# Spin-fermion hamiltonian

(a preliminary for a an auxiliary field QMC)

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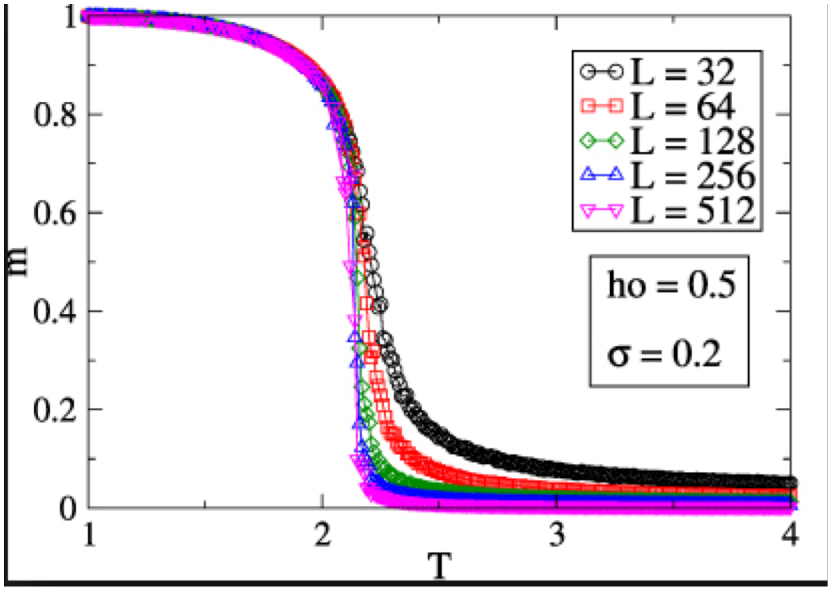
# •Brief review - Classical Monte Carlo for the Ising Model

The model: **Ising model** (classical model to describe **magnetism**/**paramagnetism** in a lattice)

$$\mathcal{H} \equiv -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z \;\; ; \;\; \sigma_i^z = \pm 1$$




$J > 0$ : **Ferromagnetic** interactions (lower energies for aligned moments)

$J < 0$ : **Anti-Ferromagnetic** interactions (lower energies for anti-aligned moments)

•Critical temperatures separating both regimes:

$$\begin{cases} T_c = 0(1d) \\ T_c = \dfrac{2}{\ln(1+\sqrt{2})}(2d\ square\ lattice) \\ T_c = 3.6410(triangular\ lattice) \end{cases}$$

## •Comparison of single flip update and cluster updates in Classical Monte Carlo

The model: **Ising model** (classical model to describe magnetism/paramagnetism in a lattice)

$$\mathcal{H} \equiv -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z \quad ; \quad \sigma_i^z = \pm 1 \quad \Rightarrow \quad \mathcal{Z} = \sum_{\{\alpha\}} e^{-E_{\{\alpha\}}/k_b T}$$

Sum with $2^{N_s}$ terms!

•***Motto*** of statistical physics: not all of those configurations are actually relevant

•Configuration $\alpha$ : Occurrence probability→

$$p(\alpha) = \underbrace{e^{-E(\alpha)/k_b T}}_{\text{Can be } \ll 1}$$

: Boltzmann factor

•No need to generate all the configurations… ***Importance sampling*** ?

