

A Quantum Cavity Method

and some applications to Monte-Carlo simulations

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Collaborators:

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G. Semerjian, ENS Paris

*Phys. Rev. B 78,
134428 (2008)*

See also: (Cavity)

C. Laumann, A. Scardicchio, S.L. Sondhi

Phys.Rev.B 78, 134424 (2008)

S. Knysh, V.N. Smelyanskiy

arXiv:0803.0149

See also (Monte-Carlo):

Beard-Wiese 96,

Prokof'ev et al. 98,

Rieger-Kawashima 99

Generalize the cavity method to quantum systems

Why?

- A consistent mean field theory for finite-connectivity quantum models:
 - ▶ distance between variables (correlation length)
 - ▶ fluctuations of the local environment (disorder)
 - ▶ localization phenomena (e.g. Anderson localization)
- Exact solution of quantum models on random graphs
 - ▶ phase diagram of random K-sat, q-col, ...
- Studies of quantum annealing or quantum information
- Monte-Carlo methods for disordered systems

Quantum Spins Model in Transverse Field

Hilbert space: $(|+\rangle, |-\rangle)^{\otimes N}$


$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$


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$$\mathcal{H} = E(\{\sigma^z\}) - \Gamma \sum_i \sigma_i^x$$

Classical part *Original interaction* 

Transverse field *New quantum interaction* 


Partition Function: $Z = \text{Tr } e^{-\beta \mathcal{H}}$


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Example: The Ising Ferromagnet

$$E = -J \sum_{\langle i,j \rangle} S_i S_j \quad \Rightarrow \quad \mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$

Two technically related questions:

- 1) How to simulate such models using the Heat Bath Monte Carlo Simulation ?
- 2) How to apply the Bethe-Peierls (Cavity/Message Passing/TAP...) approach to such models ?

Overview

- Heat bath for classical and quantum spins
- Cavity Method for classical and quantum spins
- Conclusions and perspectives

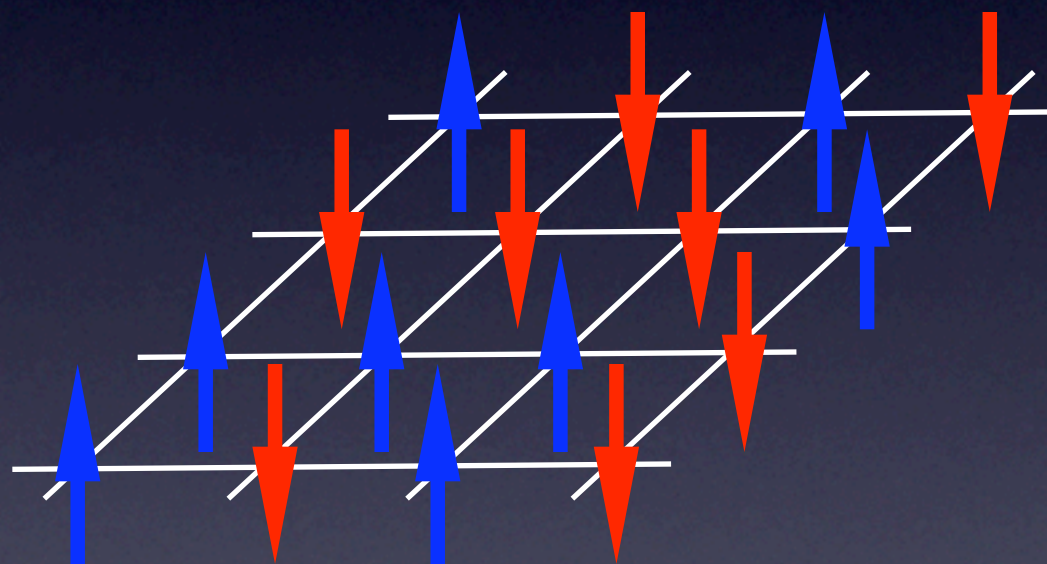
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How to perform classical Monte-Carlo Simulations ?

The Heat-Bath Monte-Carlo algorithm

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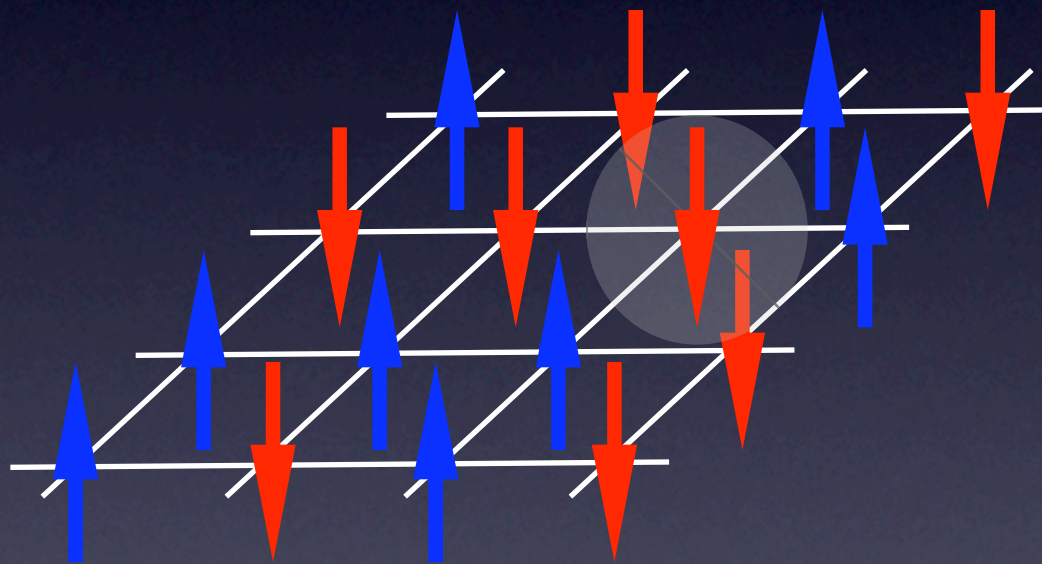


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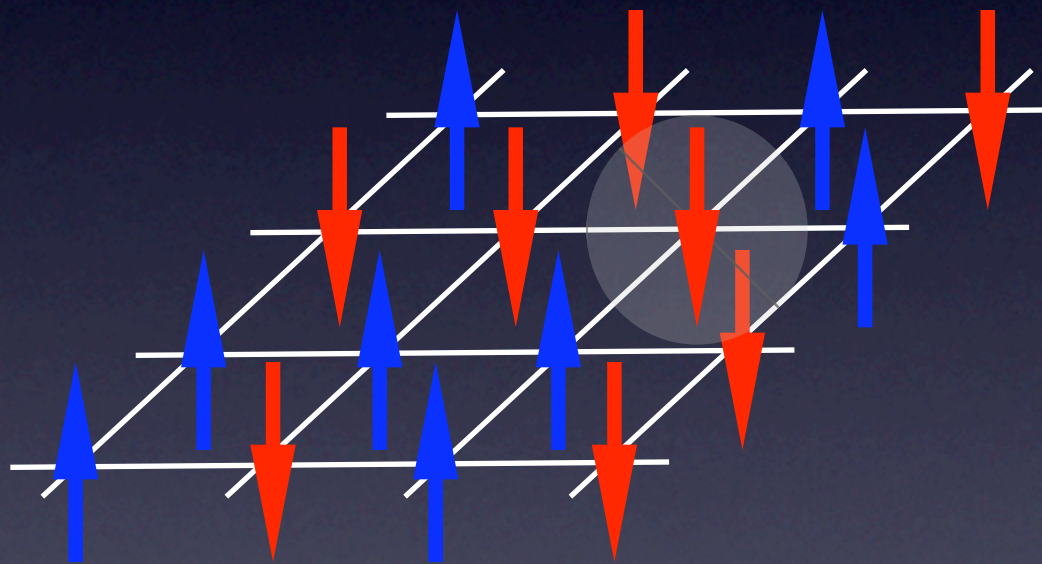
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- 2) Compute its “local field”

