Gino Del Ferraro

from Italy - Velletri (Rome)

KTH Royal Institute of Technology
- Department of Computational Biology -
Stockholm

Supervisor
Prof. Erik Aurell

Educational Background :

Academic Studies:

Università degli studi di Roma
"La Sapienza"

- Bachelor Degree: → " Regular and Chaotic Motion in Hamiltonian Systems"
  - Supervisor: Angelo Vulpiani

- Brief Period in Ireland (Dublin) to work

- Master Degree → " Models for self non-self discrimination in the immune system"
  - Supervisors:

    Francesco Guerra

(Submitted) Paper **arXiv:1212.2574**

"Anergy in self-directed B lymphocytes
from a statistical mechanics perspective"

E. Agliari, A. Barra, G.D.F., F. Guerra, D. Tantari

Adriano Barra

NETADIS Project outlines:

Title:

" Cavity Method for non-equilibrium states"

- Supervisor: Erik Aurell

↓

Develop **dynamic BP (Belief Propagation) methods** to give a description of **non-equilibrium states** → Compare the results with **naive mean field** and **dynamic TAP methods**

- Applications: To dynamics of spin glasses and neural networks models, disease spreading models, communicate systems...

Other formative experiences so far:

First secondment:

Trieste, ICTP, SISSA

the end of October - the end of December

- Matteo Marsili

  - Advanced topics in probability theory

  - Winter school in Quantitative System Biology (ICTP)

Second secondment:

Paris, Université Paris-Sud

- Silvio Franz

  - dynamics cavity methods on spin glasses

Formative collaborations:

Helsinki, Aalto University

- Alexander Mozeika

Work done so far on the project:

General macroscopic analysis of dynamics

“Glauber dynamics of disordered Ising Chain ”

OUTLINE - MODEL

$$\mathcal{H}(\sigma) = -\sum_i J_{i,i+1}\sigma_i\sigma_{i+1} - \sum_i \theta_i\sigma_i$$

Glauber choice for updating:

$$\mathrm{Prob}(\sigma_i(t+1)) = \frac{1}{2}(1+\sigma_i(t+1)\tanh(\beta h_i(\sigma(t))),$$

→ it will satisfy detailed balance for symmetric interactions

- **Equilibrium:** → Boltzmann-Gibbs distribution $p_\infty(\sigma) = \frac{1}{Z}\mathrm{e}^{-\beta E(\sigma)}$

- **Dynamics:** **- Parallel,** **- Sequential**

- Microscopic description,

probability distribution of microstates

Macroscopic description

macroscopic observables

- Microscopic (sequential) dynamics -

General case:

- $\boldsymbol{\sigma}(t)$ unknown $$p_{t+\Delta}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W(\boldsymbol{\sigma}, \boldsymbol{\sigma}') p_t(\boldsymbol{\sigma}')$$

where $$W(\boldsymbol{\sigma}, \boldsymbol{\sigma}') = \frac{1}{N} \sum_{i=1}^{N} \left\{ \frac{1}{2} [1 + \sigma_i \tanh \beta h_i(\boldsymbol{\sigma}')) \prod_{j \neq i} \delta_{\sigma_j, \sigma'_j} \right\}$$

Current project: Glauber dynamics of Ising chain

- Microscopic (sequential) dynamics -

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- Continuous time

$$p_{t+1/N}(\boldsymbol{\sigma}) - p_t(\boldsymbol{\sigma}) \approx \frac{1}{N} \frac{d}{dt} p_t(\boldsymbol{\sigma})$$

- Master equation →

$$\frac{d}{dt} p_t(\boldsymbol{\sigma}) = \sum_{i=1}^{N} [w_i(F_i \boldsymbol{\sigma}) p_t(F_i \boldsymbol{\sigma}) - w_i(\boldsymbol{\sigma}) p_t(\boldsymbol{\sigma})]$$

where:

$$F_i \boldsymbol{\sigma} = (\sigma_1, ..., \sigma_{i-1}, -\sigma_i, \sigma_{i+1}, ..., \sigma_N)$$ - Spin-flip operator

$$w_i(\boldsymbol{\sigma}) = \frac{1}{2} [1 - \sigma_i \ \tanh[\beta h_i(\boldsymbol{\sigma})]]$$ - Transition rate

Current project: Glauber dynamics of Ising chain
- Macroscopic dynamics -

set of macroscopic observables

$$\boldsymbol{\Omega}(\boldsymbol{\sigma}) = (\Omega_1(\boldsymbol{\sigma}), ..., \Omega_n(\boldsymbol{\sigma}))$$

