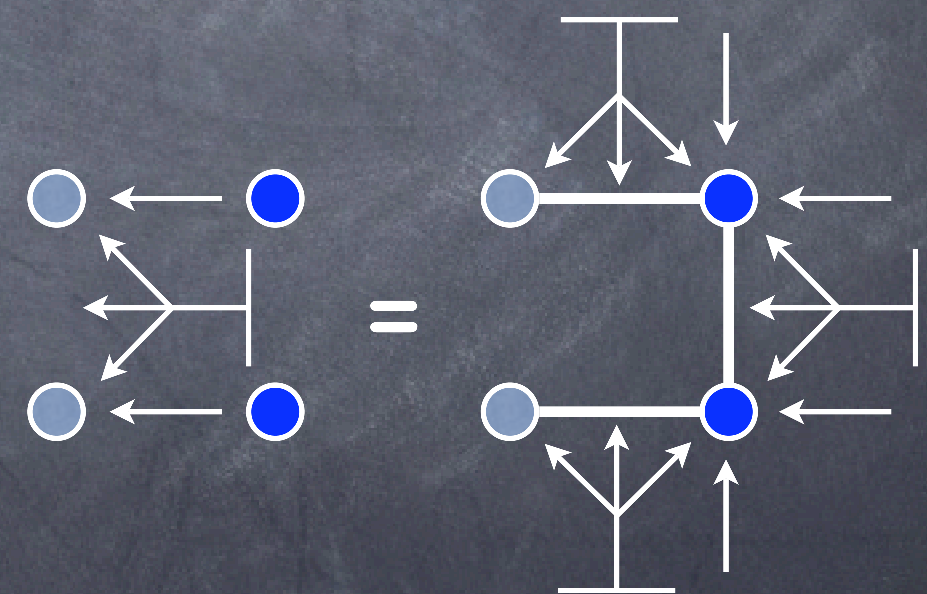


$$m \propto e^{-\beta u}$$



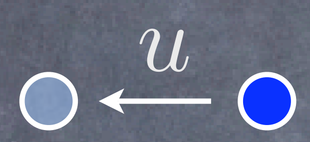
- 2 kind of equations



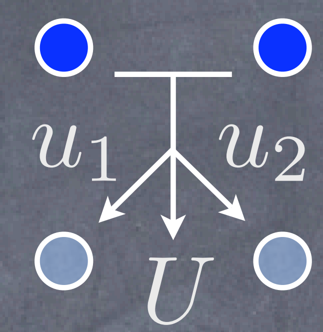


Plaquette CVM

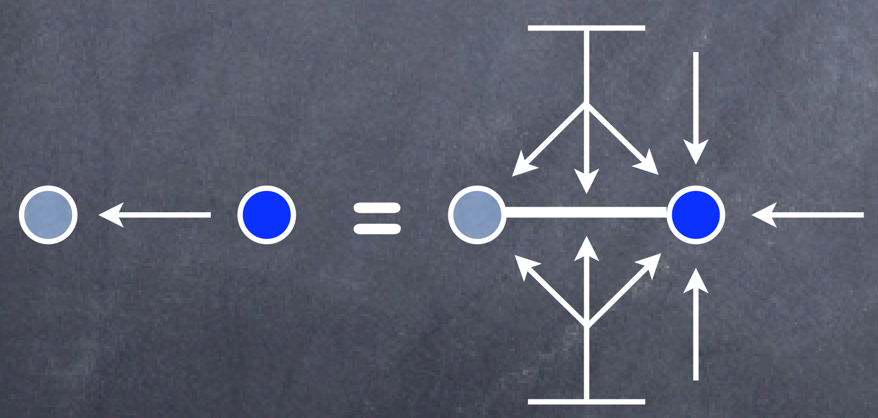
- 2 kind of messages

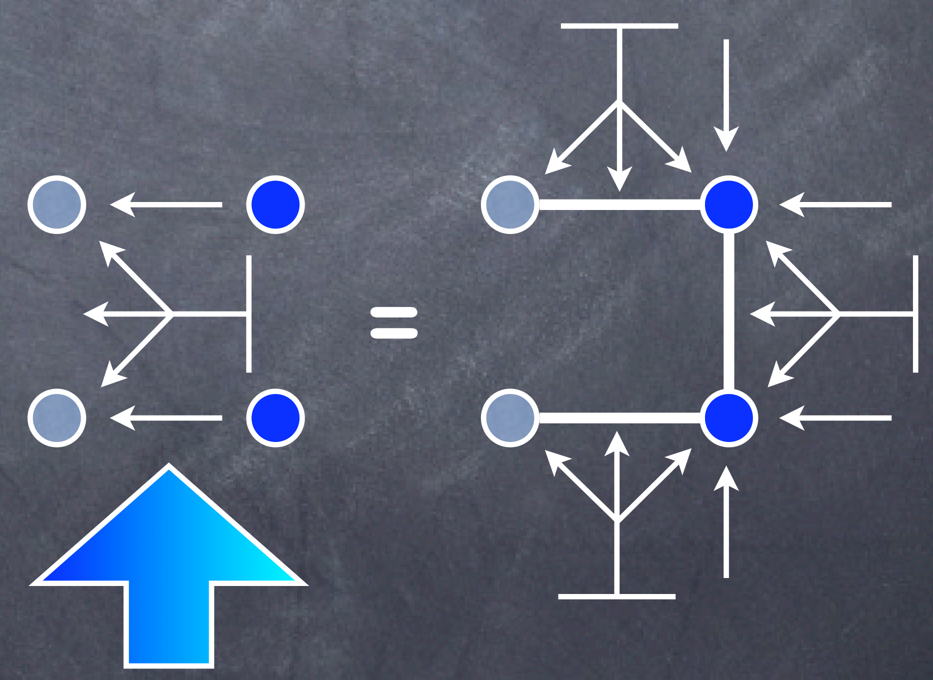


$m \propto e^{-\beta u}$



- 2 kind of equations





Single and triple messages appear together!

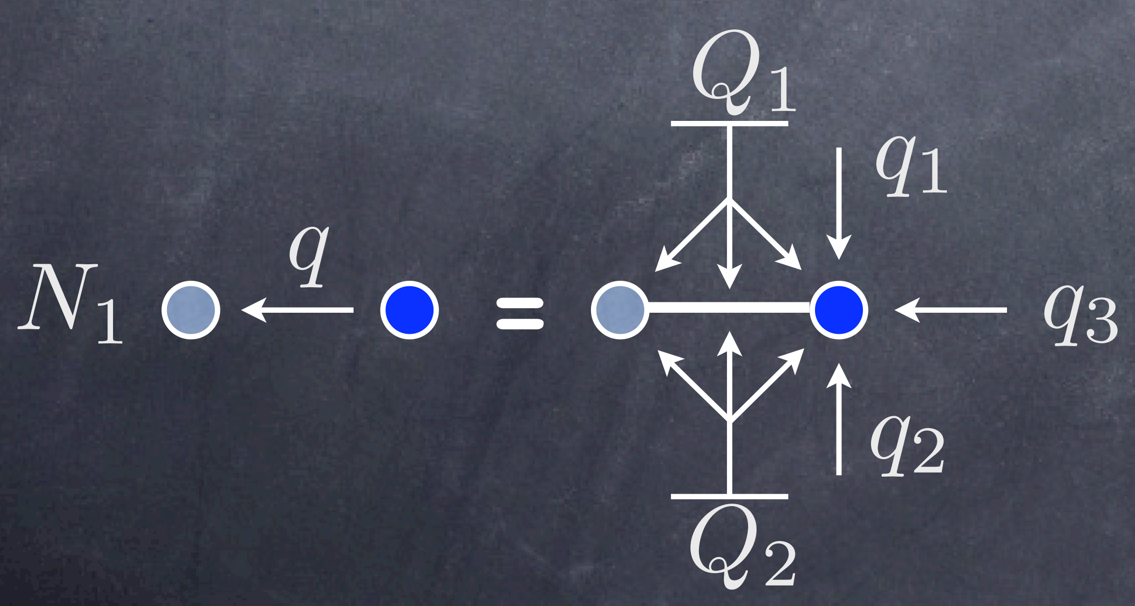
Introducing RSB

- The cavity interpretation of messages turns out to be wrong beyond Bethe
- We came back to the replica trick and the hierarchical ansatz
- We obtained general expressions for the free-energy at any level of RSB and any set of regions in the CVM

1RSB CVM for a given sample (GSP)

messages become functions of messages $q(u)$ and $Q(U, u_1, u_2)$ satisfying $\forall$ region

$$q(u) = \frac{\int dQ_1()dQ_2()dq_1()dq_2()dq_3()\ \delta[u - f()]\ N_1^m}{\langle N_1^m \rangle}$$

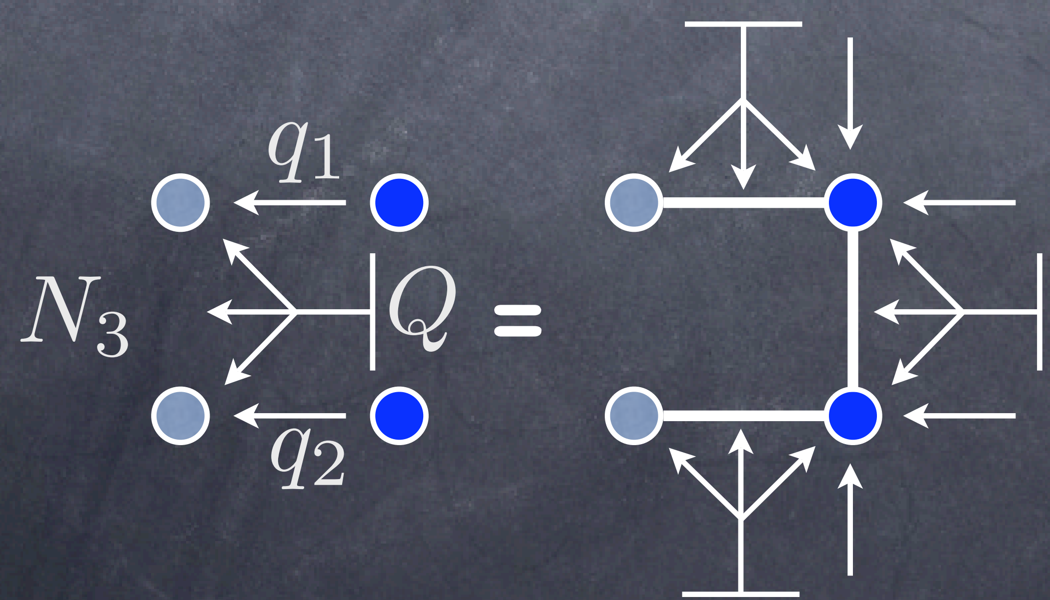


1RSB CVM for a given sample (GSP)

$$\int Q(U,x_1,x_2)q_1(u_1-x_1)q_2(u_2-x_2) =$$

$$\frac{1}{\langle N_3^m \rangle}\int dQ_1()dQ_2()dQ_3()dq_3()dq_4()dq_5()dq_6()$$

$$\delta[U-F()]\delta[u_1-f_1()]\delta[u_2-f_2()]N_3^m$$



1RSB CVM for a given sample (GSP)

