Mean-field method with correlations determined by linear response

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joint work with Jack Raymond

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Outline

- Mean field approx. (MFA)
- Linear response (LR)
- Limits of MFA and LR
- General framework for MFA + LR
- Numerical results on 2D models
  (both ordered and with disorder)

The main pb. in Stat Mech

- Compute the free-energy

$$F(\boldsymbol{J}, \boldsymbol{h}) = \log Z(\boldsymbol{J}, \boldsymbol{h}) = \log \sum_{\{s_i\}} \exp\left(\sum J_{ij} s_i s_j + \sum_i h_i s_i \right)$$

  The sum is over exponentially many terms

- Resort to mean field approximations (MFA)
  - few parameters to be fixed self-consistently
  - fast to compute, but inexact!

MFA to the free-energy

- naive mean-field (nMF)
  only N parameters $m_i = \langle s_i \rangle$

$$H(x) \equiv -x\ln(x)$$

$$F_{\mathrm{nMF}} = \sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + \sum_i h_i m_i + \sum_{i\neq j} J_{ij} m_i m_j$$

$$\frac{\partial F_{\mathrm{nMF}}}{\partial m_i} = \sum_j J_{ij} m_j + h_i - \mathrm{atanh}(m_i) = 0$$

$$\boxed{m_i = \tanh\left[h_i + \sum_j J_{ij} m_j\right]}$$

MFA to the free-energy

- nMF + Onsager reaction term (TAP)

$$F_{\mathrm{TAP}} = \sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + \\ + \sum_i h_i m_i + \sum_{i \neq j} \left(J_{ij} m_i m_j + \frac{1}{2} J_{ij}^2 (1-m_i^2)(1-m_j^2) \right)$$

$$\boxed{m_i = \tanh\left[h_i + \sum_j J_{ij} \Big(m_j - \underbrace{J_{ij}(1-m_j^2) m_i}_{\text{reaction term}} \Big) \right]}$$

MFA to the free-energy

Expansion in small J

(correct at high temperature or in fully connected models)

$$F_{\mathrm{nMF}} = \sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + \sum_i h_i m_i + \sum_{i\neq j} J_{ij} m_i m_j$$

$$F_{\mathrm{TAP}} = \sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + $$
$$+ \sum_i h_i m_i + \sum_{i\neq j} \left(J_{ij} m_i m_j + \frac{1}{2} J_{ij}^2 (1-m_i^2)(1-m_j^2) \right)$$

MFA to the free-energy

- Bethe approximation (BA)
  nMF + nearest neighbors correlations parameters

$$c_{ij} = \langle s_i s_j \rangle - m_i m_j$$

$$F_{\mathrm{BA}} = \sum_{i \neq j} \left[H\left(\frac{(1+m_i)(1+m_j)+c_{ij}}{4}\right) + H\left(\frac{(1-m_i)(1-m_j)+c_{ij}}{4}\right) + \right.$$
$$\left. + H\left(\frac{(1+m_i)(1-m_j)-c_{ij}}{4}\right) + H\left(\frac{(1-m_i)(1+m_j)-c_{ij}}{4}\right) \right] +$$
$$+ \sum_i (1-d_i) \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right) \right] + \sum_i h_i m_i + \sum_{i \neq j} J_{ij}(c_{ij} + m_i m_j) \; ,$$

MFA to the free-energy

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$$c_{ij} = \langle s_i s_j \rangle - m_i m_j$$

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$$\left. + H\left(\frac{(1+m_i)(1-m_j)-c_{ij}}{4} \right) + H\left(\frac{(1-m_i)(1+m_j)-c_{ij}}{4} \right) \right] +$$

$$+ \sum_i (1-d_i) \left[H\left(\frac{1+m_i}{2} \right) + H\left(\frac{1-m_i}{2} \right) \right] + \sum_i h_i m_i + \sum_{i \neq j} J_{ij}(c_{ij} + m_i m_j) \; ;$$

entropy

energy

MFA to the free-energy

- Bethe approximation (BA)

$$f(m_1, m_2, t) = \frac{1 - t^2 - \sqrt{(1-t^2)^2 - 4t(m_1 - m_2 t)(m_2 - m_1 t)}}{2t(m_2 - m_1 t)}$$

$$\boxed{m_i = \tanh\left[h_i + \sum_j \operatorname{atanh}\Big(t_{ij} f(m_j, m_i, t_{ij})\Big)\right]}$$

$$c_{ij}(m_i, m_j, t_{ij}) = \frac{1}{2t_{ij}}\left(1 + t_{ij}^2 - \sqrt{(1-t_{ij}^2)^2 - 4t_{ij}(m_i - t_{ij}m_j)(m_j - t_{ij}m_i)}\right) - m_i m_j$$

$$t_{ij} = \tanh(J_{ij})$$

Computing correlations by linear response (LR)

- Correlations are trivial in MFA

$C_{ij} = 0$ in nMF, TAP and BA (between distant spins)