$$\uparrow + \uparrow + \uparrow + \downarrow = 2$$



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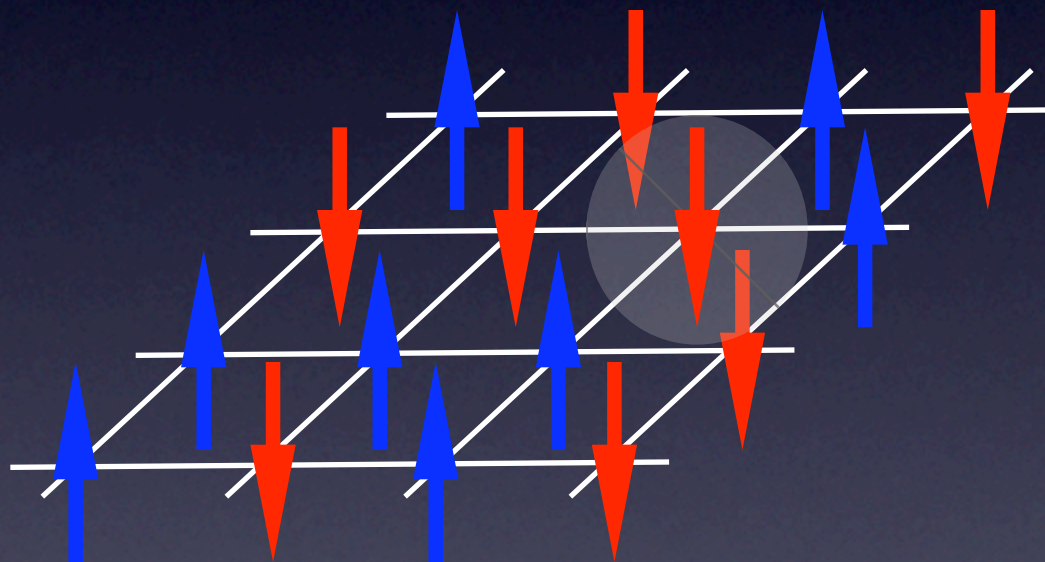
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3) Choose the new value of the spin with Boltzman probability

$$p_{up} = \frac{e^{2\beta}}{Z}$$

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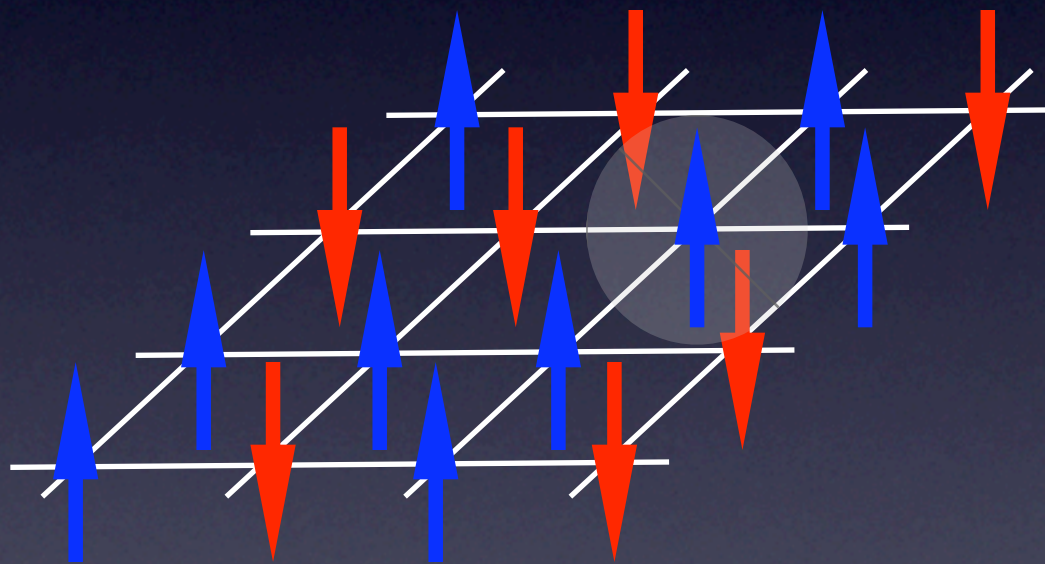
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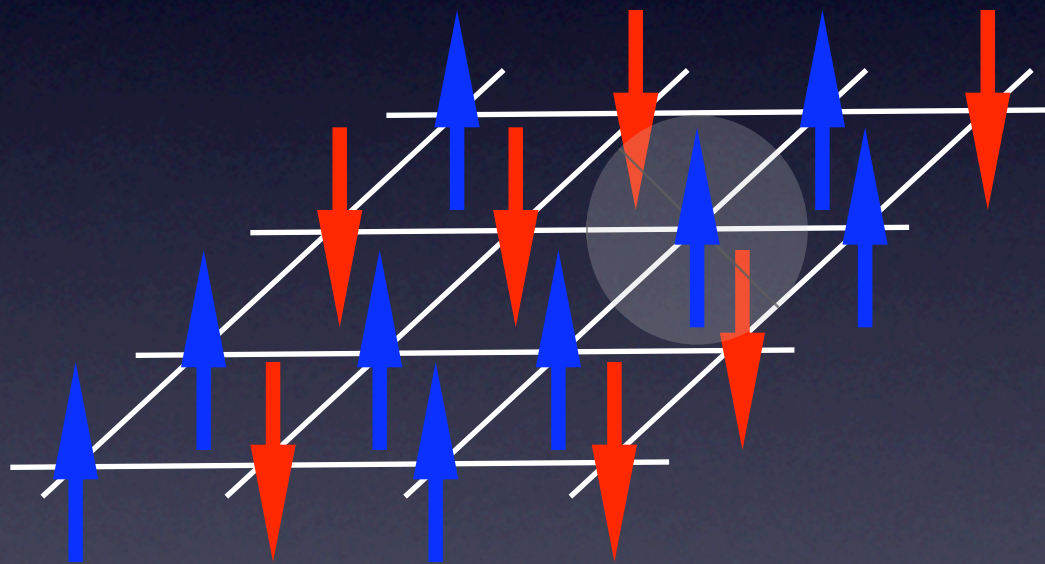
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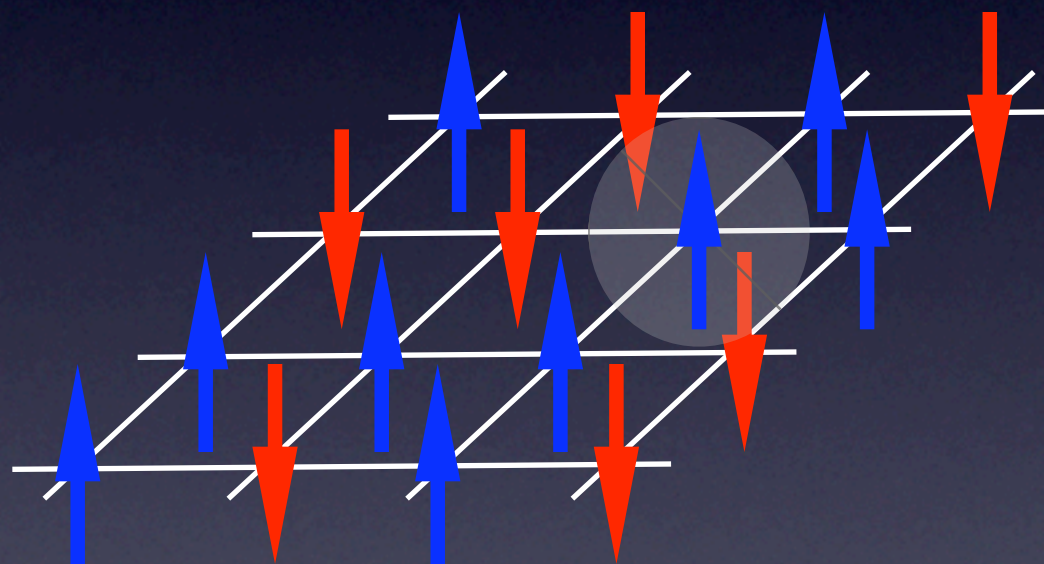
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How to generalize this procedure to the quantum case?

Suzuki-Trotter

$$Z = \text{Tr} \left(e^{-\beta \hat{E} + \beta \Gamma \sum_{i=1}^N \sigma_i^x} \right)$$

Suzuki-Trotter

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Use N_s relation
(in the “z-base”)

$$\sum_{\underline{\sigma}^\alpha} |\underline{\sigma}^\alpha\rangle \langle \underline{\sigma}^\alpha| = 1$$

where the vector are the
set of 2^N “classical”
configurations in the z-direction