From fixed point functions $q(u)$ and $Q(U, u_1, u_2)$

compute the replicated free-energy

$$F(m) = -\sum_r c_r \ln \int dQ() \dots dq() \; [N_r()]^m$$

and by Legendre trasform the complexity $\Sigma(f)$

Marginals will depend on the free-energy value

RS CVM average case

No marginals, but just free-energy

$$F = -\sum_r c_r \ln \langle N_r \rangle_J$$

Average over the disorder

↓

Traslation invariance on the lattice

↓

Just one equation per kind of message

RS CVM average case

$$q(u) = \int dQ()dQ()dq()dq()dq()\delta[u - f()]$$

$$\int Q(U, x_1, x_2)q(u_1 - x_1)q(u_2 - x_2)dx_1 dx_2 =$$

$$\int dQ()dQ()dQ()dq()dq()dq()dq()$$

$$\delta[U - F()]\delta[u_1 - f_1()]\delta[u_2 - f_2()]$$

RS CVM average case (difficulties)

- $q(u)$ and $Q(U, u_1, u_2)$ are not distributions
  - nice cavity interpretation fails
- some numerical problems
  - signed populations or histograms
  - Fourier transform to solve the convolution

Analytical results for the Edwards-Anderson model

- Bethe: $Q(U, u_1, u_2) = \delta(U)\delta(u_1)\delta(u_2)$

  Solve for $q(u)$

  $$\exists\, T_c^{\text{Bethe}} \quad : \quad q(u) = \begin{cases} \delta(u) & \text{for } T > T_c^{\text{Bethe}} \\ \text{broad and symmetric} & \text{for } T < T_c^{\text{Bethe}} \end{cases}$$

- Paramagnetic ($m_i = 0 \; \forall i$):

  $Q(U, u_1, u_2) = Q(U)\delta(u_1)\delta(u_2) \quad q(u) = \delta(u)$

  Solve for $Q(U)$

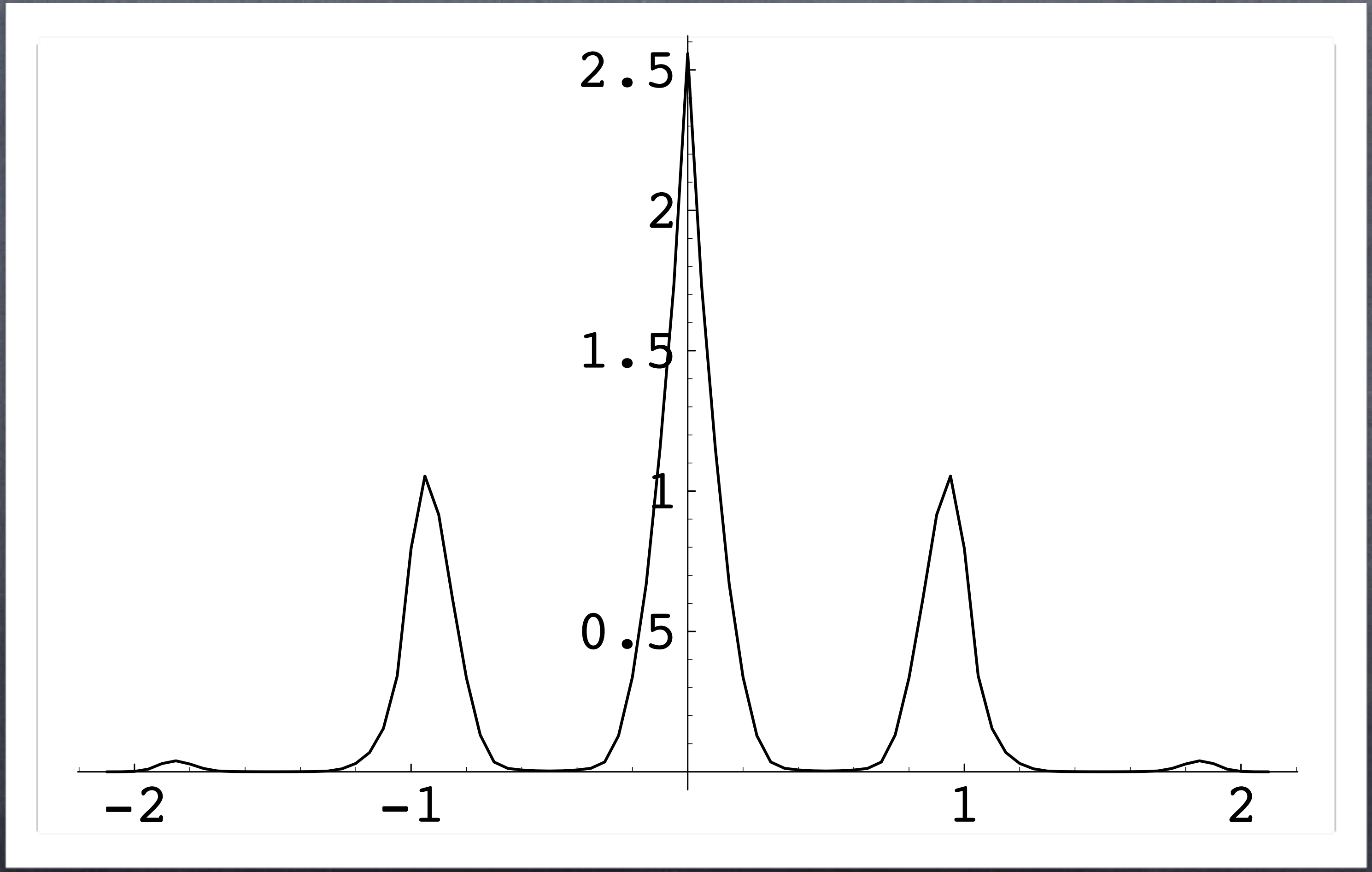
RS CVM for EA 2D

$$\tanh(\beta U) \stackrel{\mathrm{d}}{=} \tanh(\beta(J_1+U_1))\tanh(\beta(J_2+U_2))\tanh(\beta(J_3+U_3))$$