→ our considered case:

$$\boldsymbol{\Omega} = (m, E)$$

dynamical equations for $P_t(\boldsymbol{\Omega})$ $\quad N \to \infty$ ⇒ Often macroscopic dynamics becomes deterministic

Goal: to obtain a closed set of deterministic laws restricted to the number of macro-variables

define $$P_t(\boldsymbol{\Omega}) = \sum_{\boldsymbol{\sigma}} p_t(\boldsymbol{\sigma}) \delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{\sigma})]$$

- Macroscopic dynamics -

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Evolution of the probability - Kramer-Moyal expansion (keeping only first term)

- **Liouville equation**

$$\frac{d}{dt}P_t(\boldsymbol{\Omega}) = -\sum_{\mu=1}^{L}\left\{\frac{\partial}{\partial\Omega_\mu}P_t(\boldsymbol{\Omega})\underbrace{\left\langle\sum_{i=1}^{N} w_i(\boldsymbol{\sigma})\Delta_i^{\mu}(\boldsymbol{\sigma})\right\rangle_{\boldsymbol{\Omega};t}}_{F_\mu^{(1)}(\boldsymbol{\Omega},t)}\right\} = -\sum_{\mu=1}^{n}\frac{\partial}{\partial\Omega_\mu}[P_t(\boldsymbol{\Omega})F_\mu^{(1)}(\boldsymbol{\Omega},t)]$$

- **Deterministic flow**

$$\frac{d}{dt}\boldsymbol{\Omega} = F^{(1)}(\boldsymbol{\Omega},t)$$

➡ It is not closed!

requires $p_t(\boldsymbol{\sigma})$

• How to close it:

- **Equipartition assumption**

$$p_t(\boldsymbol{\sigma}) \equiv \Phi[\boldsymbol{\Omega}(\boldsymbol{\sigma}); t]$$

→ *approximation* allows us to **close the dynamics**

The averages simplify:

$$\langle f(\boldsymbol{\sigma})\rangle_{\boldsymbol{\Omega};t} = \frac{\sum_{\boldsymbol{\sigma}} p_t(\boldsymbol{\sigma})\delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{\sigma})]\, f(\boldsymbol{\sigma})}{\sum_{\hat{\boldsymbol{\sigma}}} p_t(\hat{\boldsymbol{\sigma}})\delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(\hat{\boldsymbol{\sigma}})]} \rightarrow \frac{\sum_{\boldsymbol{\sigma}} f(\boldsymbol{\sigma})\delta(\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{\sigma}))}{\sum_{\boldsymbol{\sigma}} \delta(\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{\sigma}))}$$

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From microcanonical to canonical measure

$$p_\Omega(\sigma) = \frac{\delta\,[\Omega - \Omega(\sigma)]}{\sum_{\hat{\sigma}} \delta\,[\Omega - \Omega(\hat{\sigma})]}. \Rightarrow P_{\hat{\boldsymbol{\Omega}}}(\boldsymbol{\sigma}) = \frac{\mathrm{e}^{\,\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\Omega}(\boldsymbol{\sigma})}}{\sum_{\hat{\boldsymbol{\sigma}}} \mathrm{e}^{\,\hat{\boldsymbol{\Omega}}\cdot\boldsymbol{\Omega}(\hat{\boldsymbol{\sigma}})}} = \frac{\mathrm{e}^{N\hat{m}\cdot m(\boldsymbol{\sigma}) + N\hat{E}\cdot E(\boldsymbol{\sigma})}}{Z_{\hat{m},\hat{E}}}$$

- $$P_{\hat{m},\hat{E}}(\boldsymbol{\sigma}) = \frac{\mathrm{e}^{N\hat{m}\cdot m(\boldsymbol{\sigma}) + N\hat{E}\cdot E(\boldsymbol{\sigma})}}{Z_{\hat{m},\hat{E}}} = \frac{\mathrm{e}^{\,\hat{m}\sum_i \sigma_i + \hat{E}(\sum_i J_{i,i+1}\sigma_i\sigma_{i+1} + \theta\sum_i \sigma_i)}}{Z_{\hat{m},\hat{E}}}$$

Canonical probability distribution

- **with the macroscopic analysis of dynamics:**

$$\frac{d}{dt}\mathbf{\Omega} = F^{(1)}(\mathbf{\Omega}, t) \rightarrow \begin{cases} \frac{dm_t}{dt} = -m_t + \int P(h|m_t, E_t) \tanh(\beta h) dh \\ \frac{dE_t}{dt} = -2E_t - \int P(h|m_t, E_t)\, h \tanh(\beta h) dh \end{cases}$$