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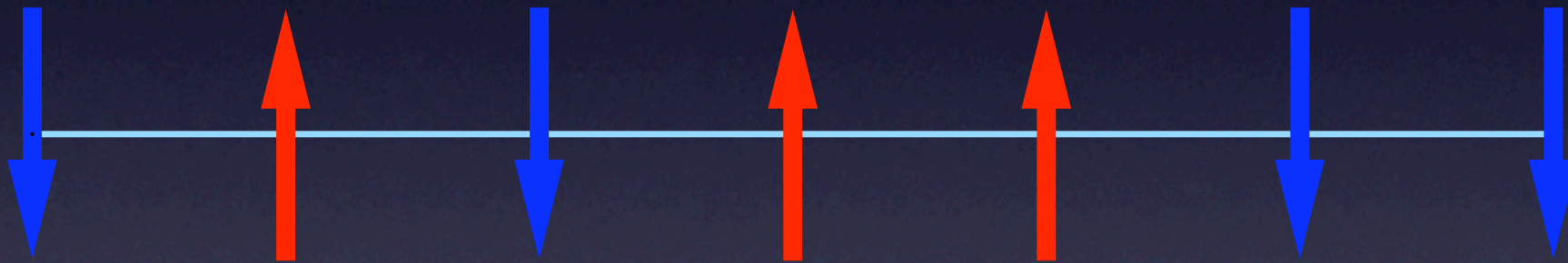
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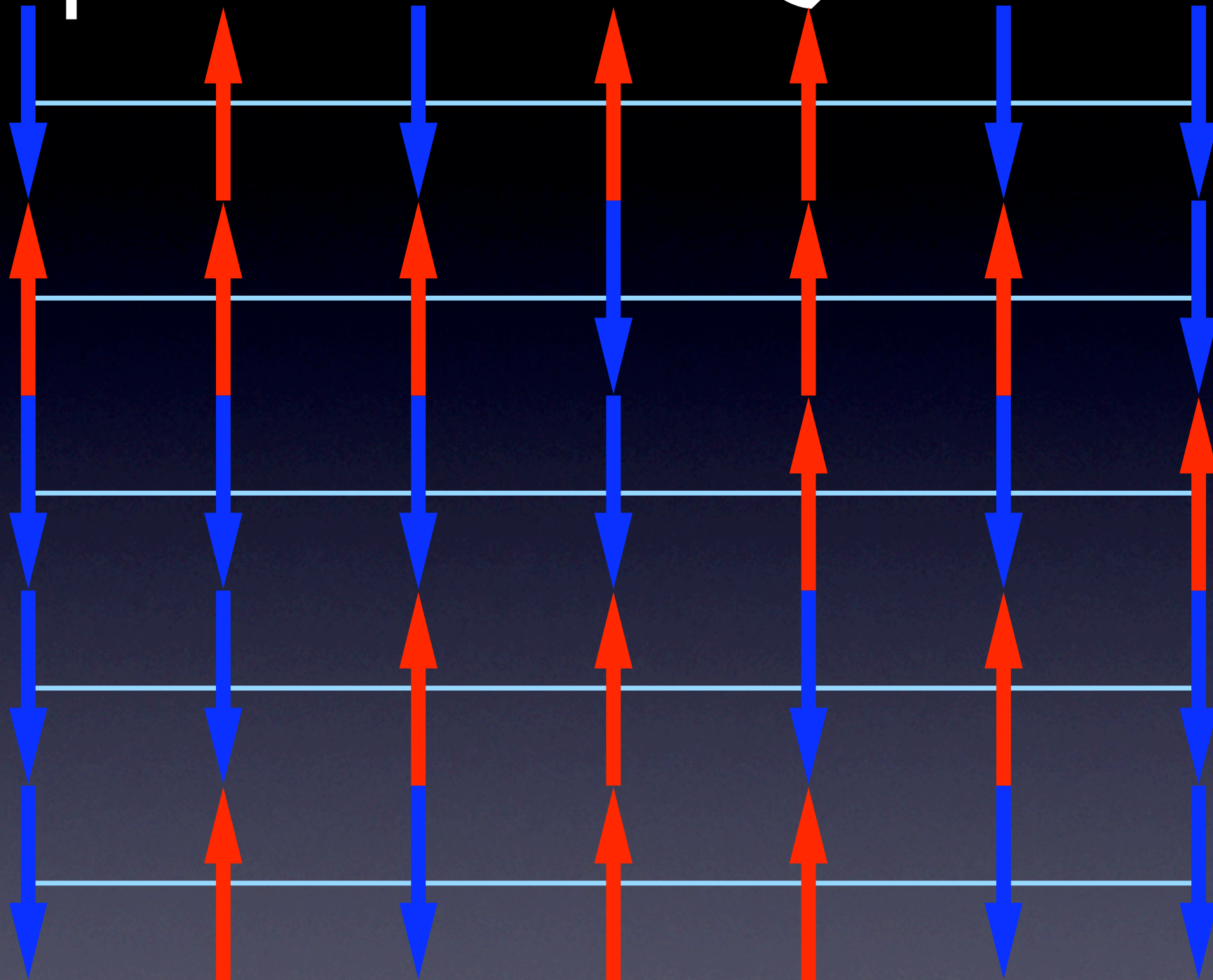
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Example for the 1d Quantum Chain



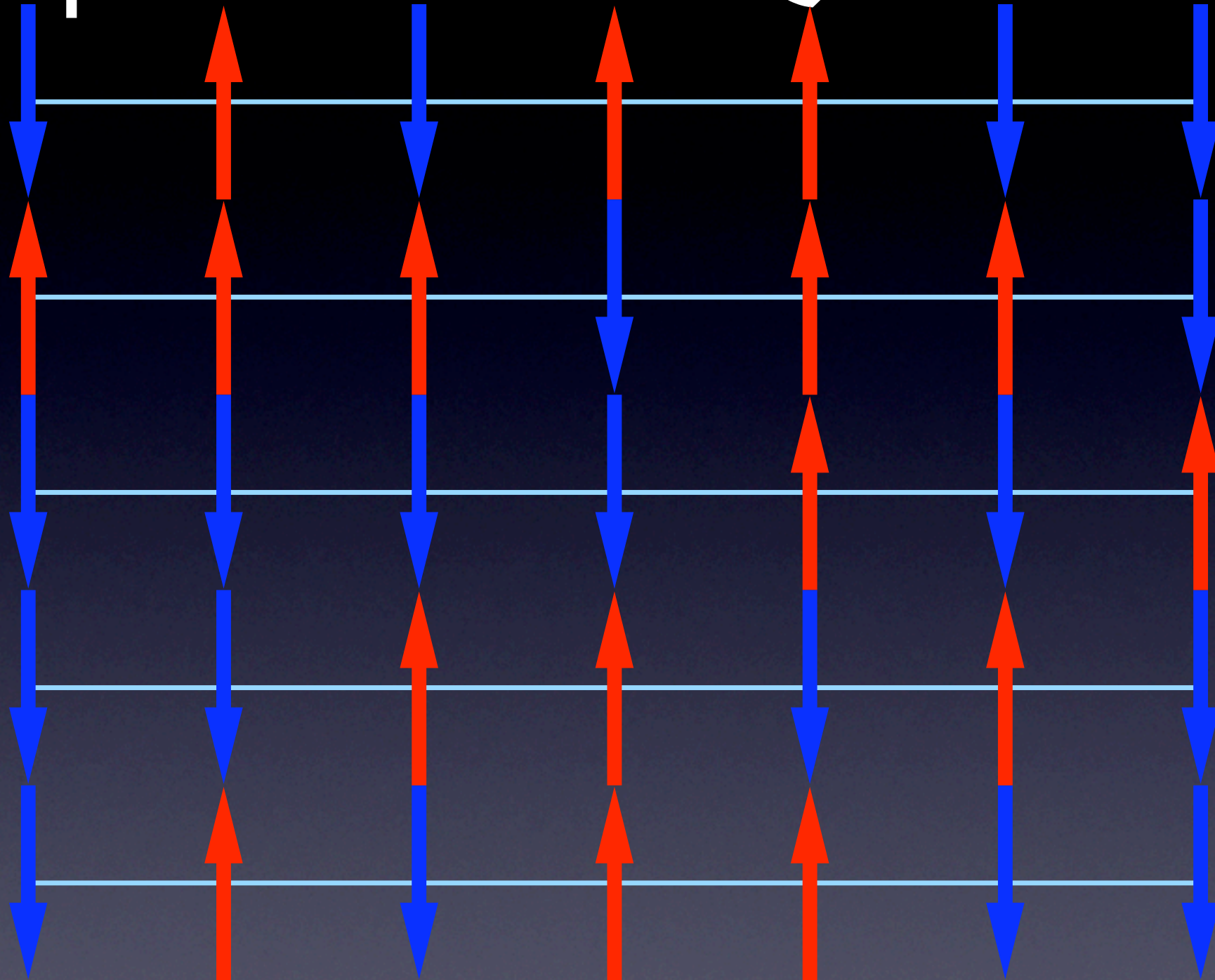
Consider the Original “classical” system