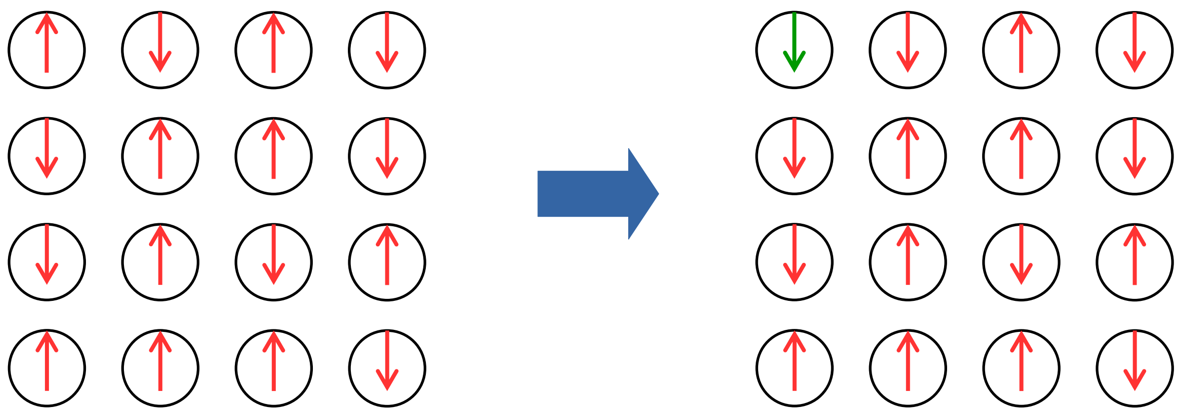
•Start from a random spin configuration $\alpha = |\sigma_1^z \sigma_2^z \ldots \sigma_{N_s}^z\rangle$

•Generate a chain of the most likely configurations (plus fluctuations) by visiting each site of the lattice and attempting a flip

## •Comparison of single flip update and cluster updates in Classical Monte Carlo

•Attempting local spin flips

$\alpha$ : $\alpha'$ :



Energy difference between configurations:

$$\Delta E = E(\alpha') - E(\alpha)$$
$$= 2J\sigma_i \sum_{j \in \text{NN of } i} \sigma_j$$

•Ratio between the correspondent Boltzmann factors: $r \equiv \dfrac{p(\alpha')}{p(\alpha)} = e^{-\Delta E/k_b T}$

- Metropolis algorithm:

  •If $\Delta E < 0$ accept the move

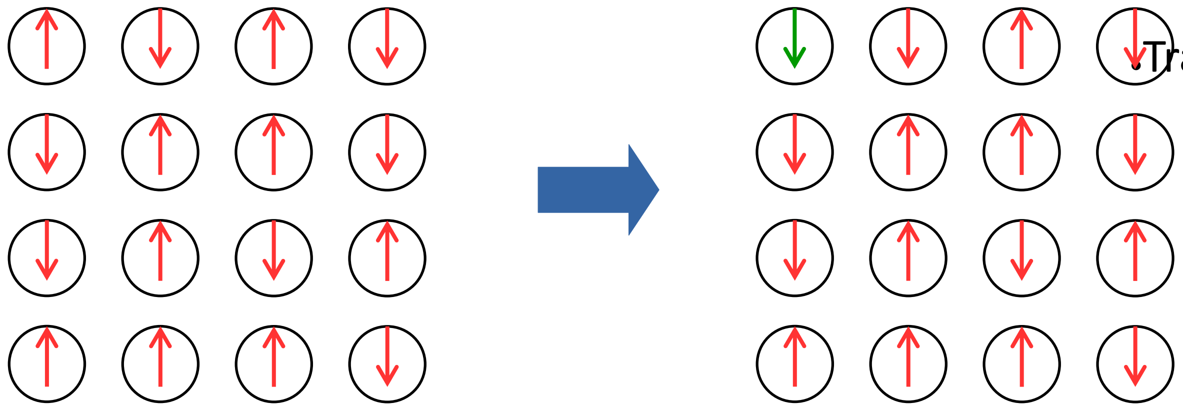
  •If $\Delta E > 0$ accept it with probability $r = e^{-\Delta E/k_b T}$

  →generate a uniform deviate and $\eta$ If $r < e^{-\Delta E/k_b T}$ $\uparrow$ Accept the flip