$Q(U)$

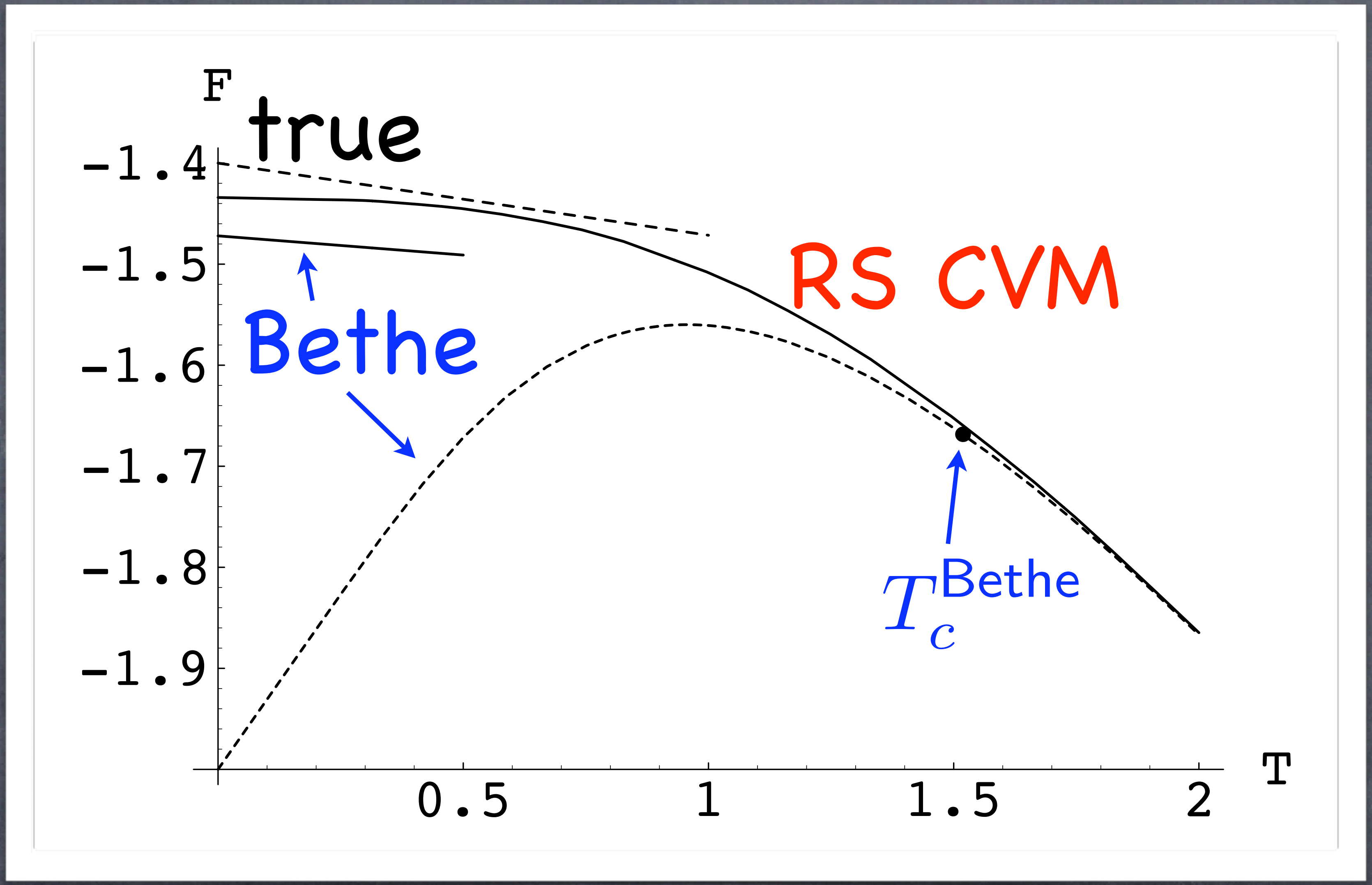
at

$T = 0.1$



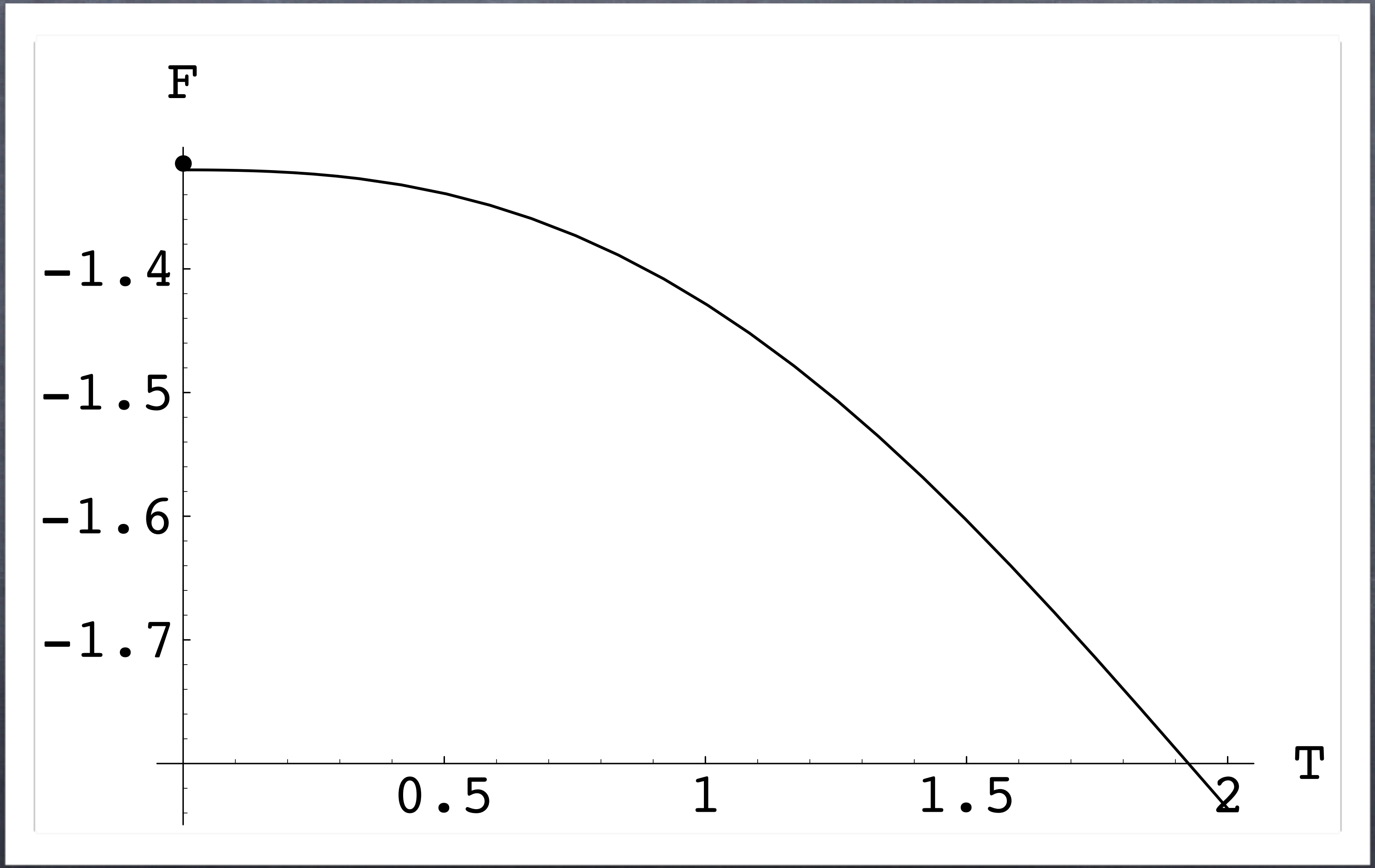
U fields concentrate over the integers for T->0

RS CVM for ±J EA 2D



Entropy is always positive
Improves the GS energy

RS CVM for Gaussian EA 2D



RS CVM for EA 2D

Local stability of the solution w.r.t. $u, u_1, u_2 \neq 0$

$$a = \int q(u) u^2 du \qquad a_{ij}(U) = \int Q(U, u_1, u_2) u_i u_j du_1 du_2 \quad j = 1, 2$$

RS CVM for EA 2D

Local stability of the solution w.r.t. $u, u_1, u_2 \neq 0$

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small

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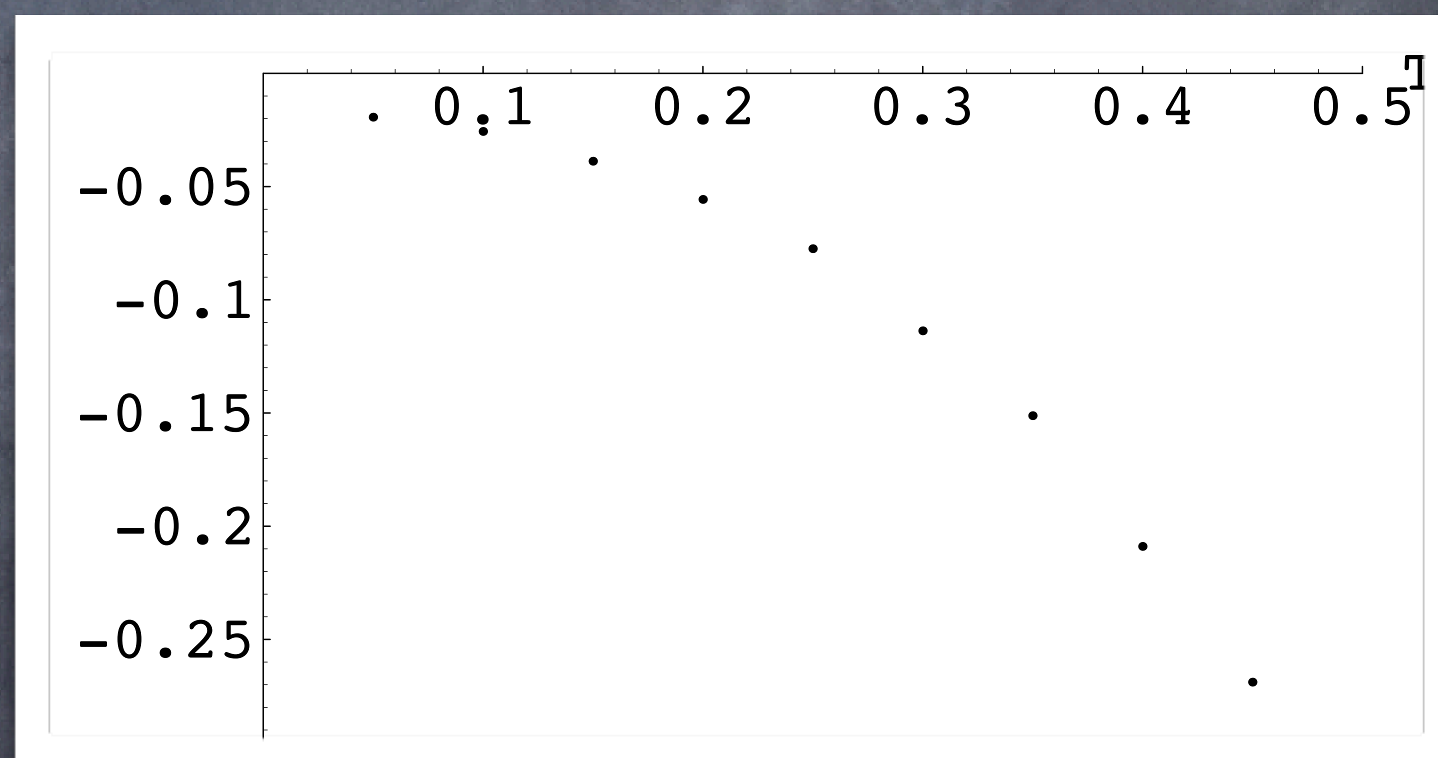
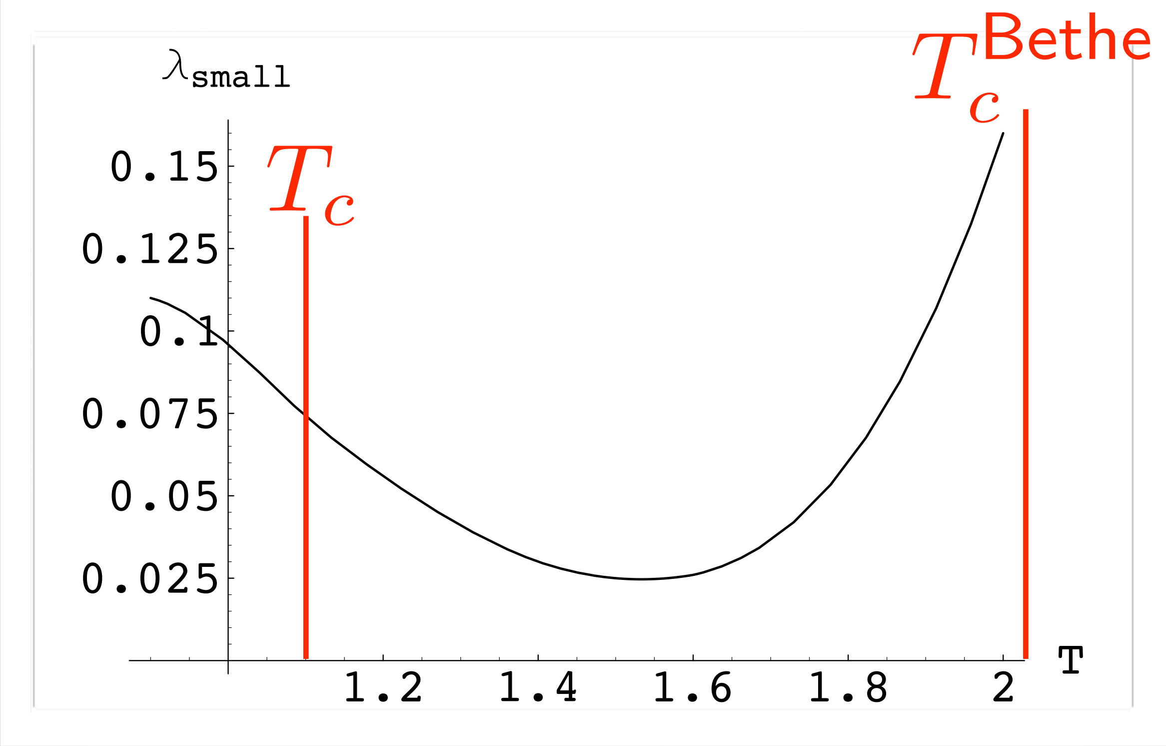
small