Differential equation for the observables

- **with the cavity method (homogeneous case):**

  - Introducing an average **spin-field distribution**

$$\langle \delta_{s,\sigma_0} \delta(h - h_0(\vec{\sigma})) \rangle = \frac{1}{Z} \sum_{\sigma_0, \sigma_1, \sigma_2} e^{[\hat{m}\sigma_0 + \hat{E}\sigma_0 h + \tilde{h}(\sigma_1 + \sigma_2)]} \delta_{s,\sigma_0} \delta(h - J(\sigma_1 + \sigma_2))$$

→ **this average over configurations is performed with the cavity method**

Current project: Glauber dynamics of Ising chain
- Back to the model -

- **with the macroscopic analysis of dynamics:**

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$$P(h|m_t, E_t) = \sum_s \langle \delta_{s,\sigma}\delta(h - h_0(\sigma))\rangle = \frac{\cosh(\hat{m} + \hat{E}h)\left(e^{2\tilde{h}}\delta(h-2J) + e^{-2\tilde{h}}\delta(h+2J) + 2\delta(h)\right)}{\cosh(\hat{m} + 2\hat{E}J)e^{2\tilde{h}} + \cosh(\hat{m} - 2\hat{E}J)e^{-2\tilde{h}} + 2\cosh(\hat{m})}$$

Probability of the real field

$$\begin{cases} m = \sum_s \int dh\, s \cdot \langle \delta_{s,\sigma_0}\delta(h - h_0(\vec{\sigma}))\rangle = \frac{\sinh(\hat{m} + 2\hat{E}J)e^{2\tilde{h}} + \sinh(\hat{m} - 2\hat{E}J)e^{-2\tilde{h}} + 2\sinh(\hat{m})}{\cosh(\hat{m} + 2\hat{E}J)e^{2\tilde{h}} \cosh(\hat{m} - 2\hat{E}J)e^{-2\tilde{h}} + 2\cosh(\hat{m})} \\ E = -\frac{1}{2}\sum_s \int dh \langle \delta_{s,\sigma_0}\delta(h - h_0(\vec{\sigma}))\rangle\, s\, h = \frac{-J\left(\sinh(\hat{m} + 2\hat{E}J)e^{2\tilde{h}} - \sinh(\hat{m} - 2\hat{E}J)e^{-2\tilde{h}}\right)}{\cosh(\hat{m} + 2\hat{E}J)e^{2\tilde{h}} + \cosh(\hat{m} - 2\hat{E}J)e^{-2\tilde{h}} + 2\cosh(\hat{m})} \\ \tilde{h} = \hat{m} + \text{arctanh}(\tanh(\hat{E}J)\tanh(\tilde{h})) \end{cases}$$