Example for the Id Quantum Chain



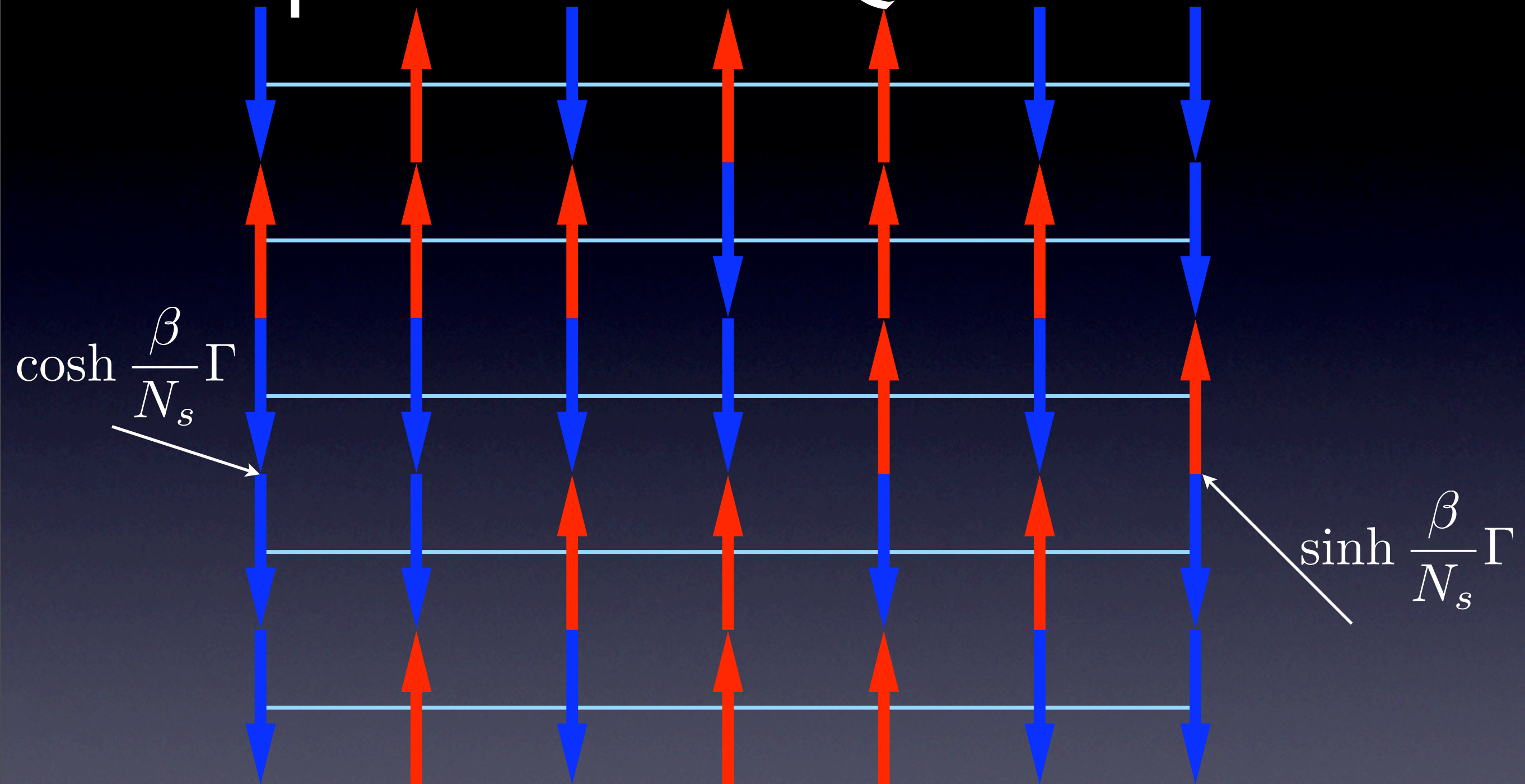
Duplicate the system N_s times

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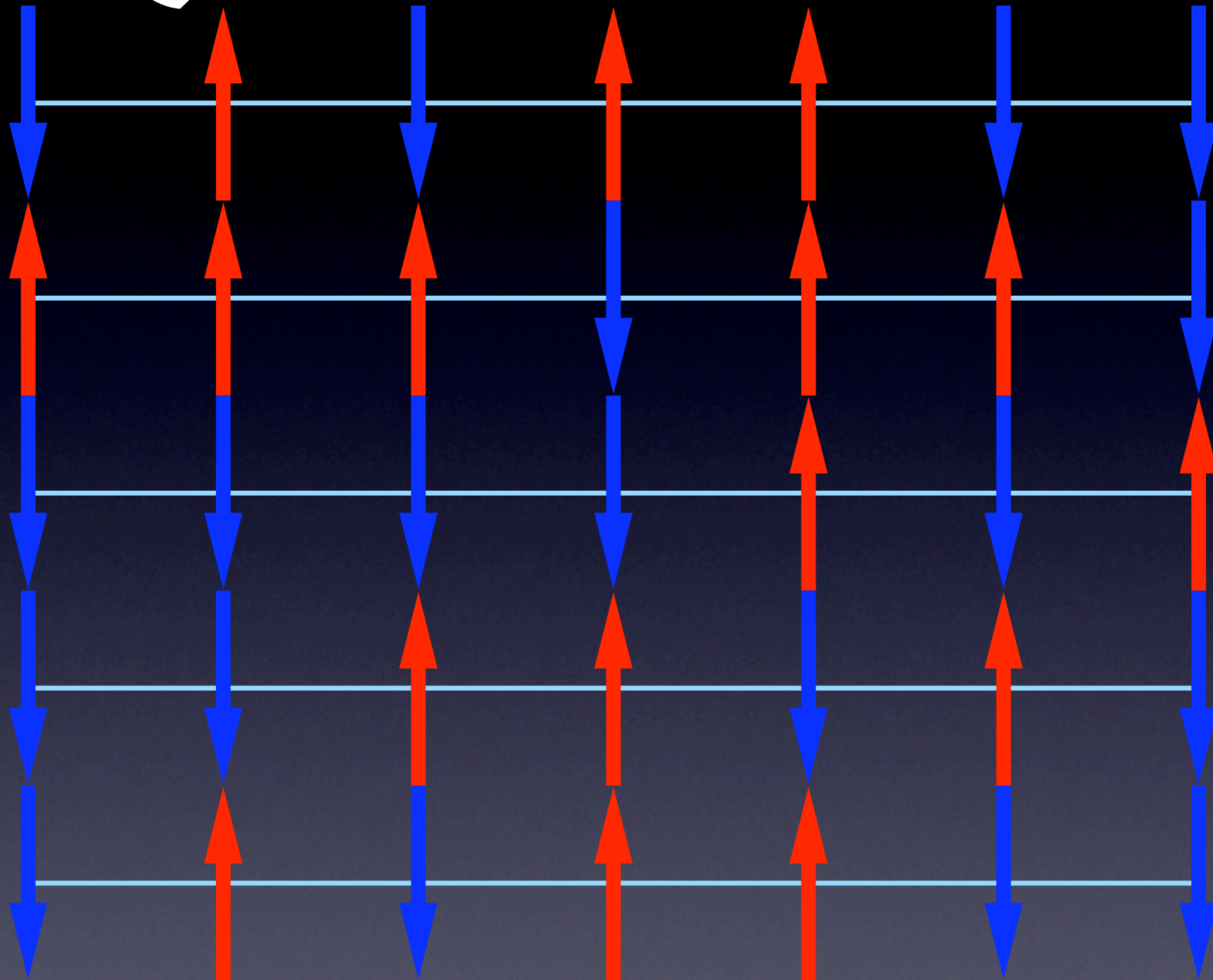
And obtain a system with $d+1$ dimension