$$\frac{1}{\ln \mathrm{Det}}$$



Summary of analytical results for the ±J EA model

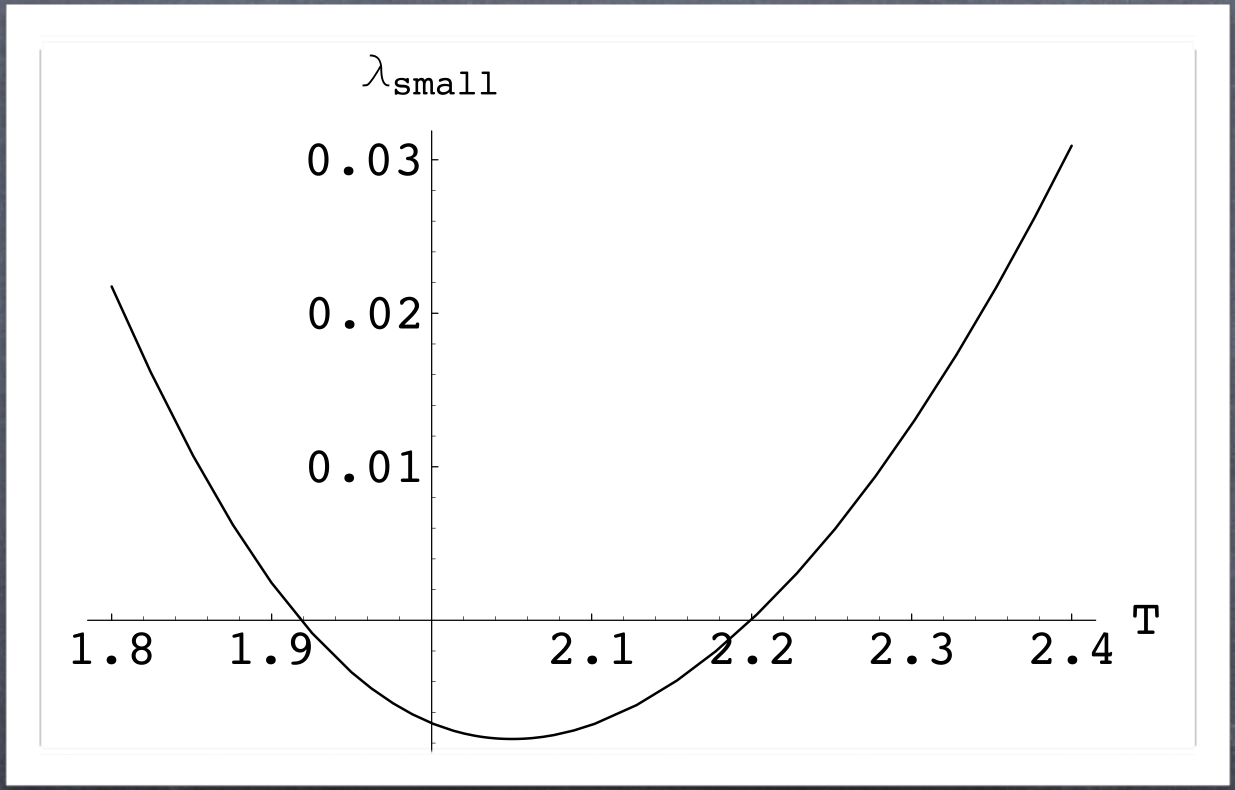
- 2D $T_c = 0$ $T_c^{\text{plaq}} = 0$ $T_c^{\text{Bethe}} = 1.5186...$
- 3D



first order transition or need to consider a larger region (the cube)

Summary of analytical results for the EA model

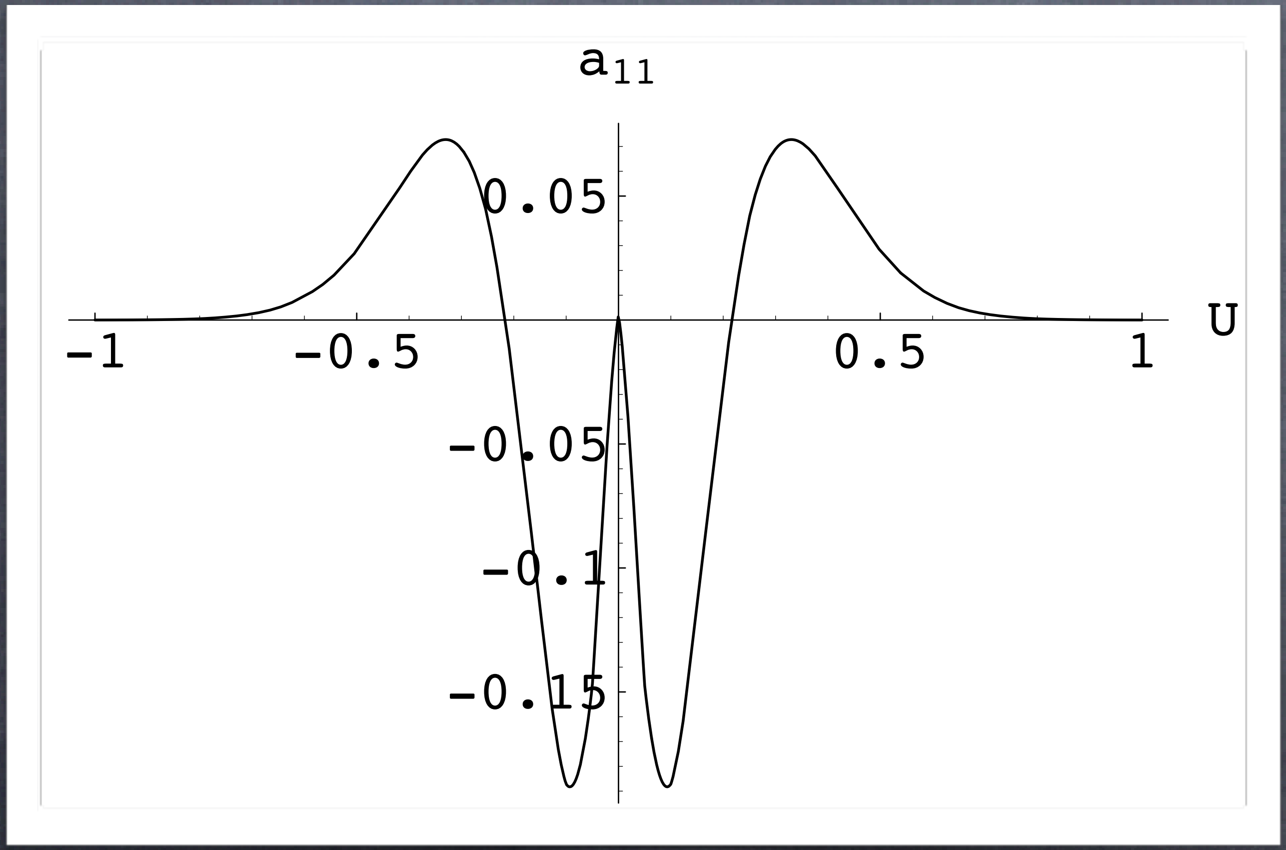
- 4D



$$T_c = 2.03 \quad T_c^{\text{plaq}} = 2.2 \quad T_c^{\text{Bethe}} = 2.515\ldots$$

Functions, not distributions!