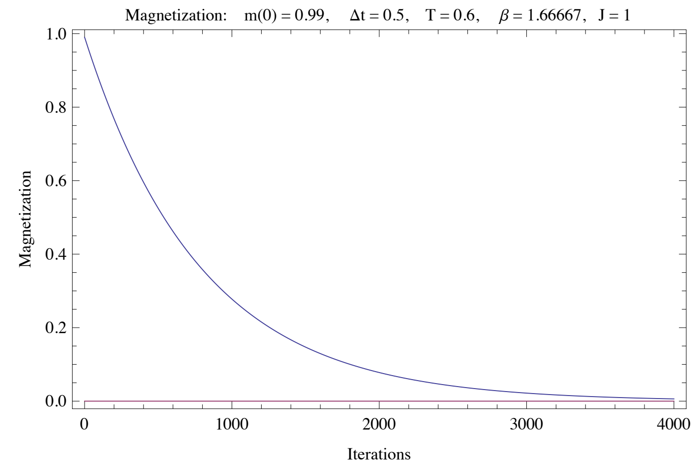
→ **Cavity Field equation**

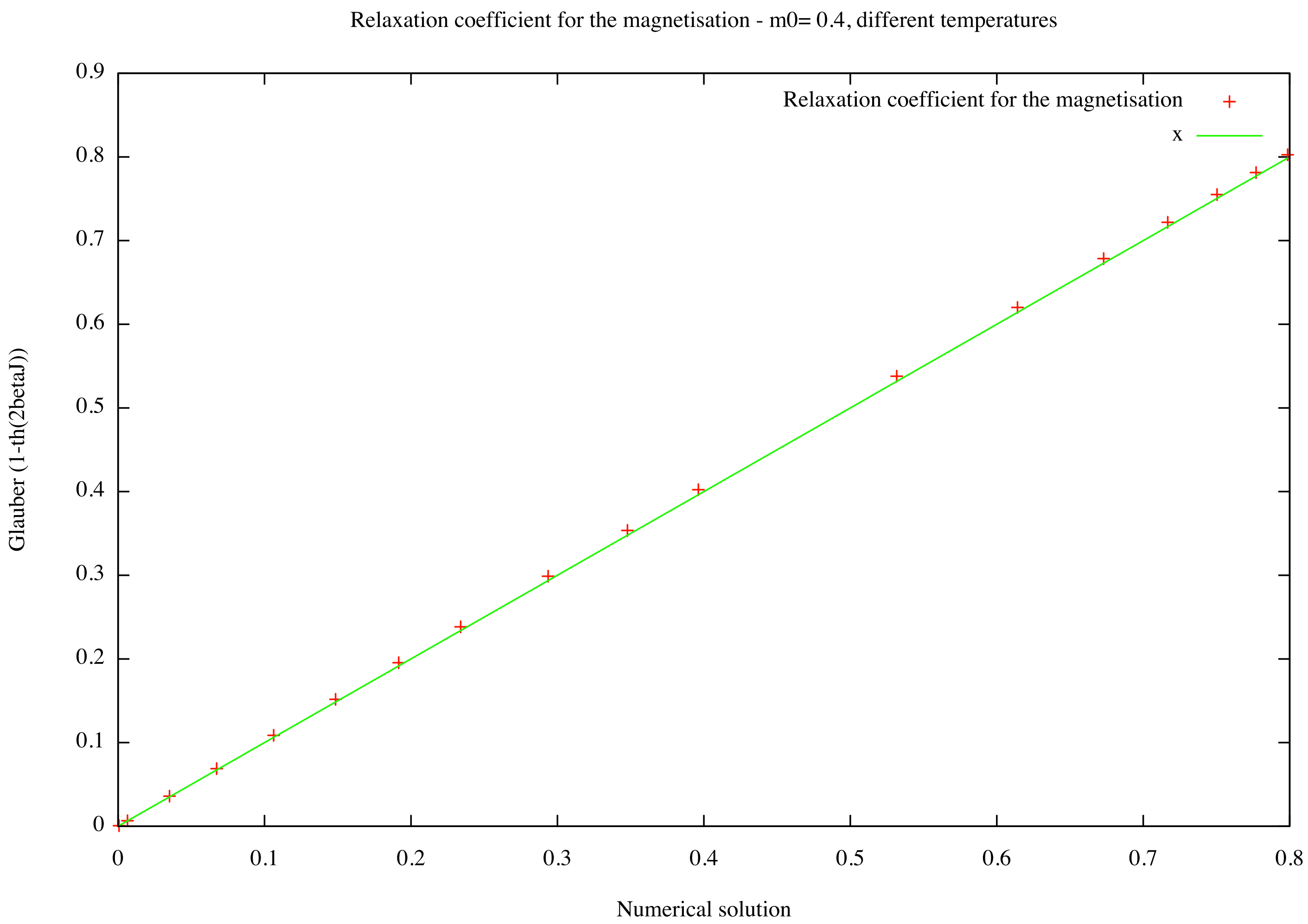
Current project: Glauber dynamics of Ising chain

Roy J. Glauber - "*TimeDependent Statistics of the Ising Model*" (1963)

evolution of the magnetization

$$m(t) = m(0)\mathrm{e}^{-(1-\tanh(2\beta J))t}$$





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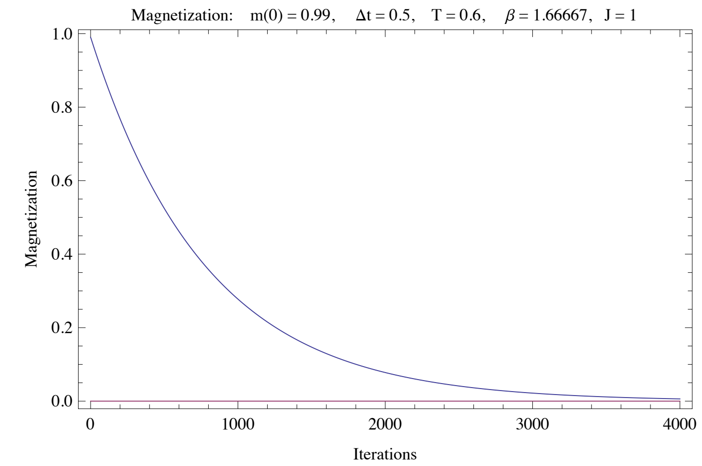