- Non trivial correlations can be obtained by using the linear response

$$\chi_{ij} = \frac{\partial m_i}{\partial h_j} \qquad (\chi^{-1})_{ij} = \frac{\partial h_i}{\partial m_j}$$

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$$\chi_{ij} = \frac{\partial m_i}{\partial h_j} \qquad (\chi^{-1})_{ij} = \frac{\partial h_i}{\partial m_j}$$

$$(\chi^{-1}_{\mathrm{nMF}})_{ij} \;=\; \frac{\delta_{ij}}{1-m_i^2} - J_{ij}\ ,$$

$$(\chi^{-1}_{\mathrm{TAP}})_{ij} \;=\; \left[\frac{1}{1-m_i^2} + \sum_k J_{ik}^2(1-m_k^2)\right]\delta_{ij} - \left(J_{ij} + 2J_{ij}^2 m_i m_j\right)$$

Computing correlations by linear response in BA

- Analytic expression for the correlations in BA
  (FRT, JSTAT, 2012)

$$(\chi^{-1}_{\mathrm{BA}})_{ij} = \left[\frac{1}{1-m_i^2} - \sum_k \frac{t_{ik} f_2(m_k, m_i, t_{ik})}{1 - t_{ik}^2 f(m_k, m_i, t_{ik})^2}\right]\delta_{ij} - \frac{t_{ij} f_1(m_j, m_i, t_{ij})}{1 - t_{ij}^2 f(m_j, m_i, t_{ij})^2}$$

- Coincide with the fixed point of Susceptibility Propagation (no need to run any algorithm!)

- PROBLEM: estimates of nearest neighbor (NN) correlations are inconsistent $\chi_{ij}^{\mathrm{BA}} \neq C_{ij}^*$

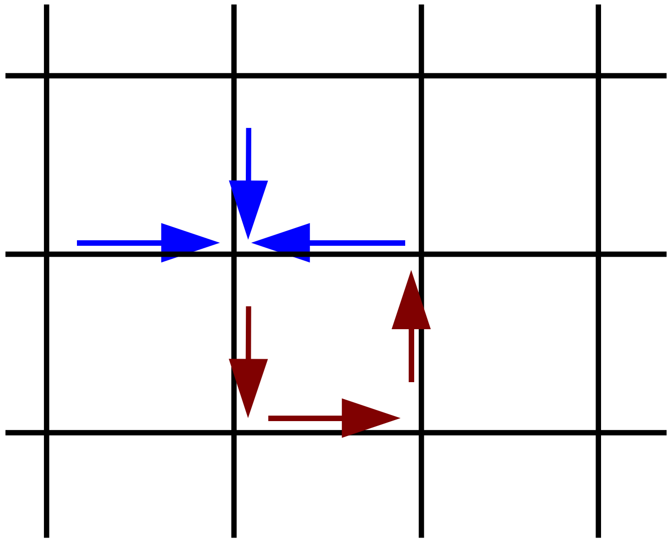
How loops make MFA fail

e.g. Bethe approximation, high temperature phase

- maximum entropy (free energy minimum)

$$\langle \sigma_i \sigma_j \rangle_c^{\mathrm{BA}} = c_{ij}^* = \tanh(\beta J_{ij}) < \langle \sigma_i \sigma_j \rangle_c^{\mathrm{exact}}$$

- linear response



$$\chi_{ii} = 1 + \sum_{j \in \partial i} u_{j \to i, i} \neq 1$$

ferromagnet $\chi_{ij}^{\mathrm{BA}} > \langle \sigma_i \sigma_j \rangle_c^{\mathrm{exact}}$

Make MFA & LR consistent

"Consistency is more important than truth" (S. Ting)

Add to the free-energy Lagrange multipliers to enforce (at the fixed point)

$$\boxed{\chi_{ii} = 1 - m_i^2 \quad \chi_{ij} = C_{ij}}$$

free energy minimum curvature

free energy minimum location

General framework (MFA + LR)

$$\boxed{F_\lambda = F_{\mathrm{MFA}}(\{m_i\}, \{C_{ij}\}, \ldots) + \sum_i \lambda_i m_i^2 + \sum_{i<j} \lambda_{ij} C_{ij}}$$

Your preferred MFA

can be set to zero to recover known approx. or used to satisfy

$$\chi_{ii} = 1 - m_i^2 \quad \chi_{ij} = C_{ij}$$

General framework (MFA + LR)

$$F_{\mathrm{MFA}}(\{m_i\},\{C_{ij}\},\ldots) = \overbrace{\sum_i h_i m_i + \sum_{ij} J_{ij}(m_i m_j + C_{ij})}^{\text{energy}}$$

$$+ \underbrace{\sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + S^{2+}(\{m_i\},\{C_{ij}\},\ldots)}_{\text{entropy}}$$