## •Comparison of single flip update and cluster updates in Classical Monte Carlo

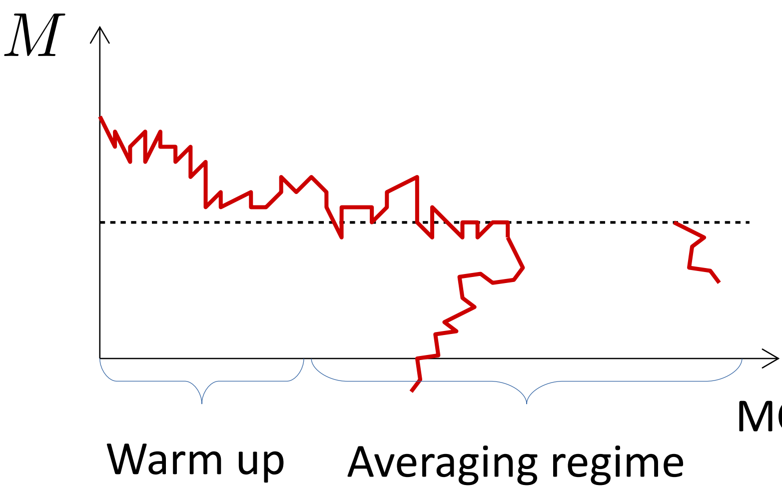
•Attempting local spin flips

$\alpha$ : $\alpha'$ :



•Traversing the whole lattice constitutes a

•or one MC step




Observables:

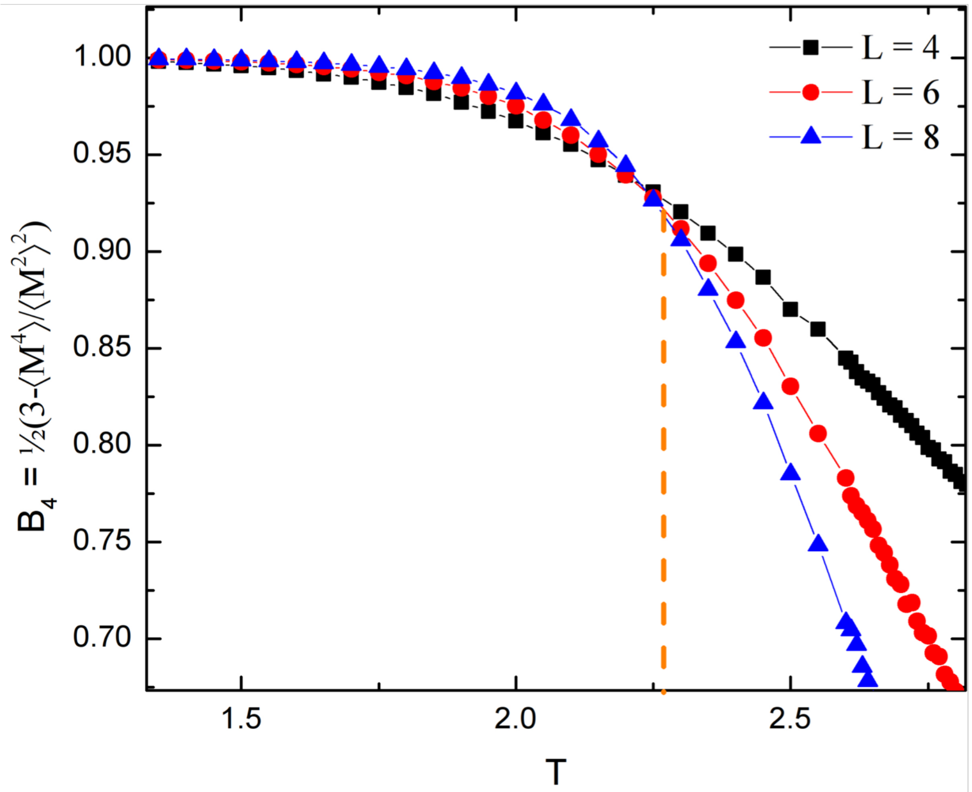
$$M = \frac{1}{N_s} \sum_i \sigma_i^z$$ : Magnetization

$$\langle M \rangle = \frac{1}{N_{\text{meas.}}} \sum_{\alpha=1}^{N_{\text{meas.}}} M_\alpha$$

$$\delta M = \sqrt{\frac{\frac{1}{N_{\text{meas.}}} \sum_\alpha^{N_{\text{meas.}}} M_\alpha^2 - \langle M \rangle^2}{N_{\text{meas.}} - 1}}$$