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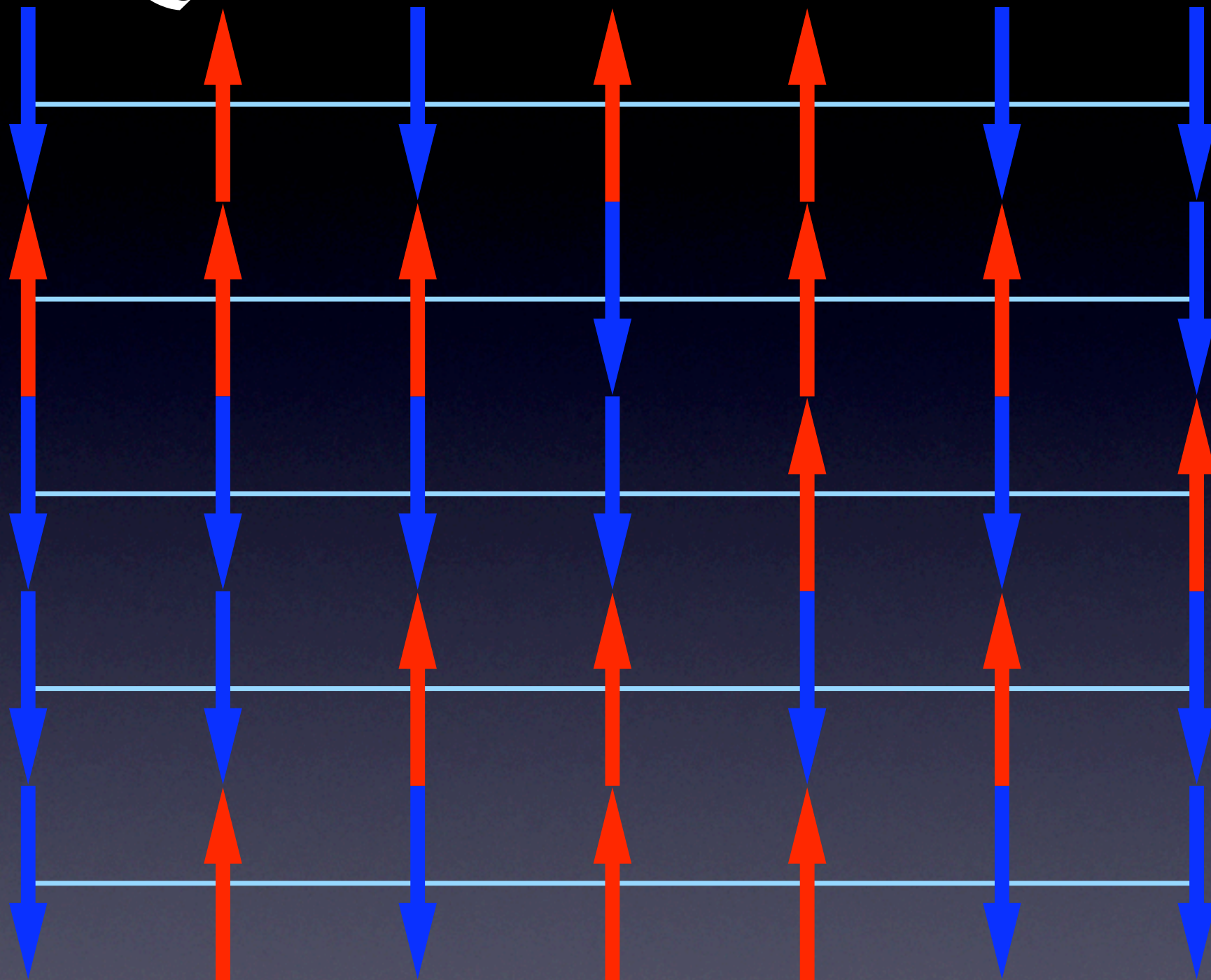
And obtain a system with $d+1$ dimension
With additional couplings

Quantum Monte Carlo

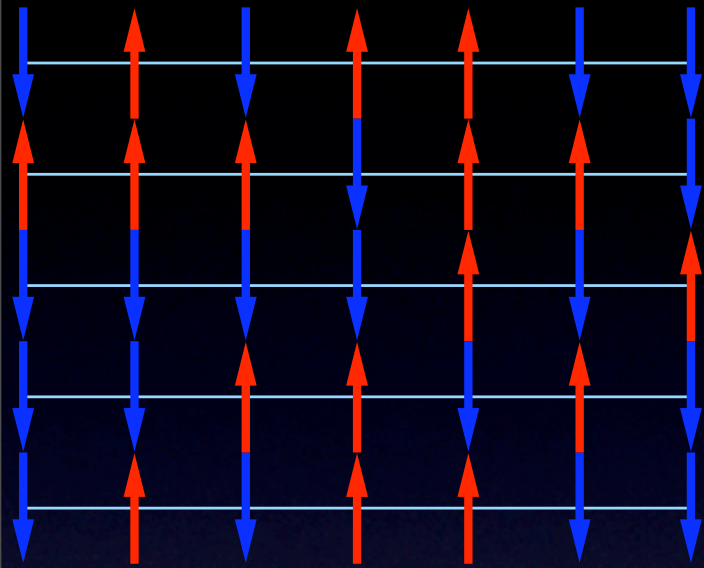


Perform a Classical Monte Carlo on the $d+1$ Lattice

Quantum Monte Carlo



Quantum Monte Carlo



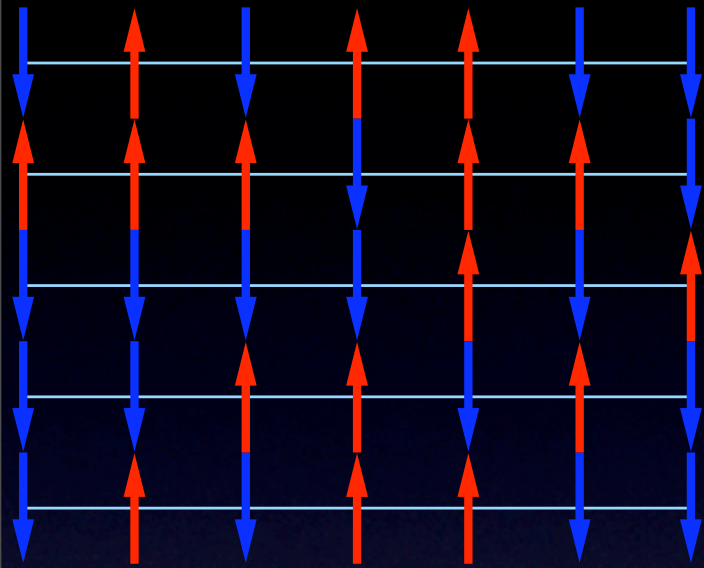
GOOD NEWS:

Very easy implementation
Just add one dimension and use your usual code

BAD NEWS:

New source of finite size effects
(finite-size in the “Trotter” Dimension)
Slow evolution, metastable states

Quantum Monte Carlo



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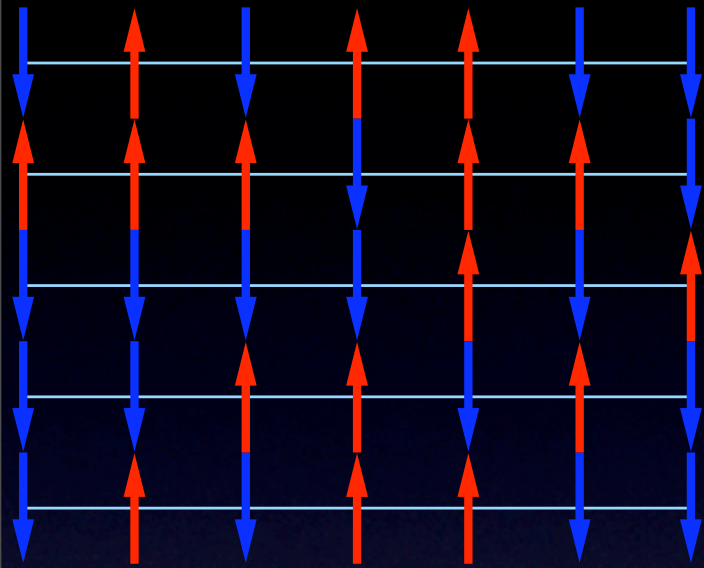
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Quantum Monte Carlo