General framework (MFA + LR)

$$F_\lambda = F_{\mathrm{MFA}}(\{m_i\}, \{C_{ij}\}, \ldots) + \sum_i \lambda_i m_i^2 + \sum_{i<j} \lambda_{ij} C_{ij}$$

Maximum Entropy equations
from free-energy minimization

$$\partial_{m_i} F_\lambda = \mathrm{atanh}(m_i) + \partial_{m_i} S^{2+} + h_i + \sum_j J_{ij} m_j + \lambda_i m_i = 0$$

$$\partial_{C_{ij}} F_\lambda = \partial_{C_{ij}} S^{2+} + J_{ij} + \lambda_{ij} = 0$$

$$\partial_{C_{ijk}} F_\lambda = \partial_{C_{ijk}} S^{2+} = 0$$

Higher order correlation parameters
are fixed by standard maximum entropy

$$\chi_{ii} = 1 - m_i^2 \quad \chi_{ij} = C_{ij}$$

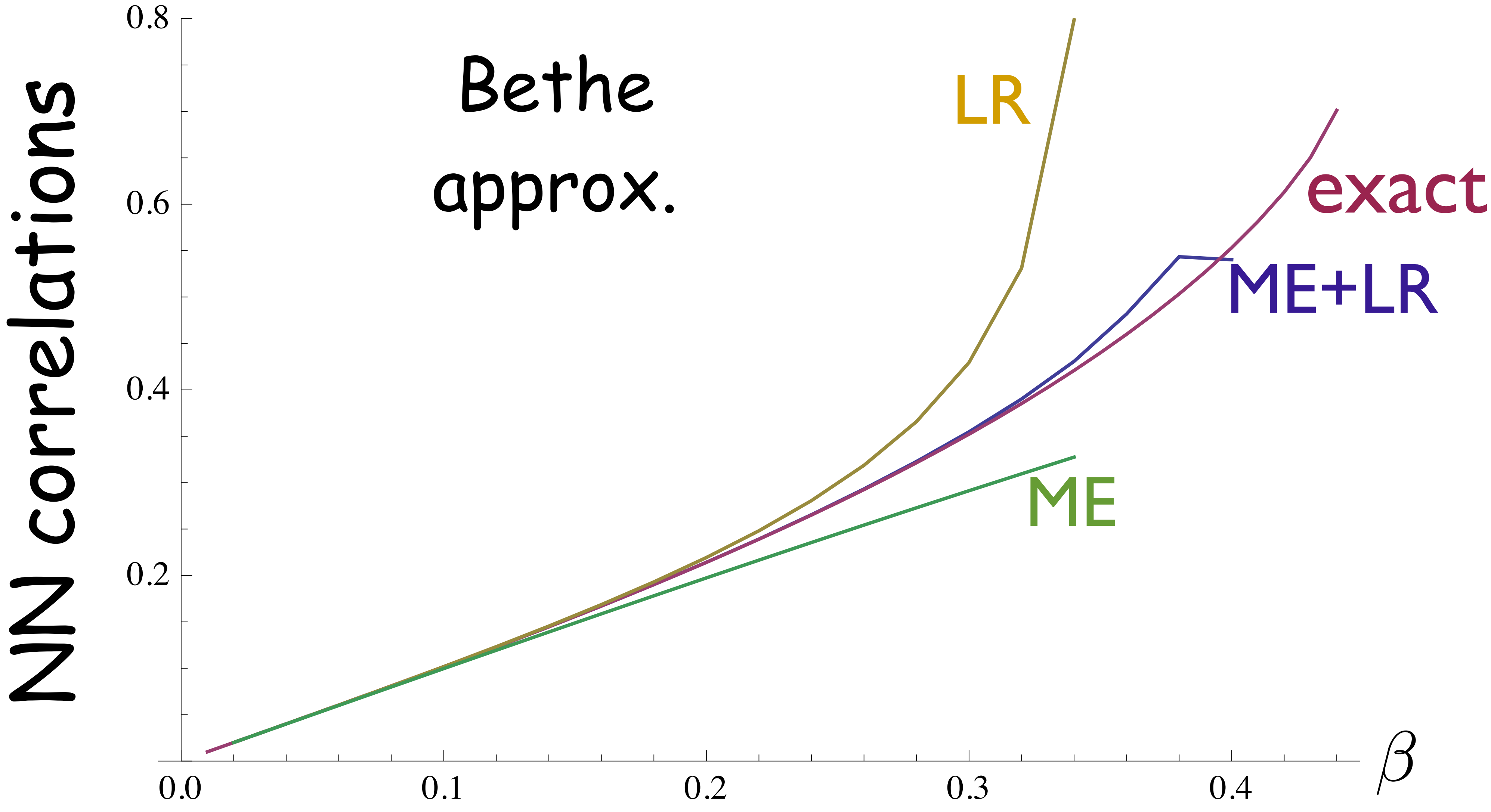
Some comments...