$$a_{11}(U) = \int Q(U, u_1, u_2)\, u_1^2 \, du_1 du_2$$



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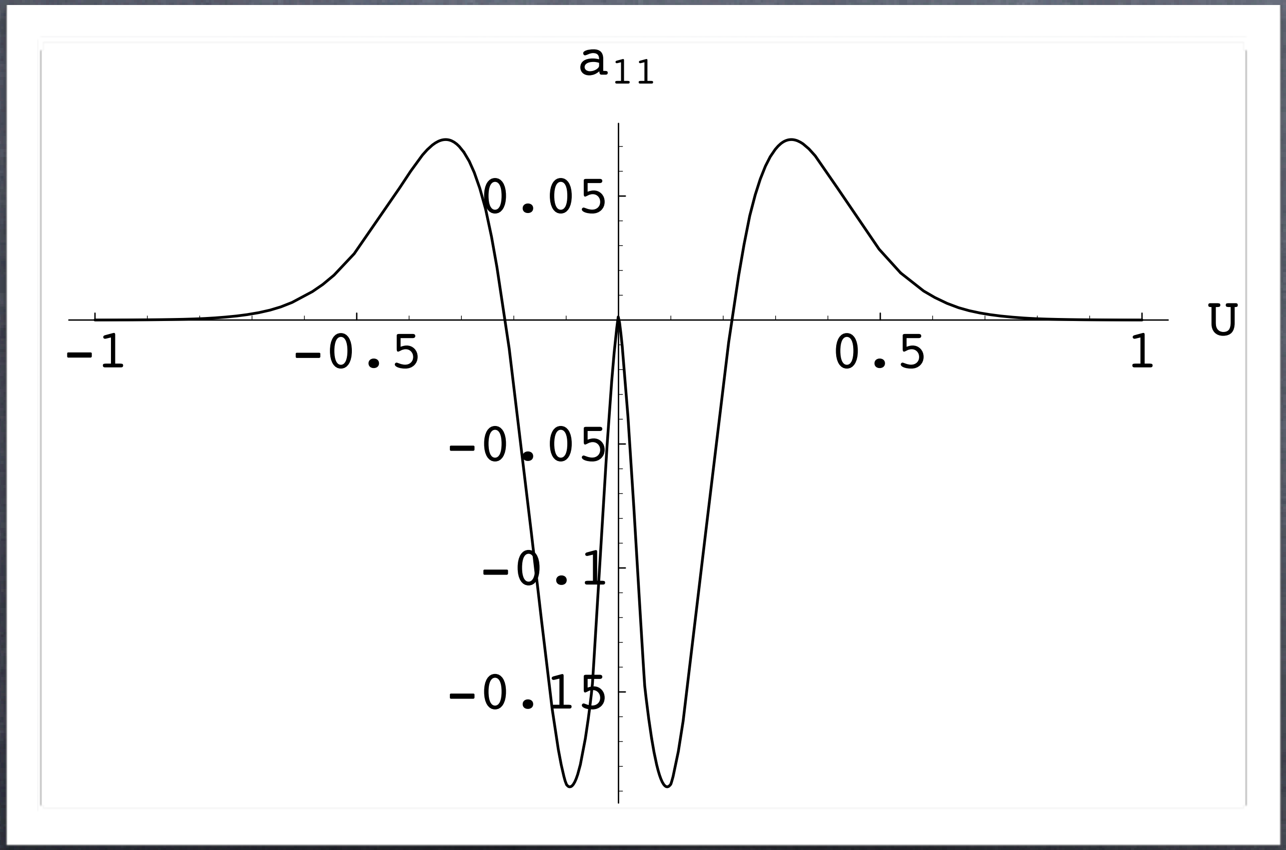
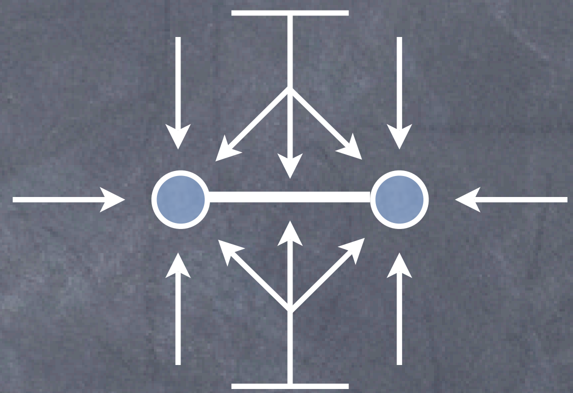
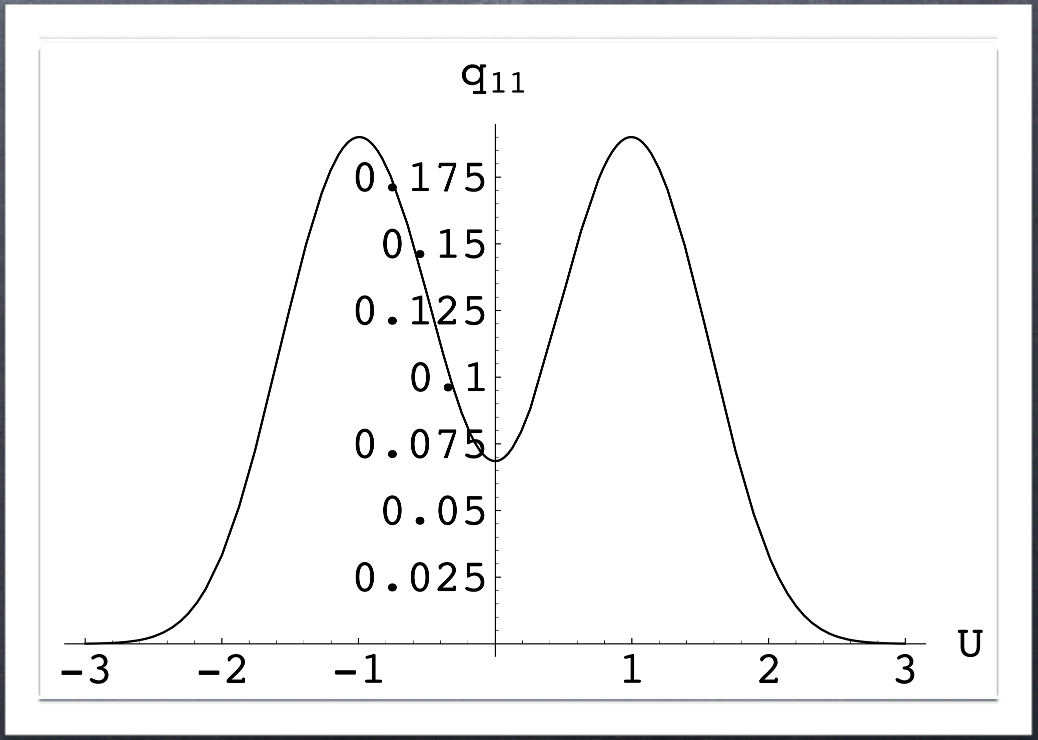
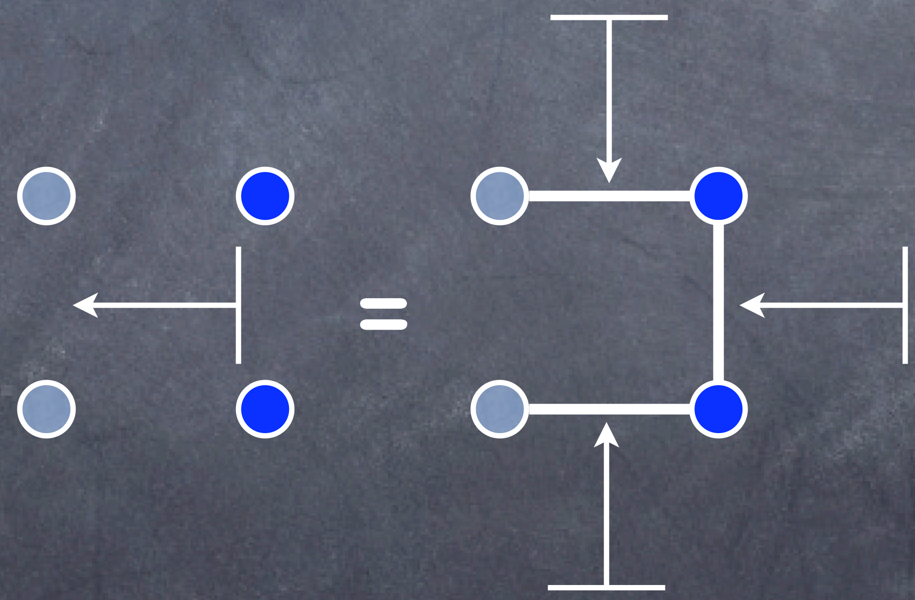