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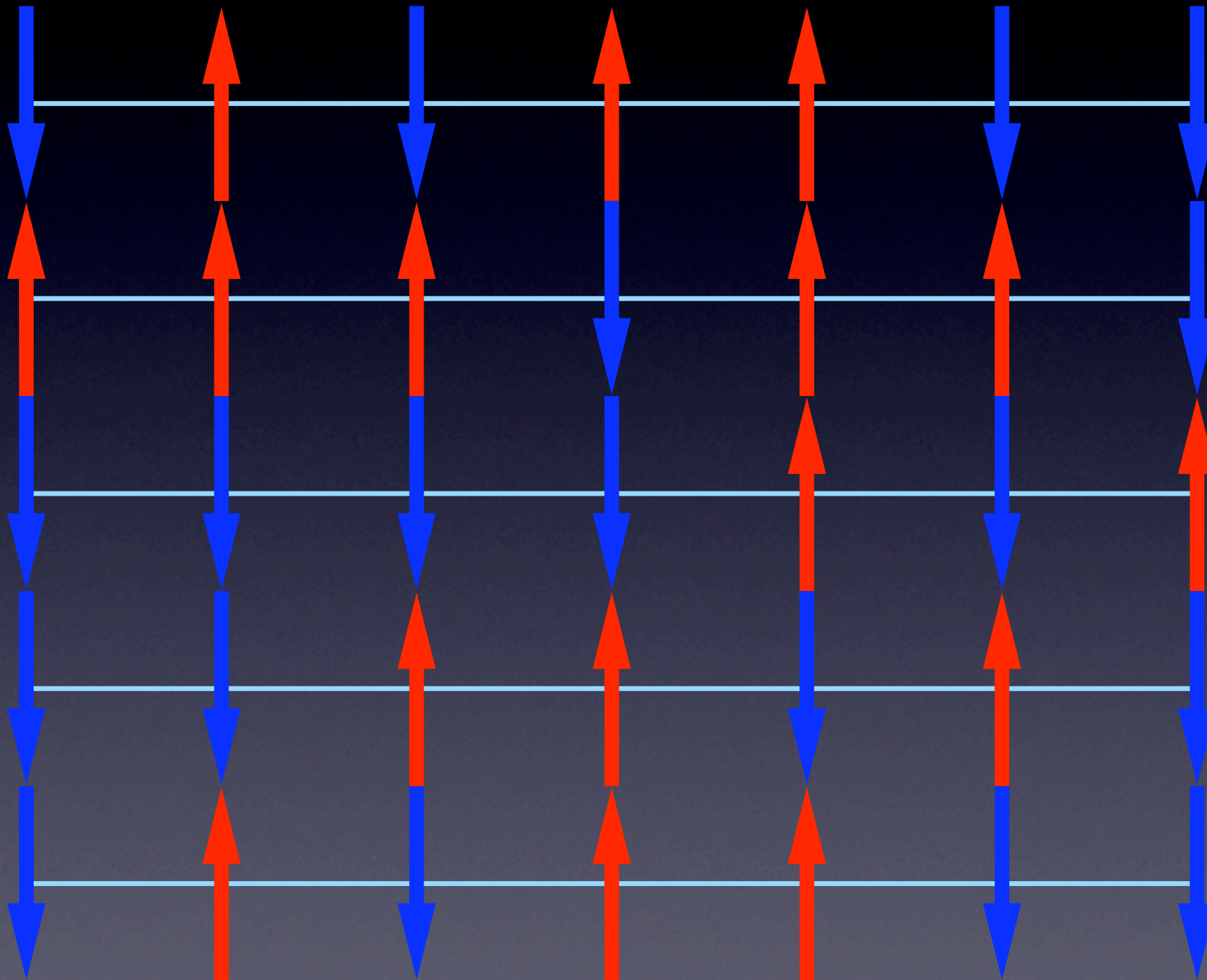
Can we work directly in the infinite N_s limit?

Work directly in the continuous limit :

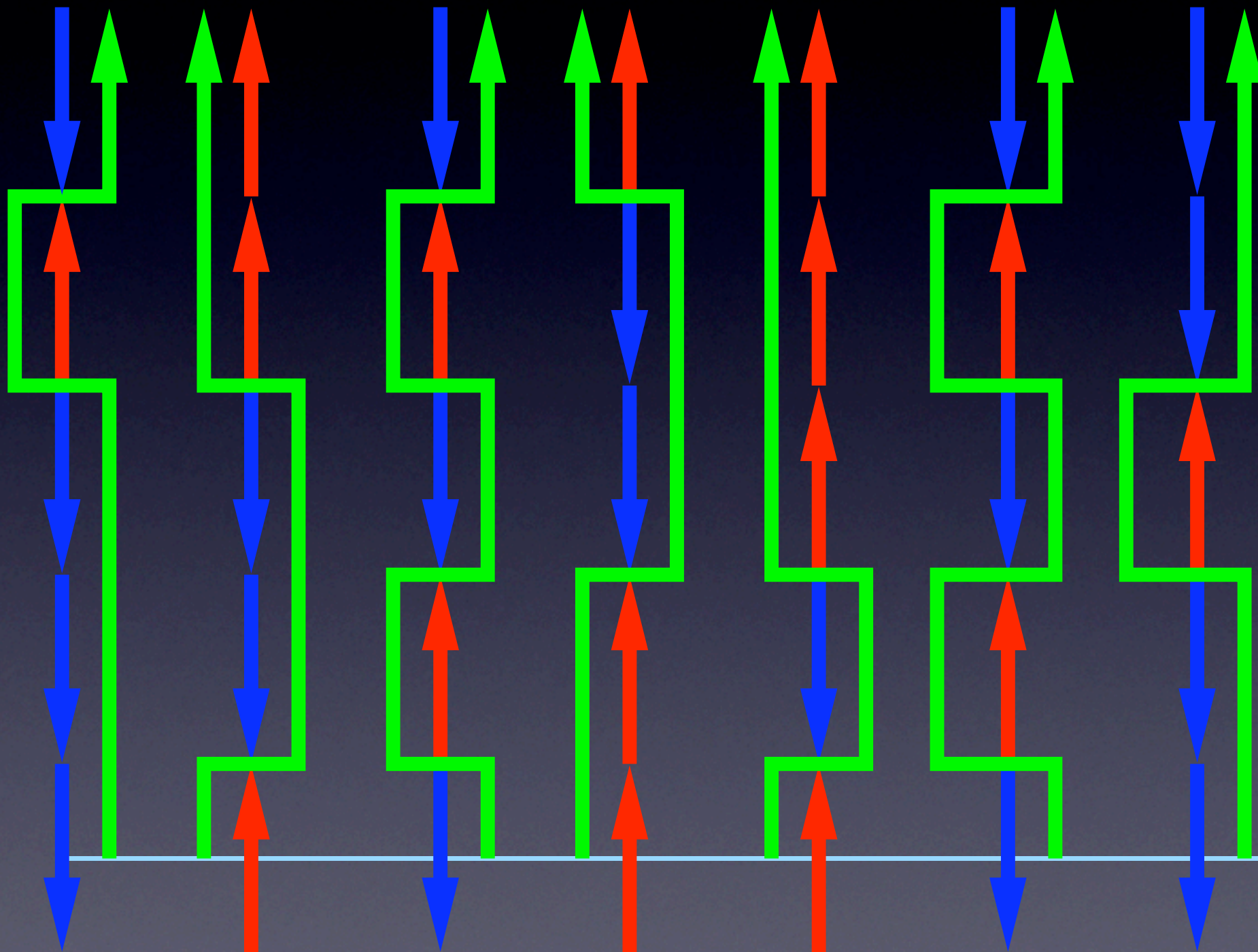
(Loop algorithm: *Beard-Wiese 96, Prokof'ev et al. 98, Rieger-Kawashima 1999*)