- Bethe/CVM free-energies are not convex adding parameters it not obvious to improve!
- λ parameters measure how wrong is the MFA e.g. on a random graph with Bethe approx. $\lambda \to 0$
- $J_{ij} \to J_{ij} + \lambda_{ij}$ would naively imply stronger correlations and also more unstable Susc. Prop. but this is not the case!

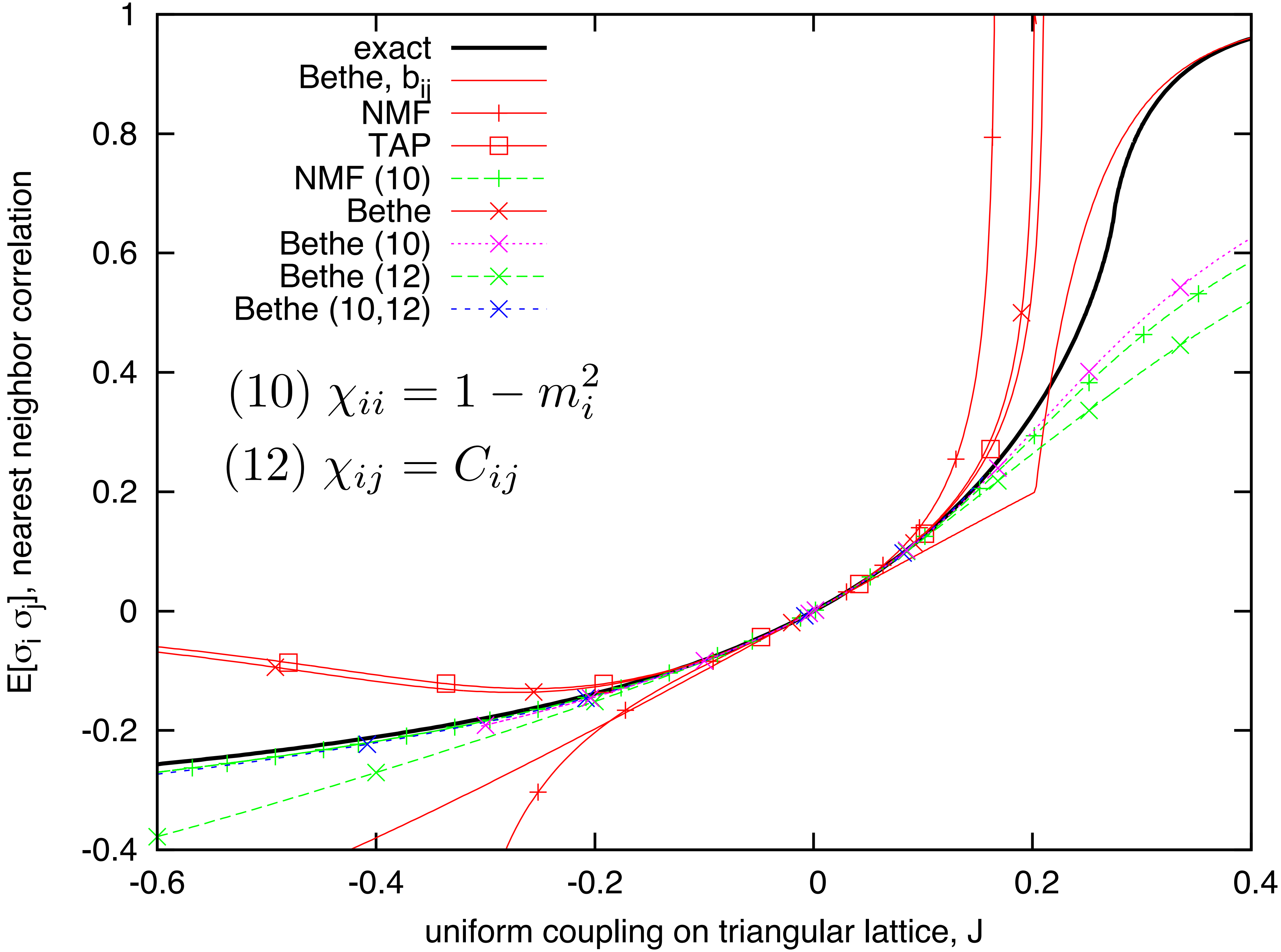
Models studied so far

- Ising variables
- 2D topology (square and triangular lattices)
- ferromagnetic
- frustrated -> triangular antiferromagnet
- frustrated & disordered -> random field