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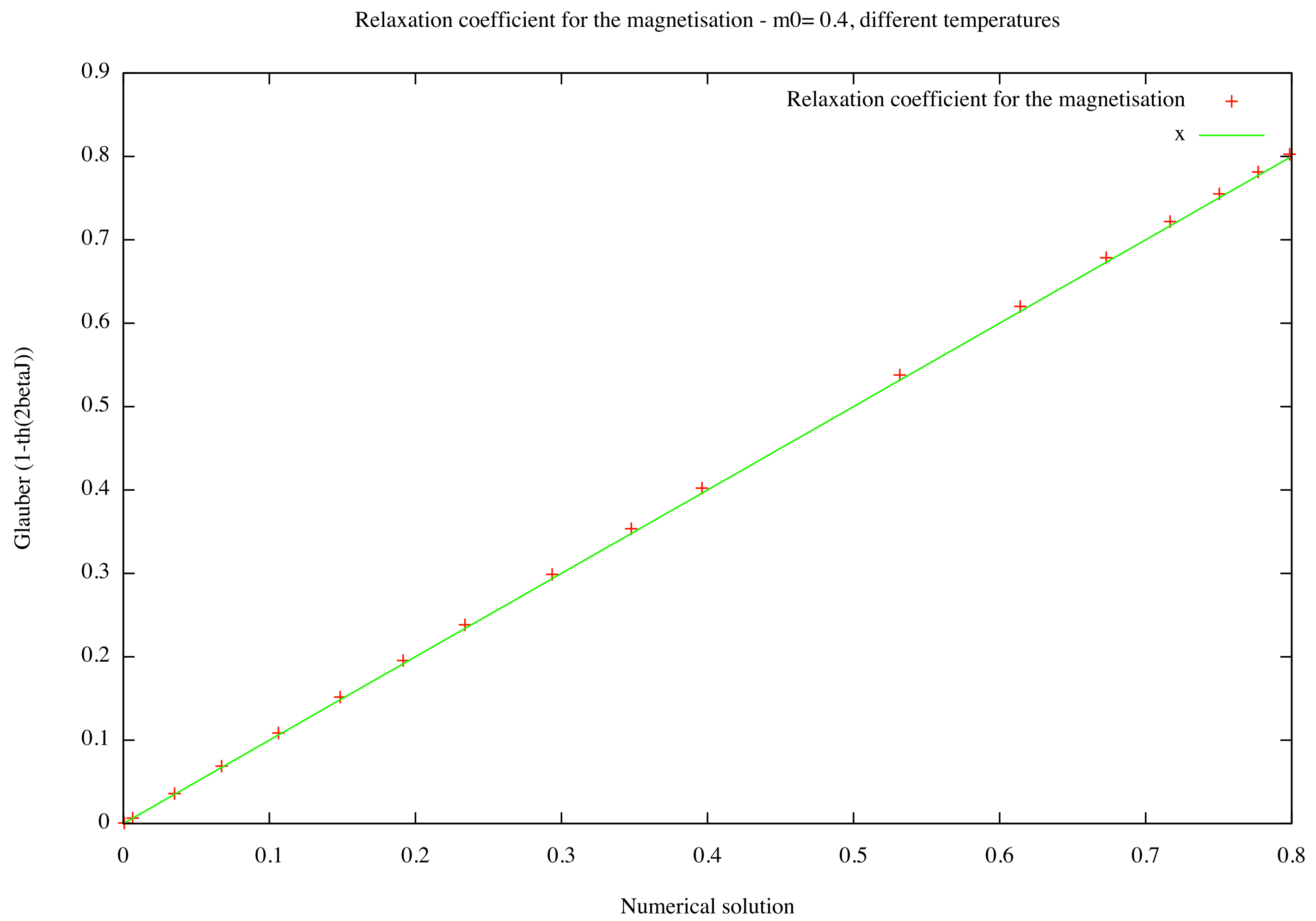
$$m(t) = m(0)\mathrm{e}^{-(1-\tanh(2\beta J))t}$$