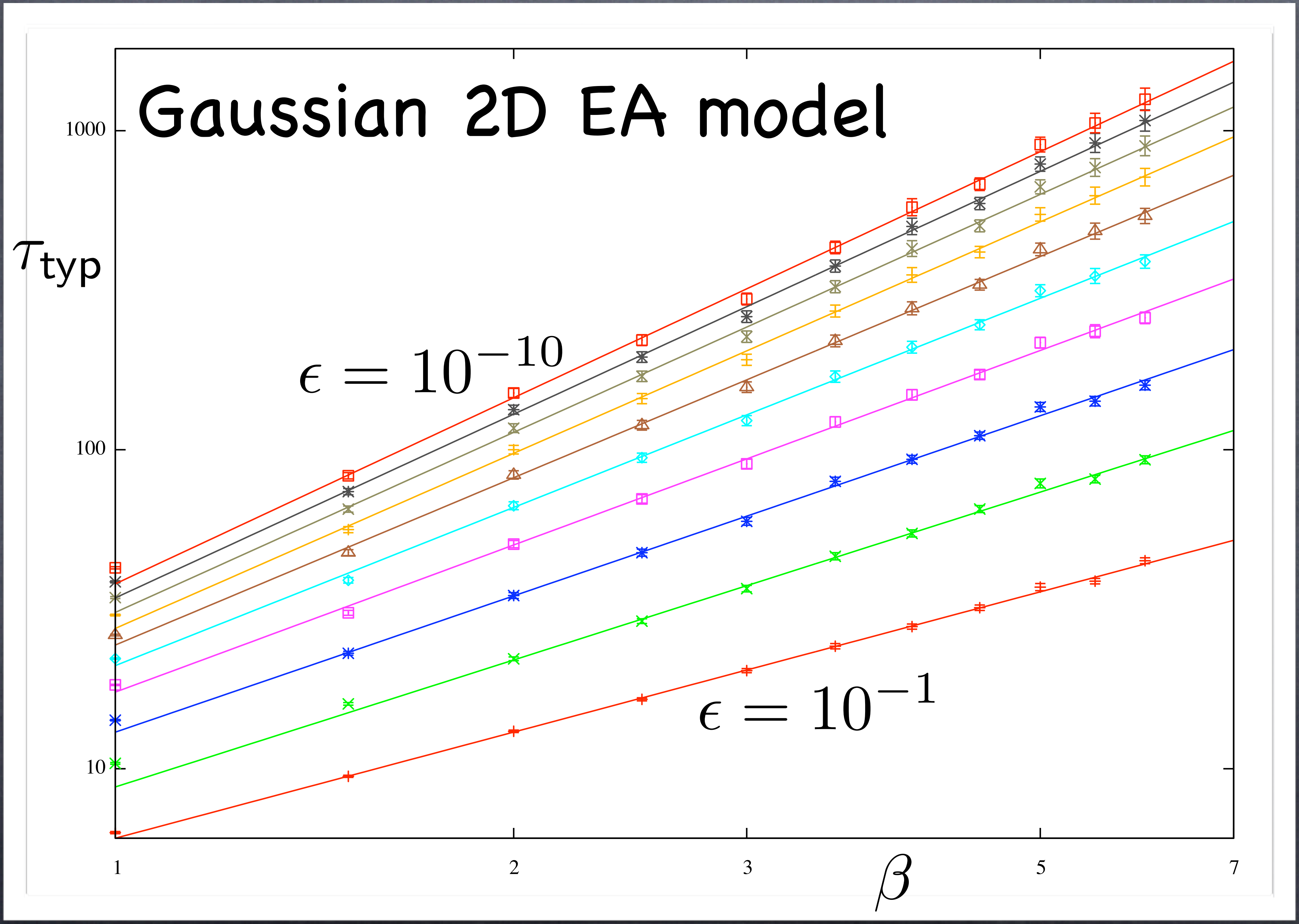


MPA for solving a given sample of 2D EA model

Set u=0 and solve iteratively for U's according to eq.

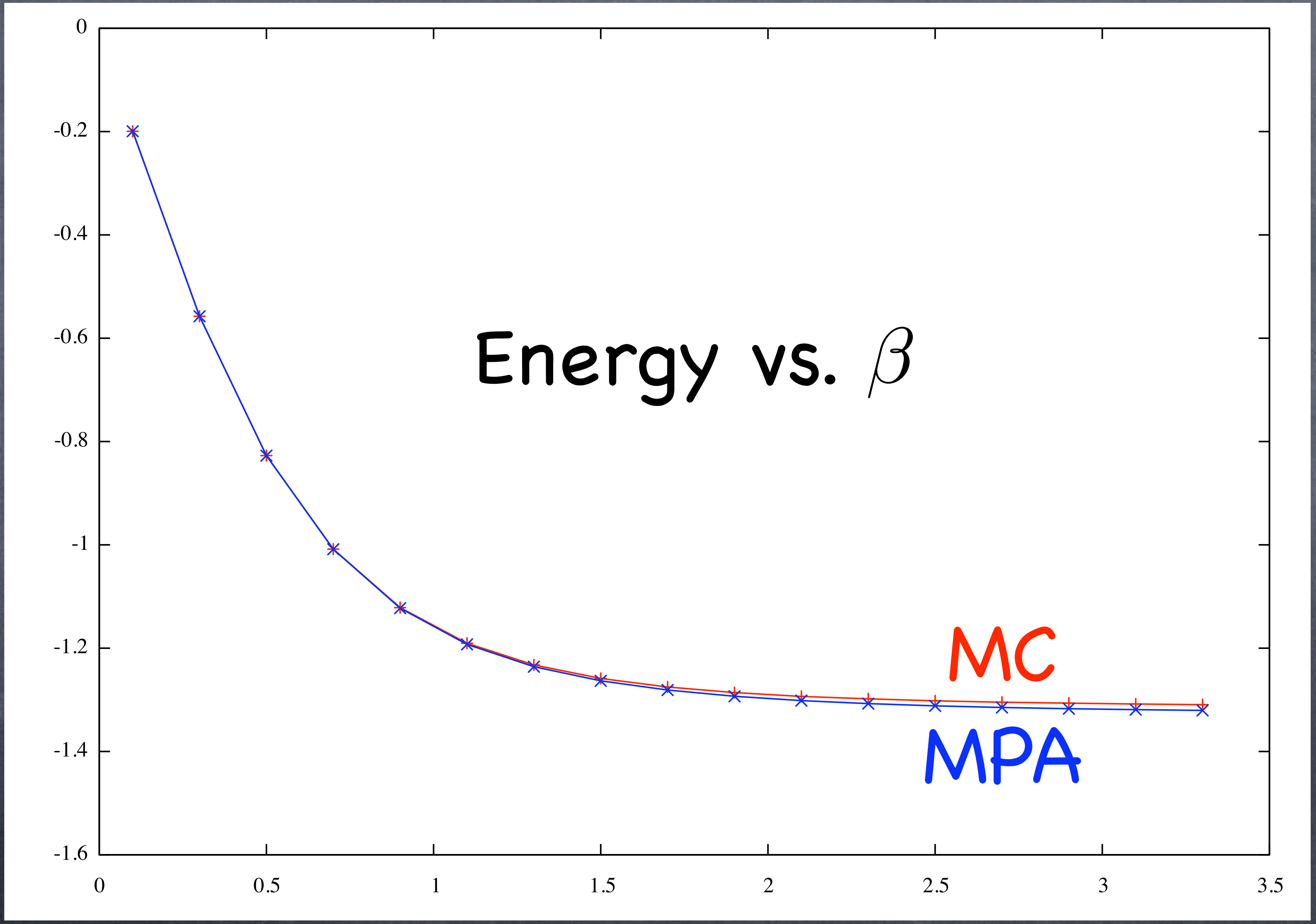


Converges for any T



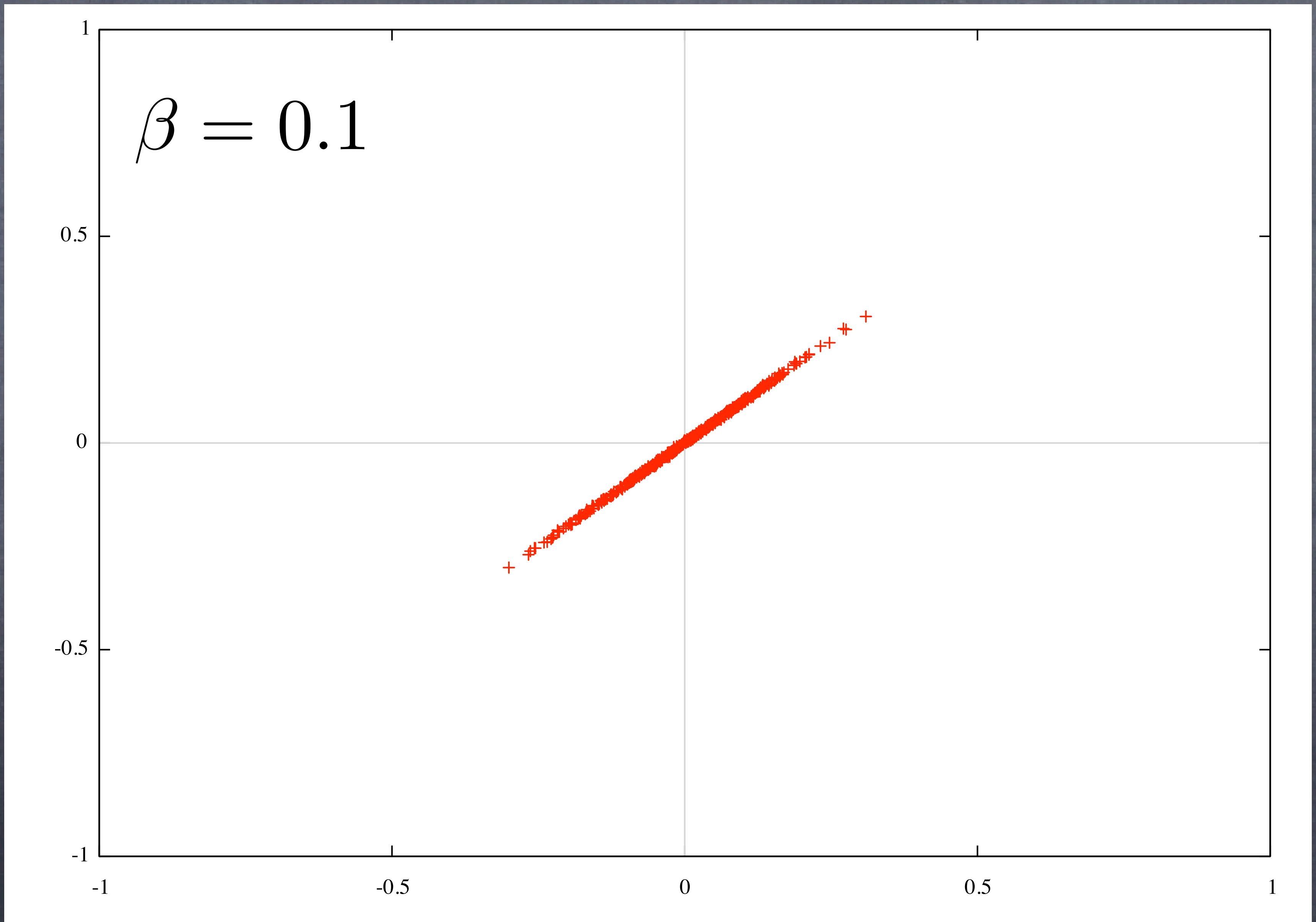
BP converges only for $\beta < 0.84$!!