## •Comparison of single flip update and cluster updates in Classical Monte Carlo

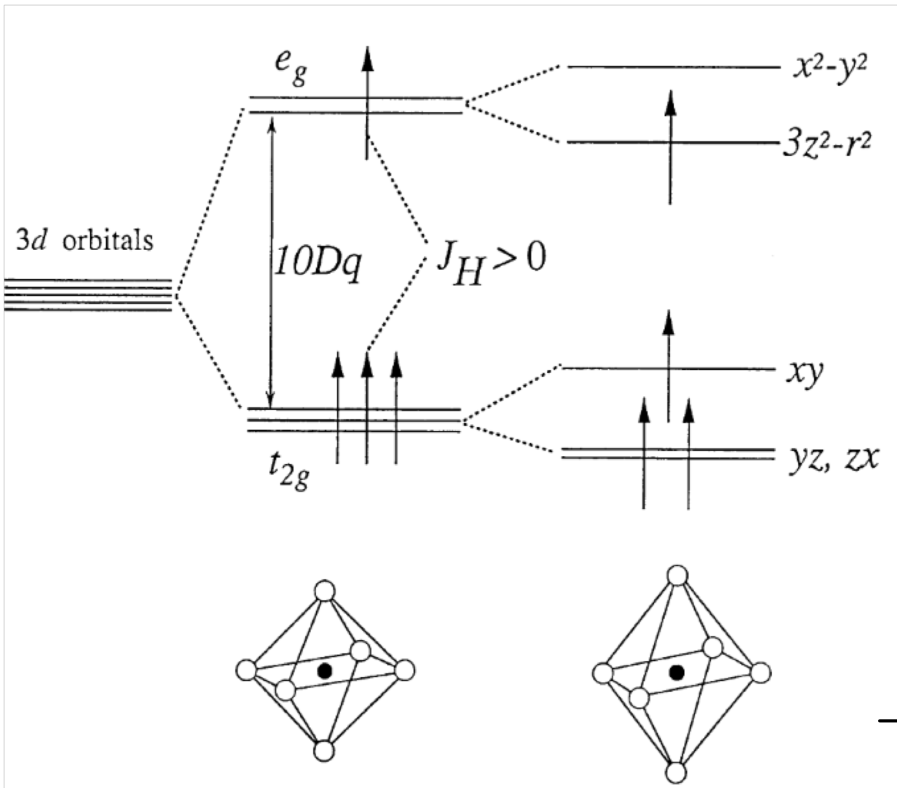
**Binder cumulant:** very precise in obtaining the critical temperature (it is a crossing of the different system sizes results)




[K. Binder, Z. Physik B **43**, 119 (1981); Phys. Rev. Lett. **47**, 693 (1981)]

# •Giant magnetoresistance – why spin-fermion?

•Typical orbital arrangement in Mn atoms:




Itinerant electrons are affected by a polarized background (spin!)

Itinerant

Localized

•Typical interaction – Hund's coupling:

$$-J_{\mathrm{H}} \sum_i \vec{\hat{c}}_i^{\dagger} \vec{\sigma} \vec{\hat{c}}_i \cdot \vec{\mathbf{S}}_i \quad \text{with} \quad \vec{\hat{c}}_i = \begin{pmatrix} \hat{c}_{i\uparrow} \\ \hat{c}_{i\downarrow} \end{pmatrix}$$

Simplification: What if the spin S is classical?

## •Realizing GMR with models of classical spins + free fermions

**Summary**:

- Itinerant fermions interacting with classical spins are thought to be sufficient
- for a minimal explanation of magnetoresistance phenomena

- One has a a slightly more complicated Monte Carlo. It is still classical Monte Carlo
- (Metropolis) but with a quantum flavor in it...

- The bottleneck is that one requires to diagonalize the fermionic matrix for every
- single configuration along the MC phase space evolution → very expensive!
- (There are simpler and more involved numerical methods, e.g. KPM,
- but this already gives you an intuition of how quantum particles interact with a
- a classical field )

- Now, let's head towards a full quantum problem again!