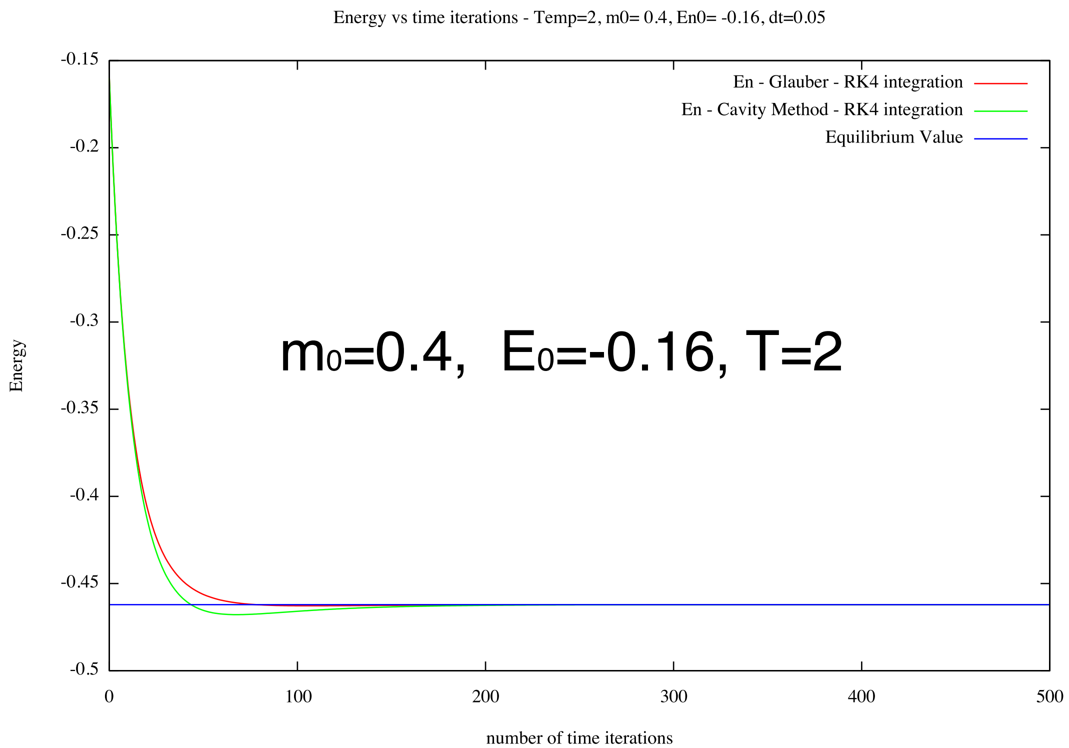
evolution of the correlation between spins in different positions

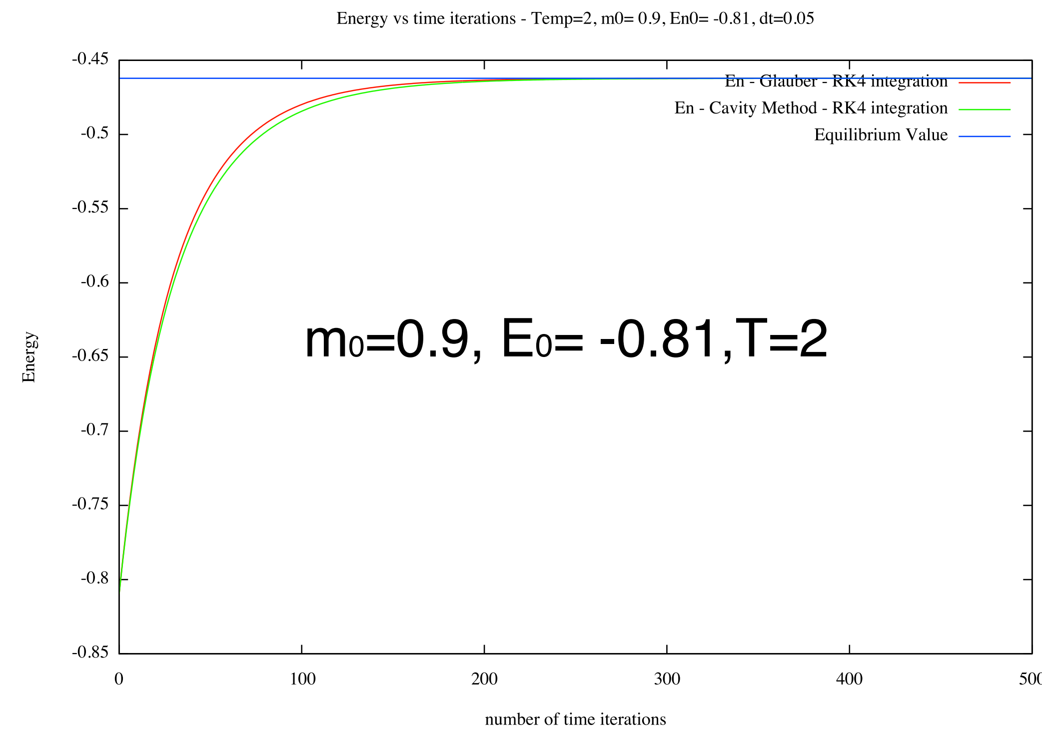
$$\begin{cases} \frac{d}{dt} r_{j,k}(t) = -2r_{j,k}(t) + \frac{1}{2}\tanh(2\beta J)\{r_{j,k-1}(t) + r_{j,k+1}(t) + r_{j-i,k}(t) + r_{j+1,k}(t)\} \\ r_{j,j}(t) = 1 \end{cases}$$