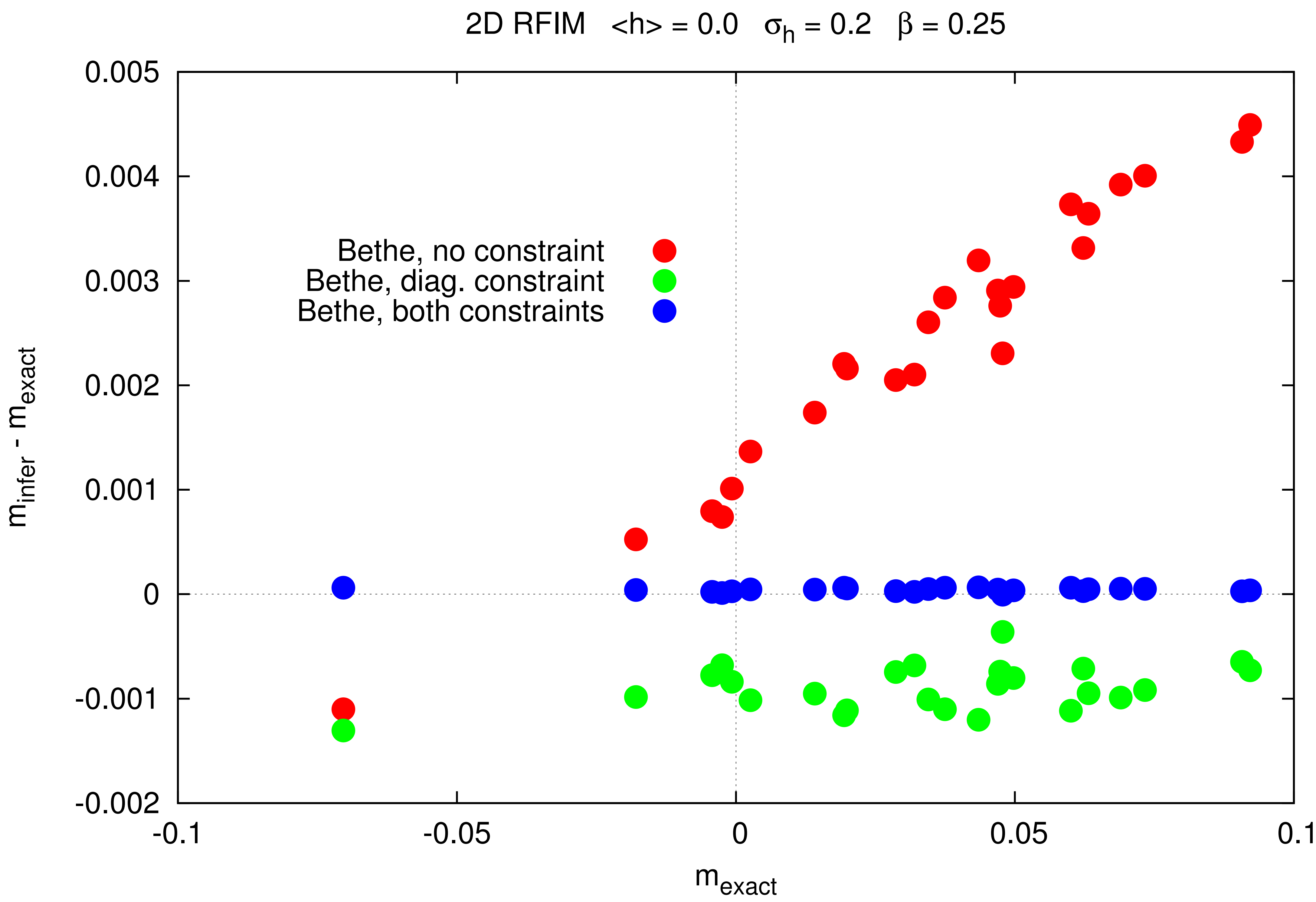
Nearest-neighbor correlation (2D square lattice)



Nearest-neighbor correlation (2D triangular lattice)