Comparison with MC



Two spins marginals

$\langle \sigma_i \sigma_j \rangle_{\text{MC}}$



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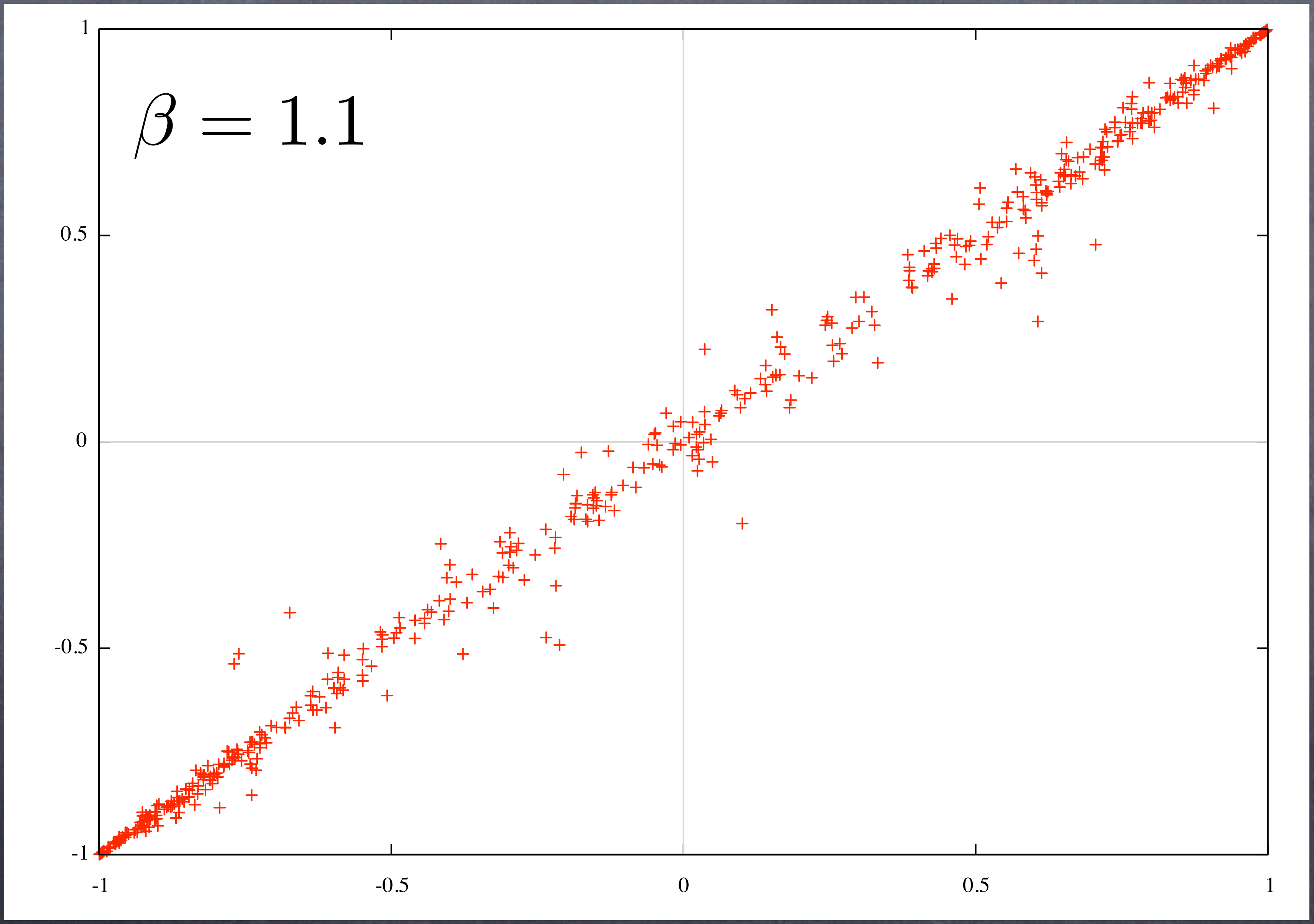

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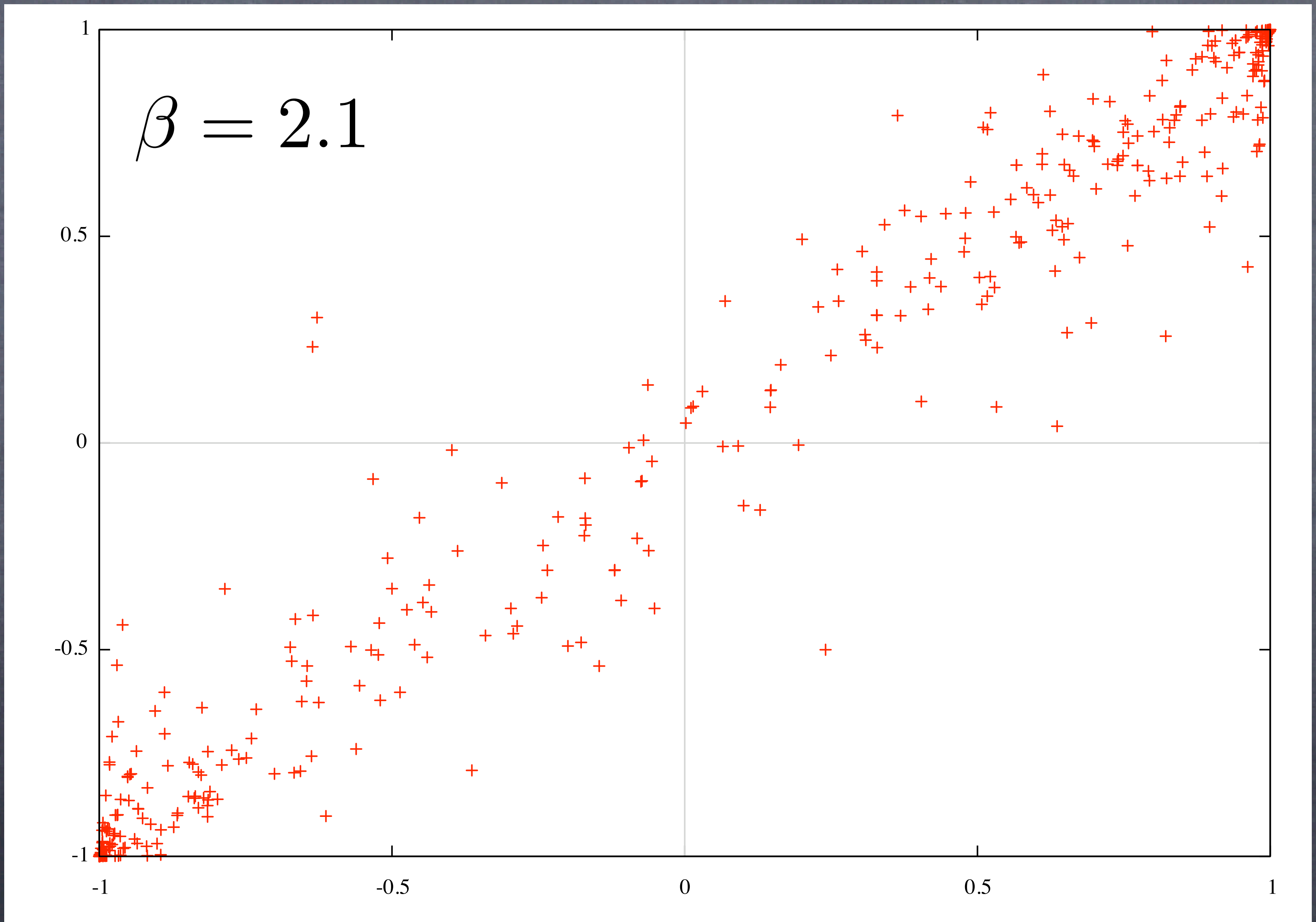

$\langle \sigma_i \sigma_j \rangle_{\text{MC}}$

$\langle \sigma_i \sigma_j \rangle_{\text{MPA}}$

Stronger test: find GS

MPA + decimation or reinforcement

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MPA + decimation or ~~reinforcement~~

never finds GS !!