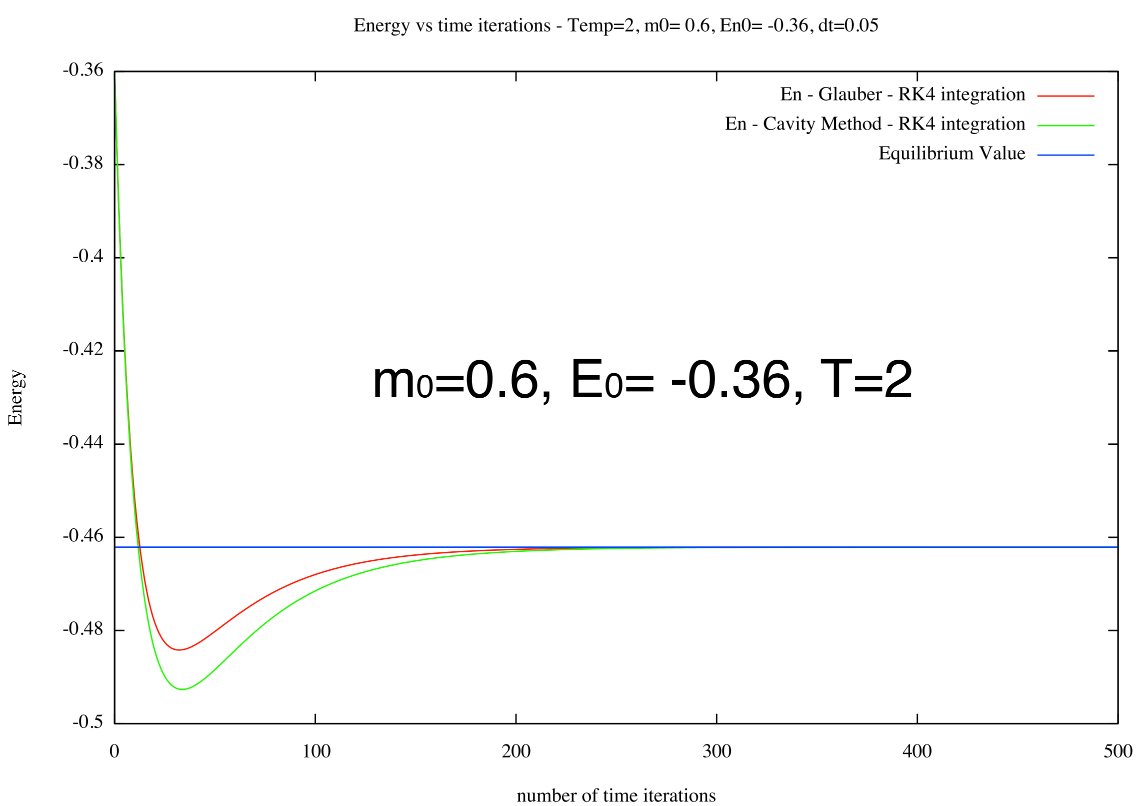
$$E(t) = -\frac{1}{N}\sum_i r_{i,i+1}(t)$$