Random field Ising model
2D square lattice



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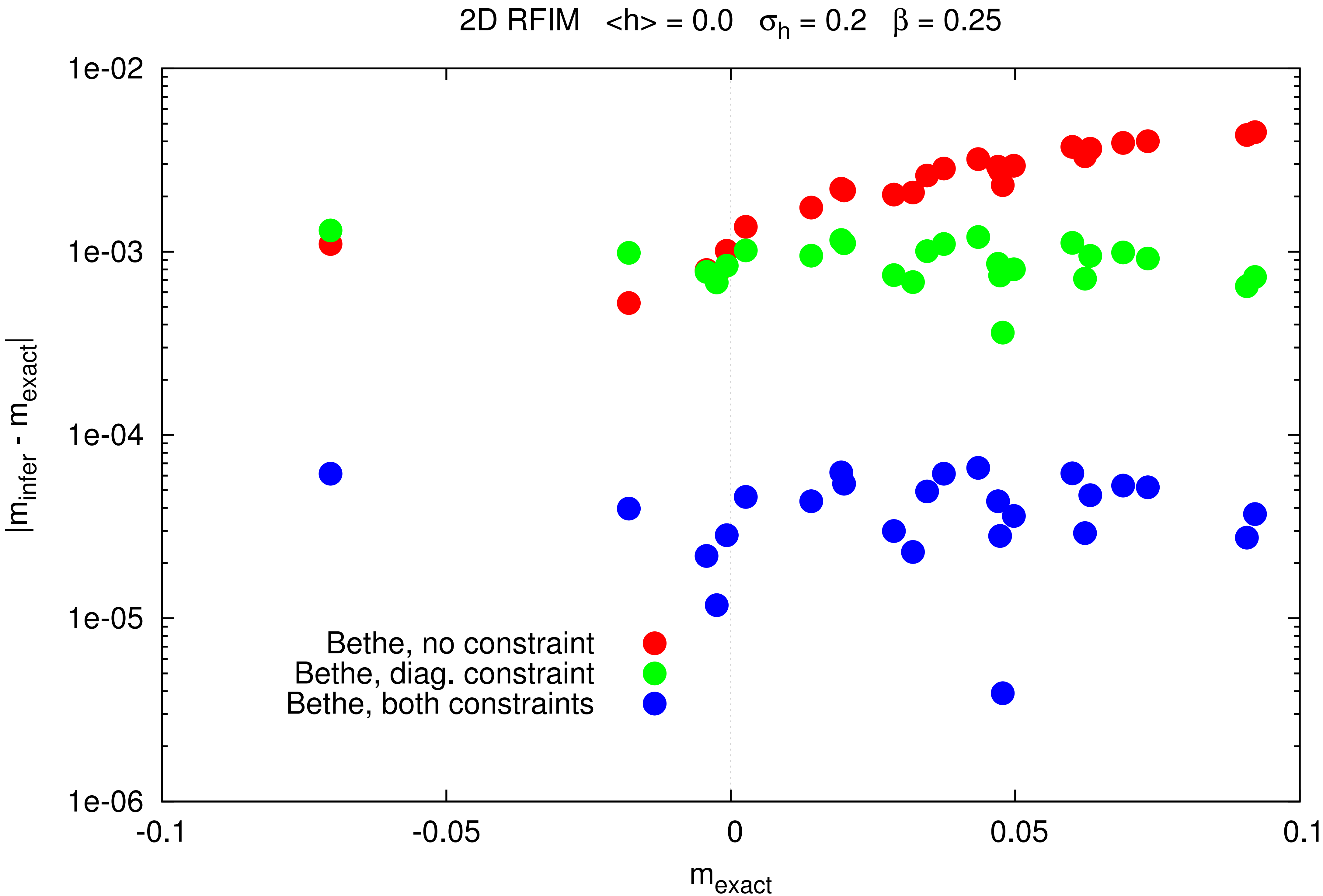