Up to now limited to non-disordered systems

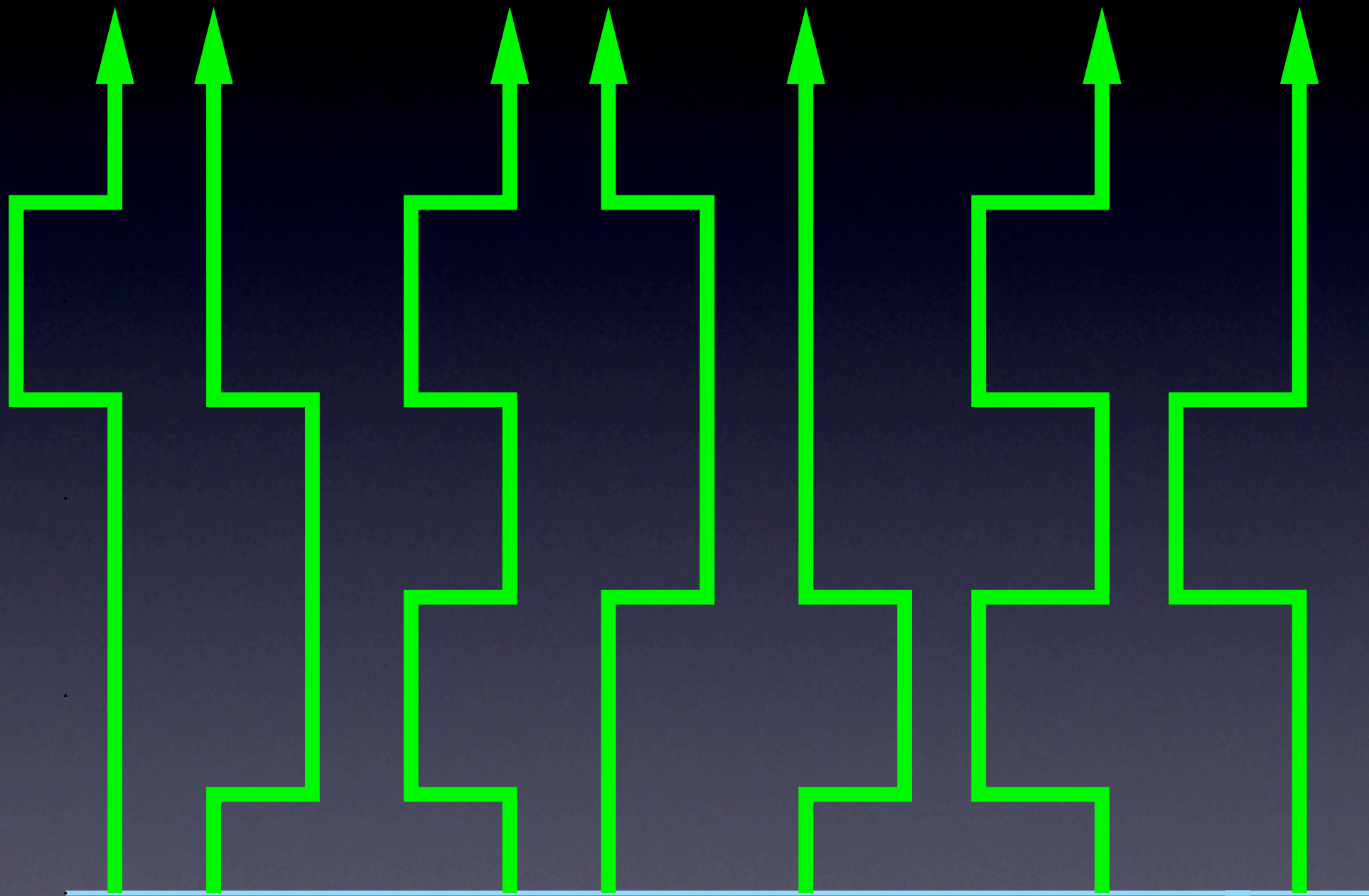
The Continuous limit



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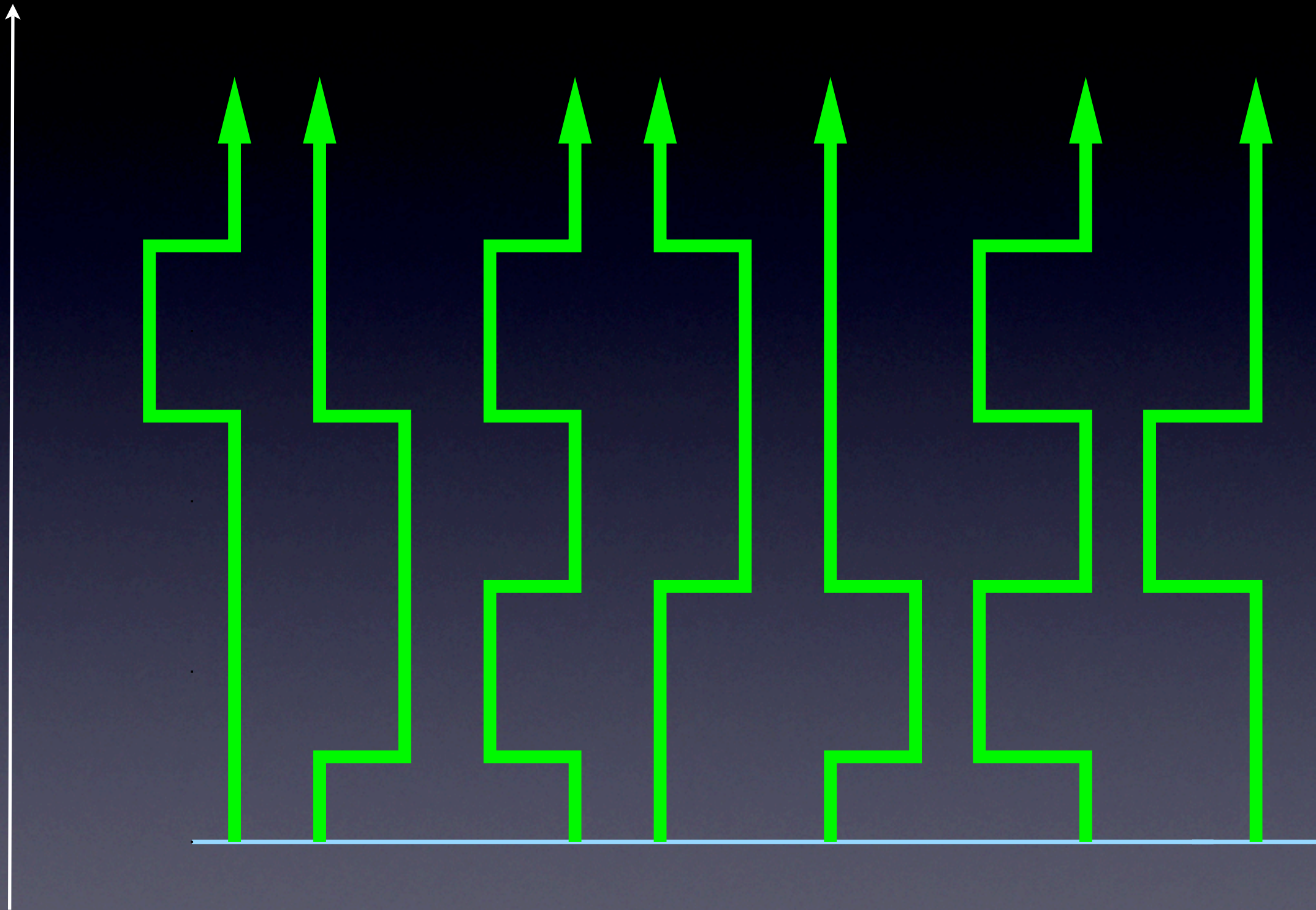


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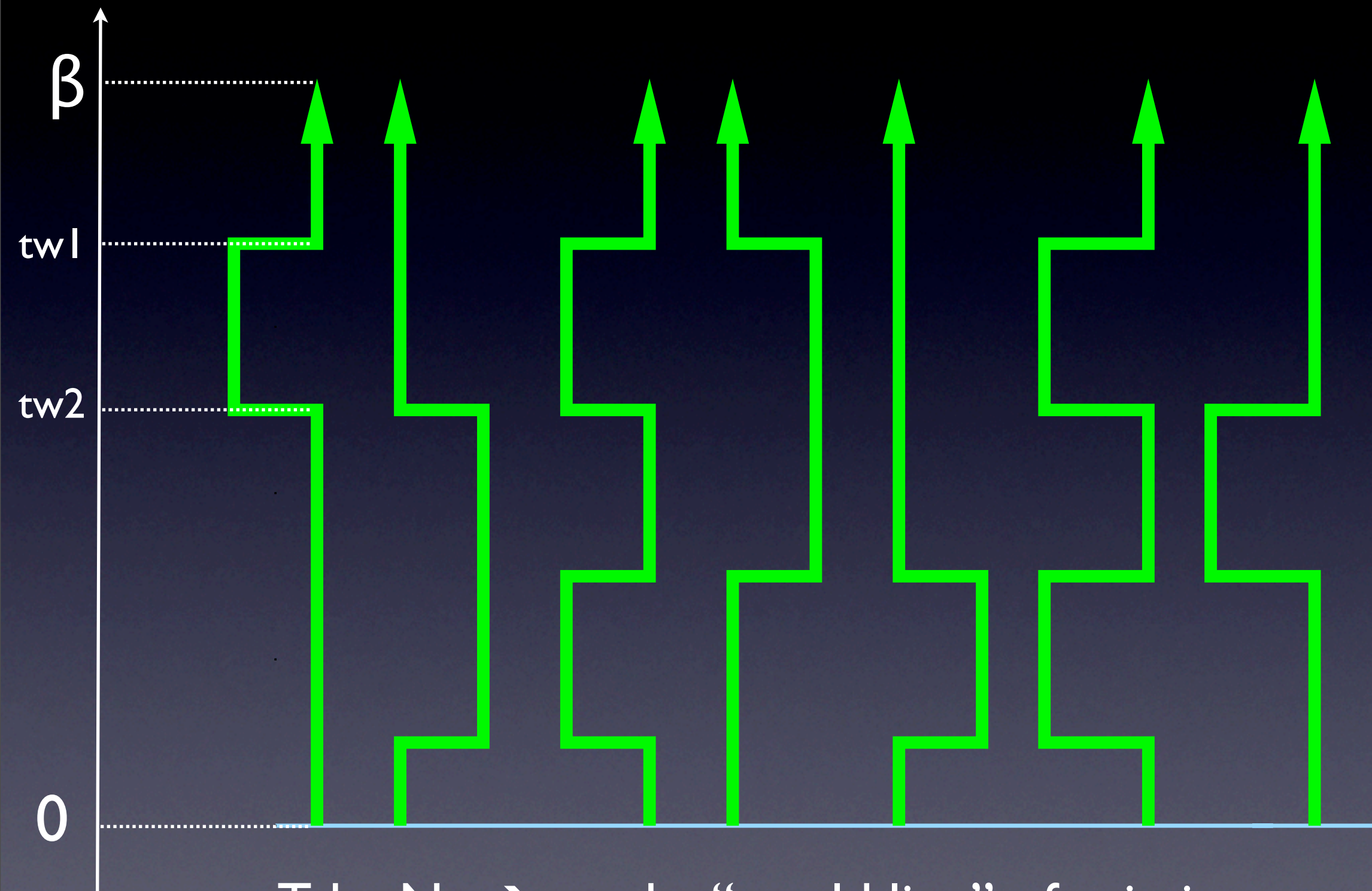
The Continuous limit