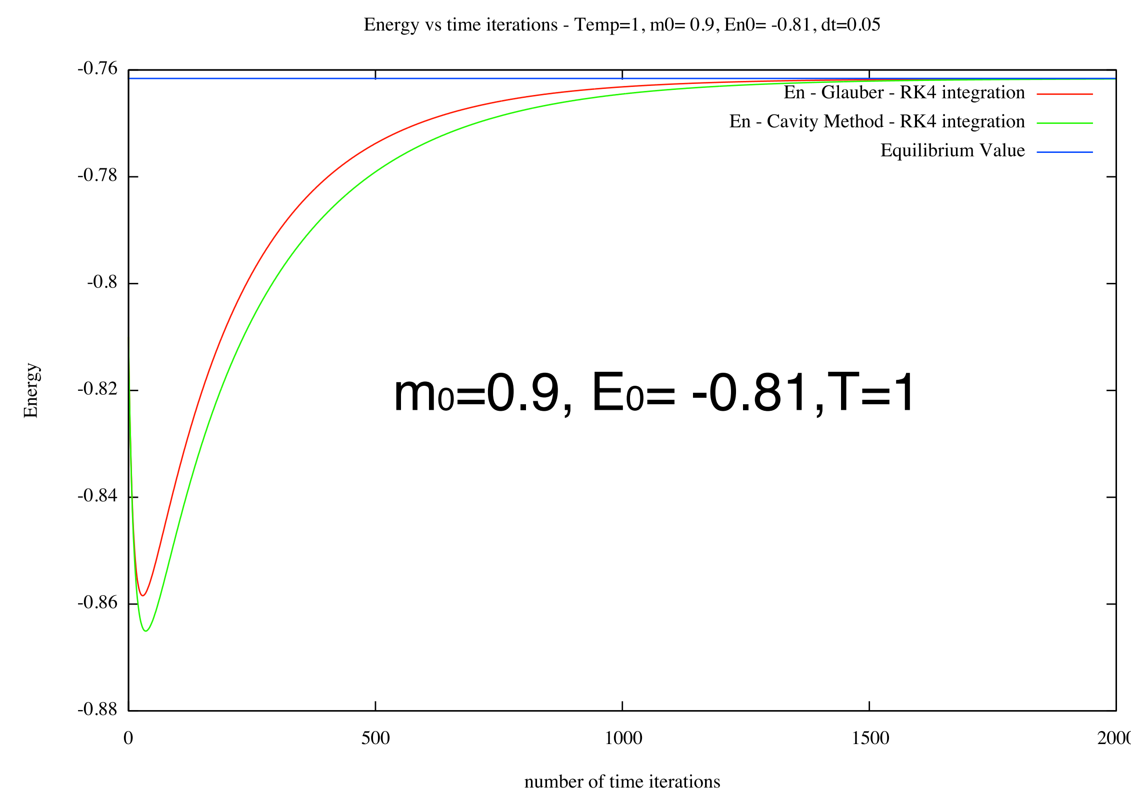


Our theory doesn’t match Glauber’s perfectly









Disordered case:

$$\mathcal{H}(\sigma) = -\sum_i J_{i,i+1}\sigma_i\sigma_{i+1} - \sum_i \theta_i\sigma_i$$

- **We assume that all the observables are self-averaging**

$$\lim_{N\to\infty} \mathbf{\Omega}(J) = \mathbf{\Omega}_\infty$$

Methods to take averages over disorder in this setting:

- Dynamical Replica Analysis *(A.C.C. Coolen and D. Sherrington)*
- Cavity Method *(G. Parisi and M. Mézard)*

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Differential equation for the observables

$$P(h|m_t, E_t) = \lim_{N\to\infty} \frac{1}{N}\sum_i \langle\langle \delta(h - h_i(\boldsymbol{\sigma}))\rangle_{m_t, E_t}\rangle_{J,\tilde{h}}$$

- **with the cavity method:**

$$m = \left\langle \frac{\sum_{\sigma_1,\sigma_2} \sinh[\hat{m} + \hat{E}(J_1\sigma_1 + J_2\sigma_2 + \theta)]\mathrm{e}^{\tilde{h}_1\sigma_1 + \tilde{h}_2\sigma_2}}{\sum_{\sigma_1,\sigma_2} \cosh[\hat{m} + \hat{E}(J_1\sigma_1 + J_2\sigma_2 + \theta)]\mathrm{e}^{\tilde{h}_1\sigma_1 + \tilde{h}_2\sigma_2}} \right\rangle_{J_1, J_2, \tilde{h}_1, \tilde{h}_2}$$

$$E = -\frac{1}{2}\left\langle \frac{\sum_{\sigma_1,\sigma_2} \sinh[\hat{m} + \hat{E}(J_1\sigma_1 + J_2\sigma_2 + \theta)]\mathrm{e}^{\tilde{h}_1\sigma_1 + \tilde{h}_2\sigma_2}(J_1\sigma_1 + J_2\sigma_2 + \theta))}{\sum_{\sigma_1,\sigma_2} \cosh[\hat{m} + \hat{E}(J_1\sigma_1 + J_2\sigma_2 + \theta)]\mathrm{e}^{\tilde{h}_1\sigma_1 + \tilde{h}_2\sigma_2}} \right\rangle_{J_1, J_2, \tilde{h}_1, \tilde{h}_2} - \frac{1}{2} m\,\theta$$

$$P_C(\tilde{h}) = \int d\tilde{h} P_C(\tilde{h}) \int d\, J P(J)\delta[\tilde{h} - (\hat{m} + \hat{E}\theta + \tanh^{-1}[\tanh(\hat{E}J)\tanh(\tilde{h})])]$$

Conclusions:

Next step on this project:

- Finish the derivations for the disordered case
- Simulation for this disordered Ising model
- Case with non-homogeneous external field
- Perhaps join Erik and Alexander in other applications of this methodology

Further work in NETADIS

- Dynamic cavity method
- Marsili (to apply this and other complex systems tools on finance)
- Go to Paris to work with S. Franz for second secondment