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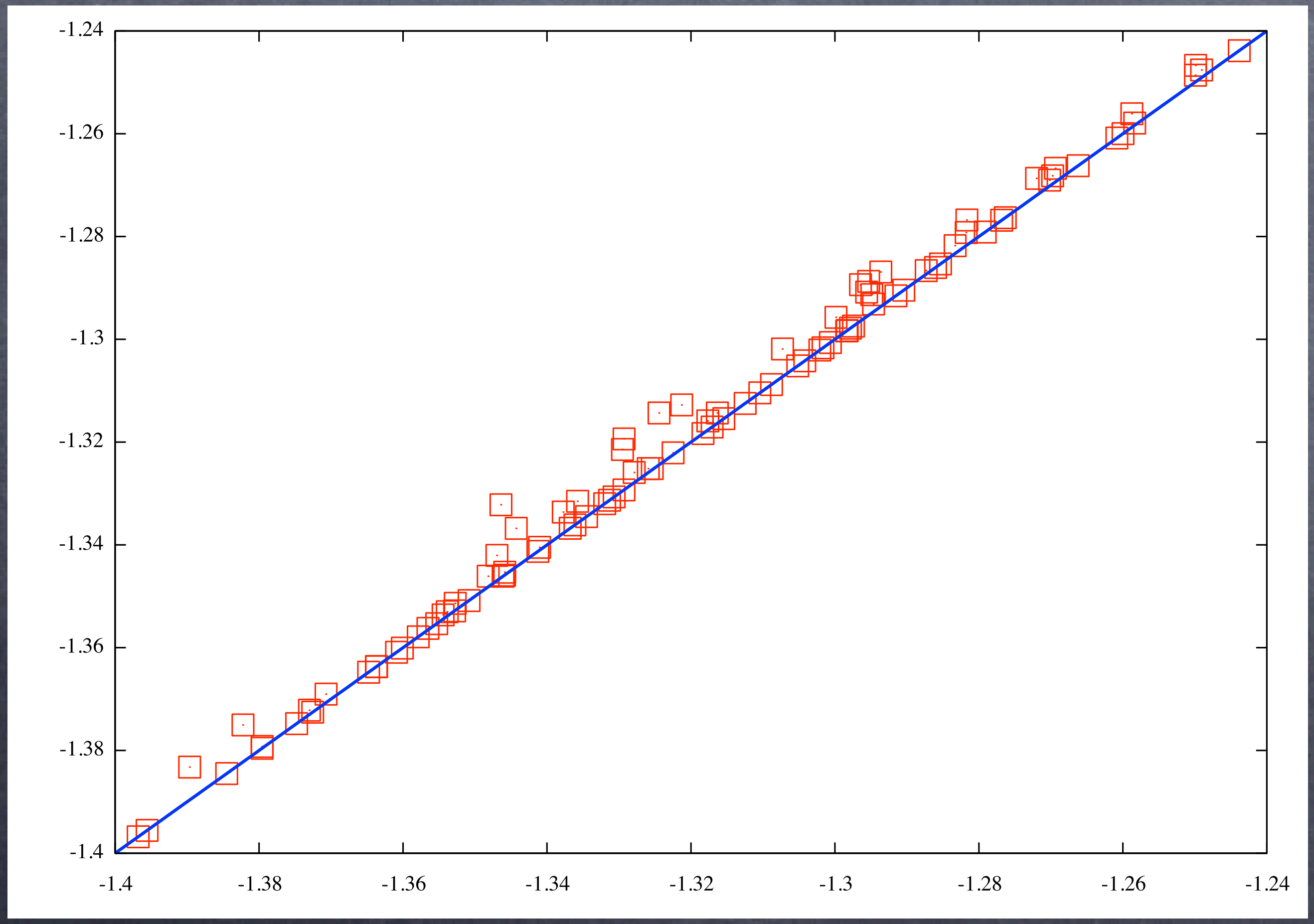
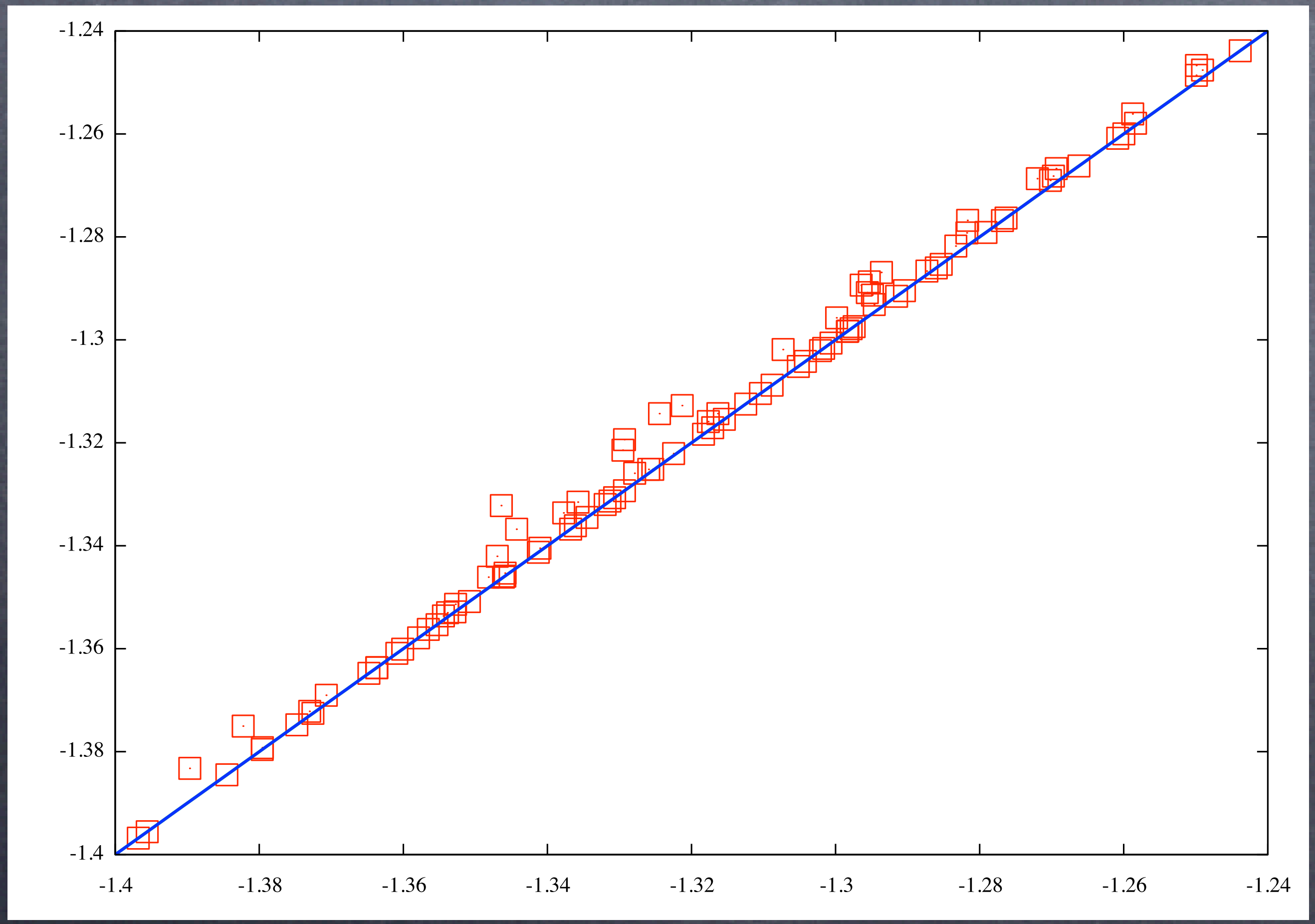


exact GS energy

Stronger test: find GS

MPA + decimation or ~~reinforcement~~

never finds GS !!



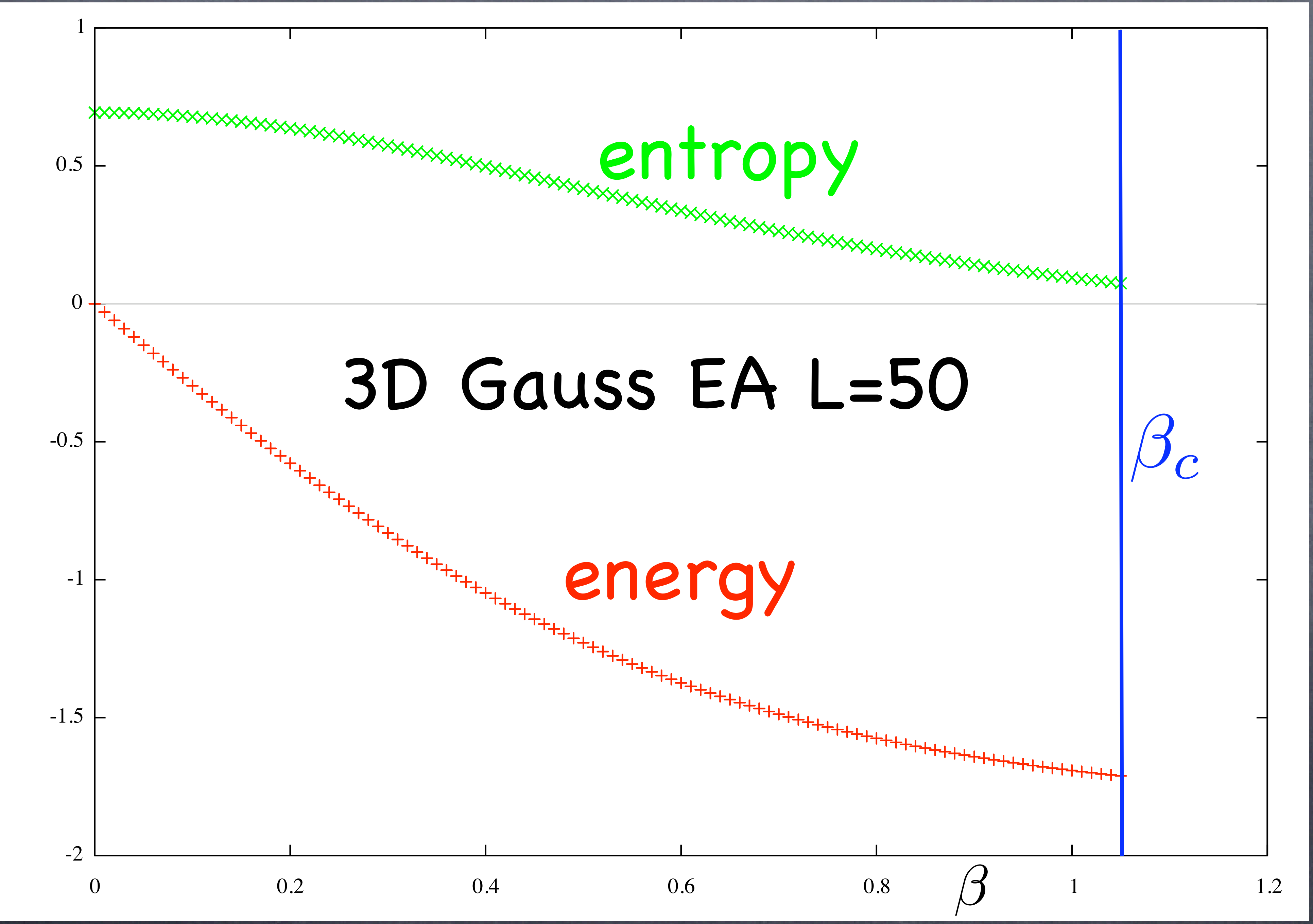
exact GS energy

mean relative error:

0.0013 for Gauss

0.00078 for ±J

It works on a 3D lattice!



Conclusions

- By the Replica CVM we derived GSP eqs.
- The solution is a computational challenge!
- Very good approximation scheme:
  - average case, no transition in 2D EA model
  - single sample, MPA for the paramagnetic phase

Future work

- find the AT line (paramagnetic phase in field)
- going in the SG phase with GSP:
  - 1RSB factorized solution
  - few first moments of Q(U,u1,u2)