Random field Ising model
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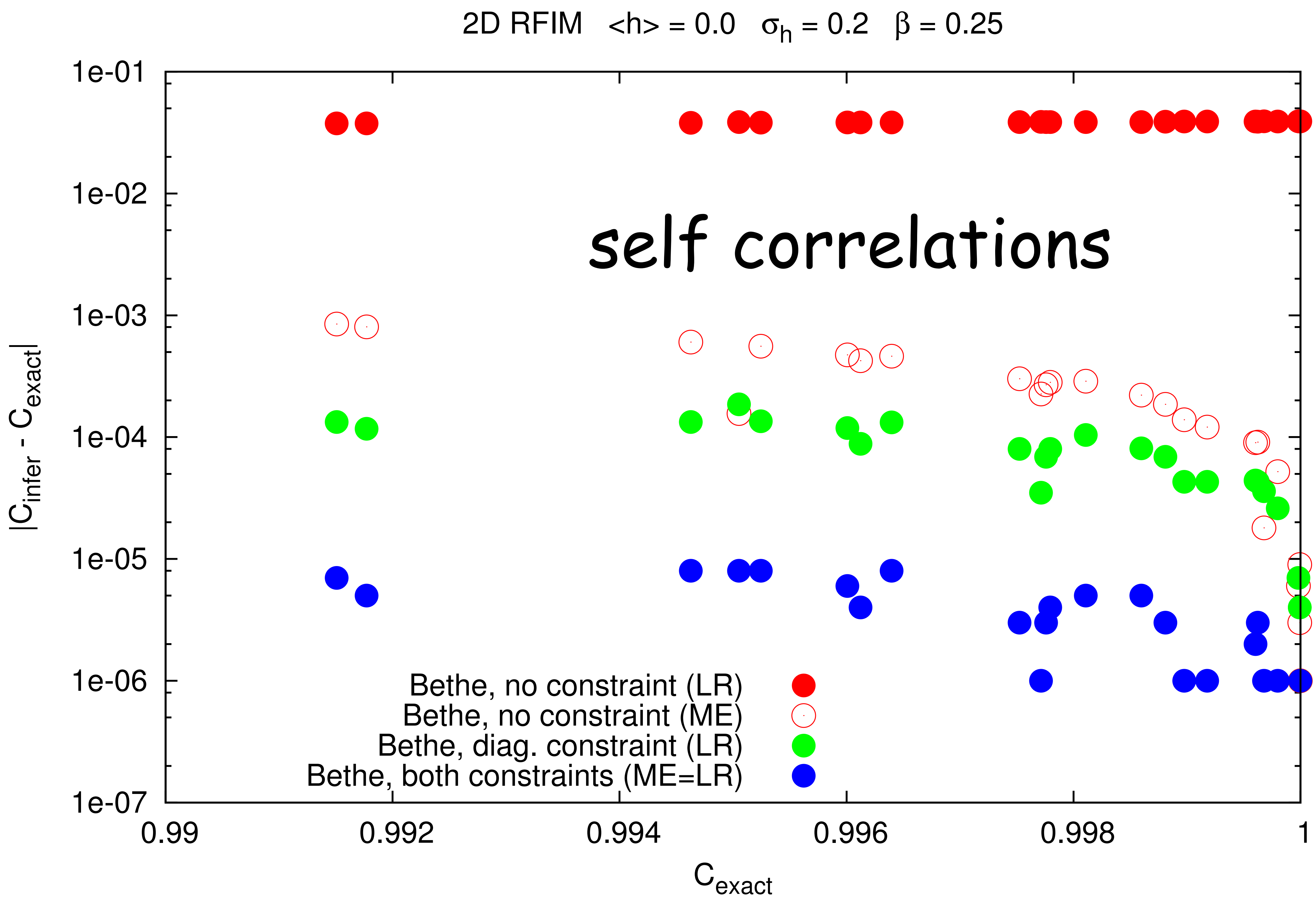
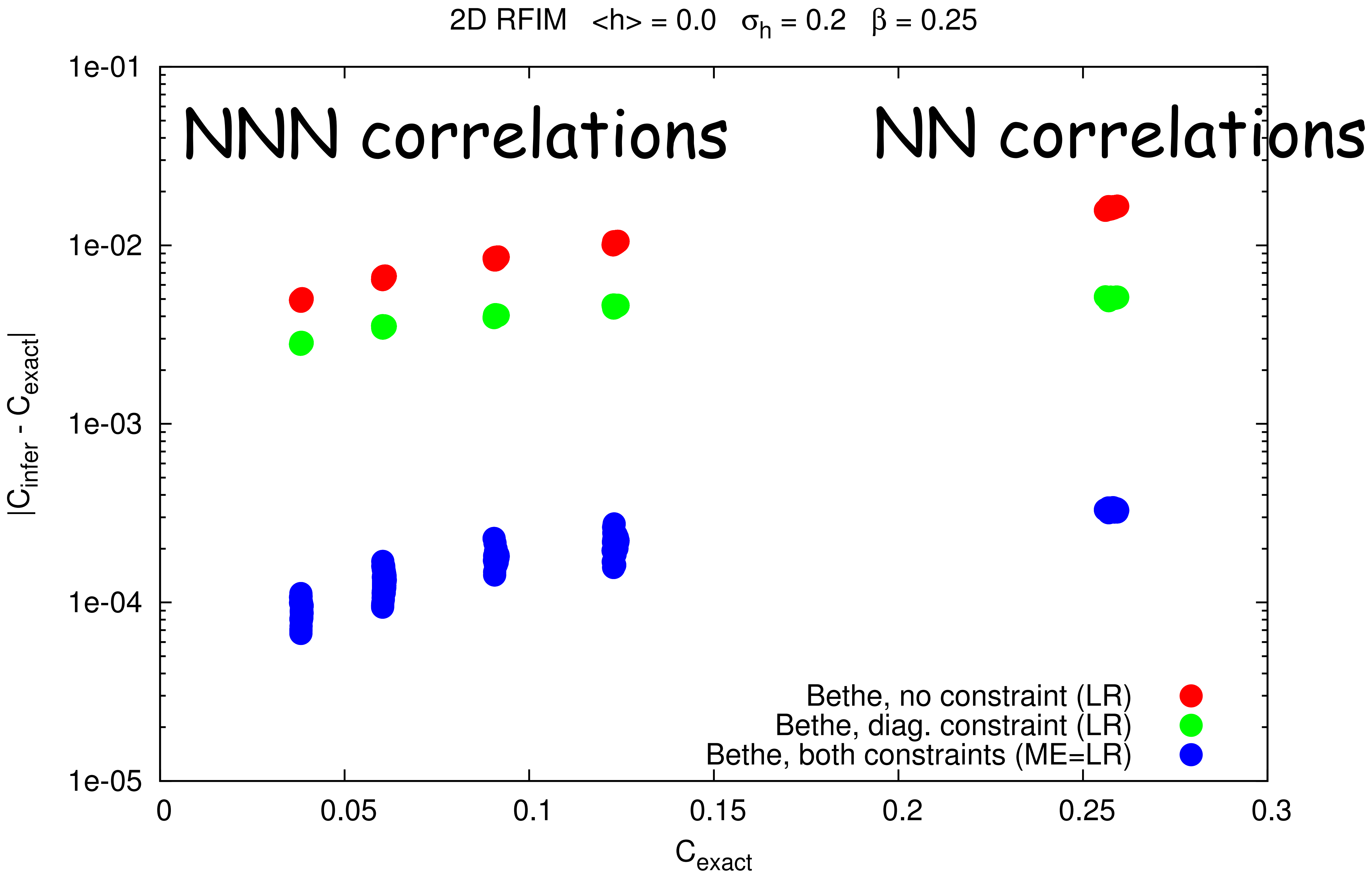
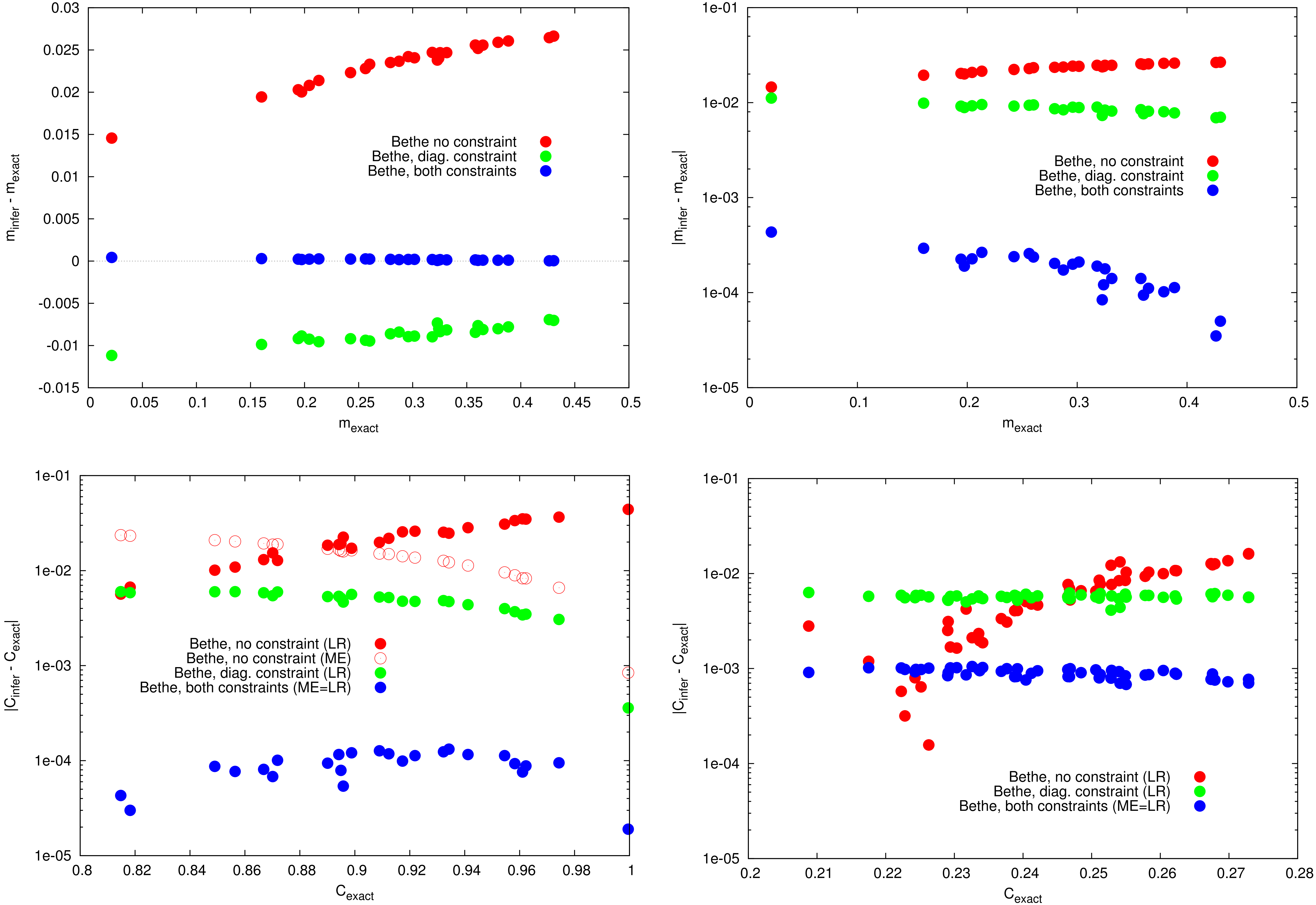


Random field Ising model
2D square lattice



Random field Ising model 2D square lattice $\langle h \rangle = 0.2 \ \ \sigma_h = 0.5$



Summary

Any MFA (even Cluster Variational Methods) can be improved by enforcing consistency between maximum entropy and linear response estimates.

Several improvements achieved

- Direct problem: better high temperature expansions & better correlation estimates
- Inverse problem: smaller errors in estimating couplings and fields

Still working for a fast message passing algorithm...