“time”



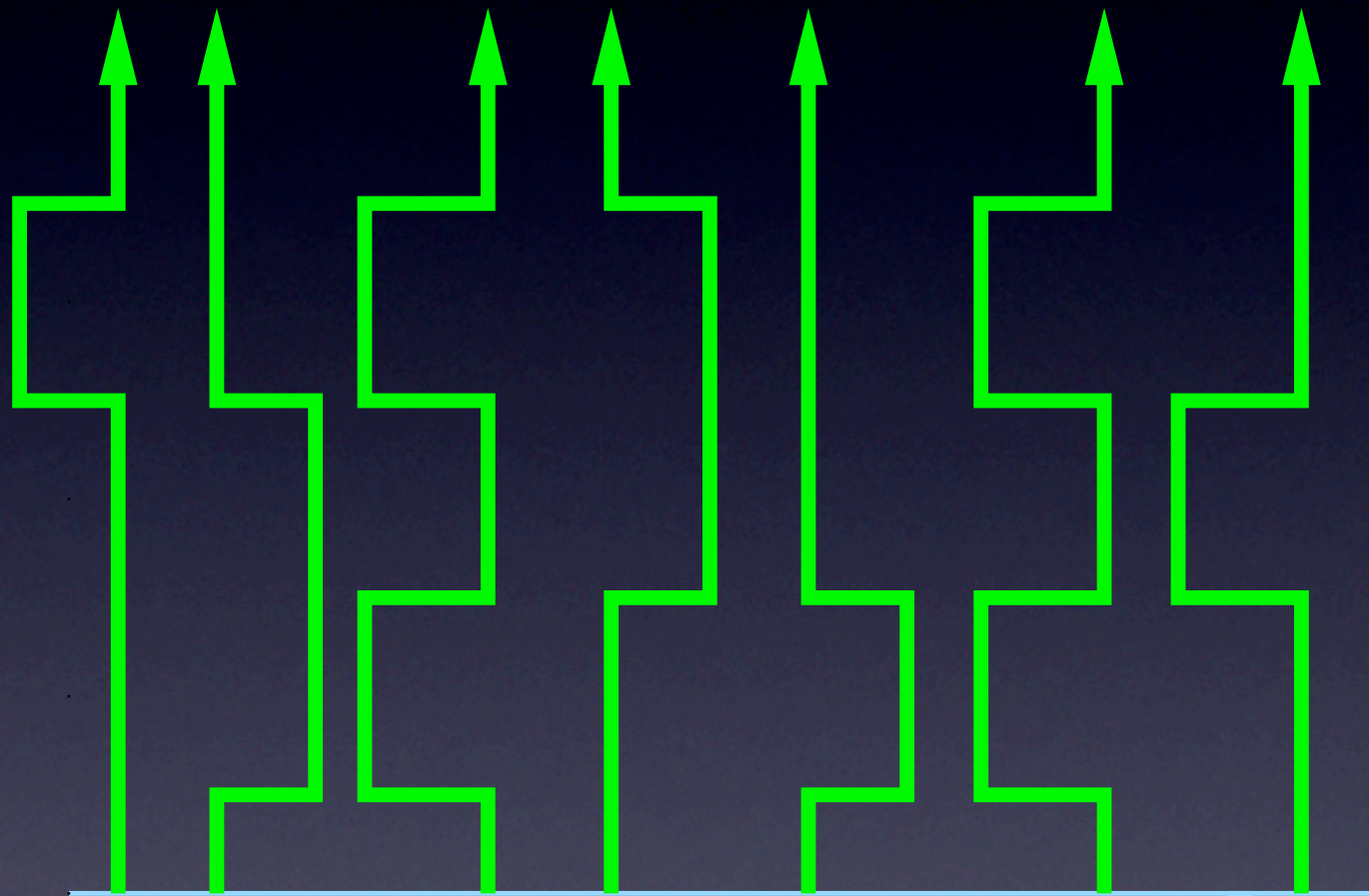
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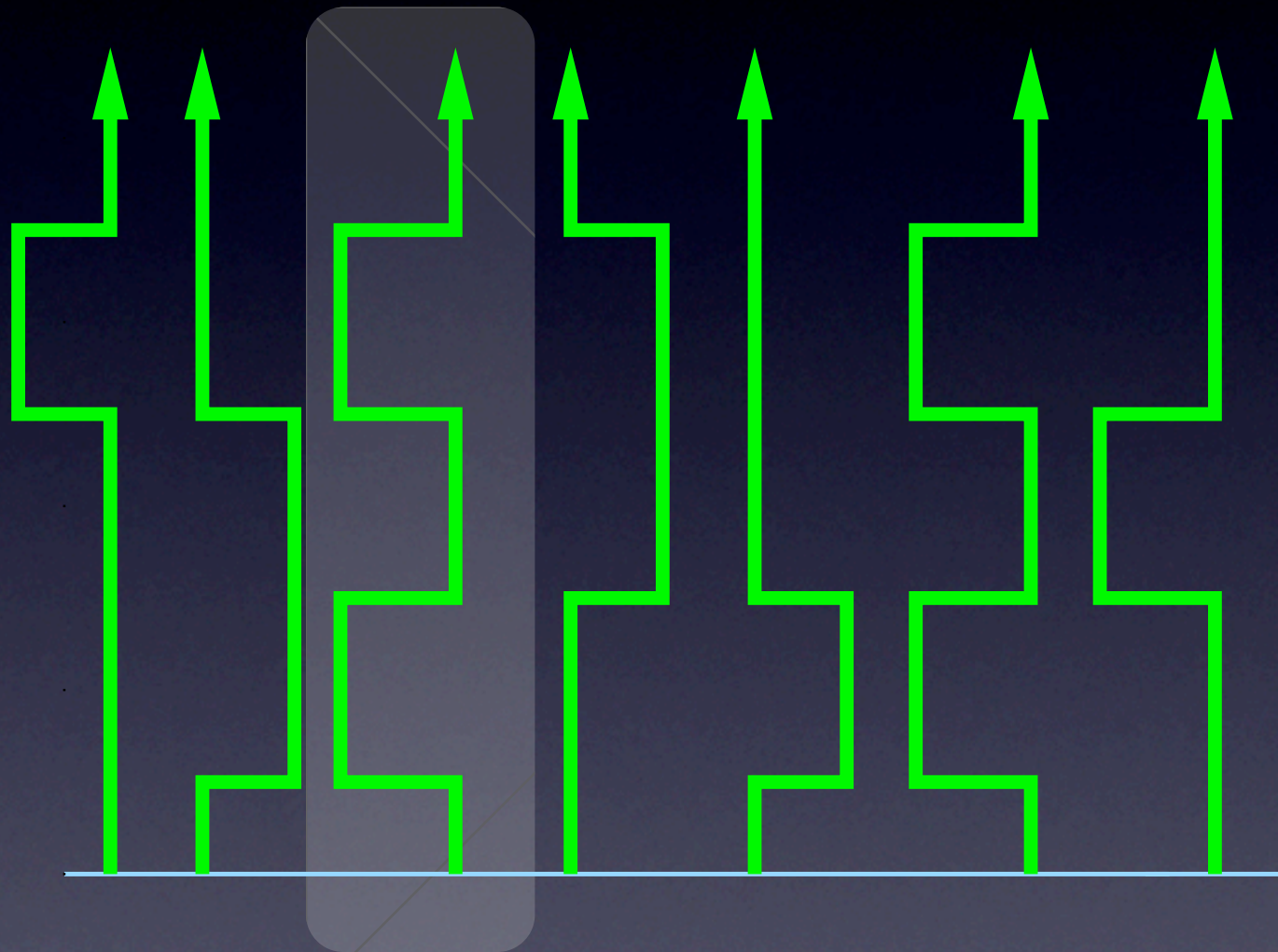
Take $N_s \rightarrow \infty$: the “world line” of spin is now entirely characterized by the set of flipping times

The “Continuous” time Heat Bath



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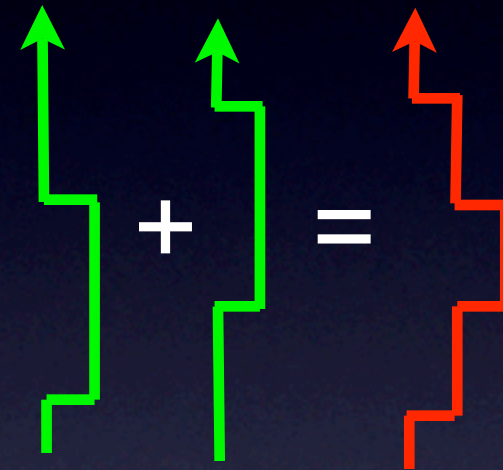
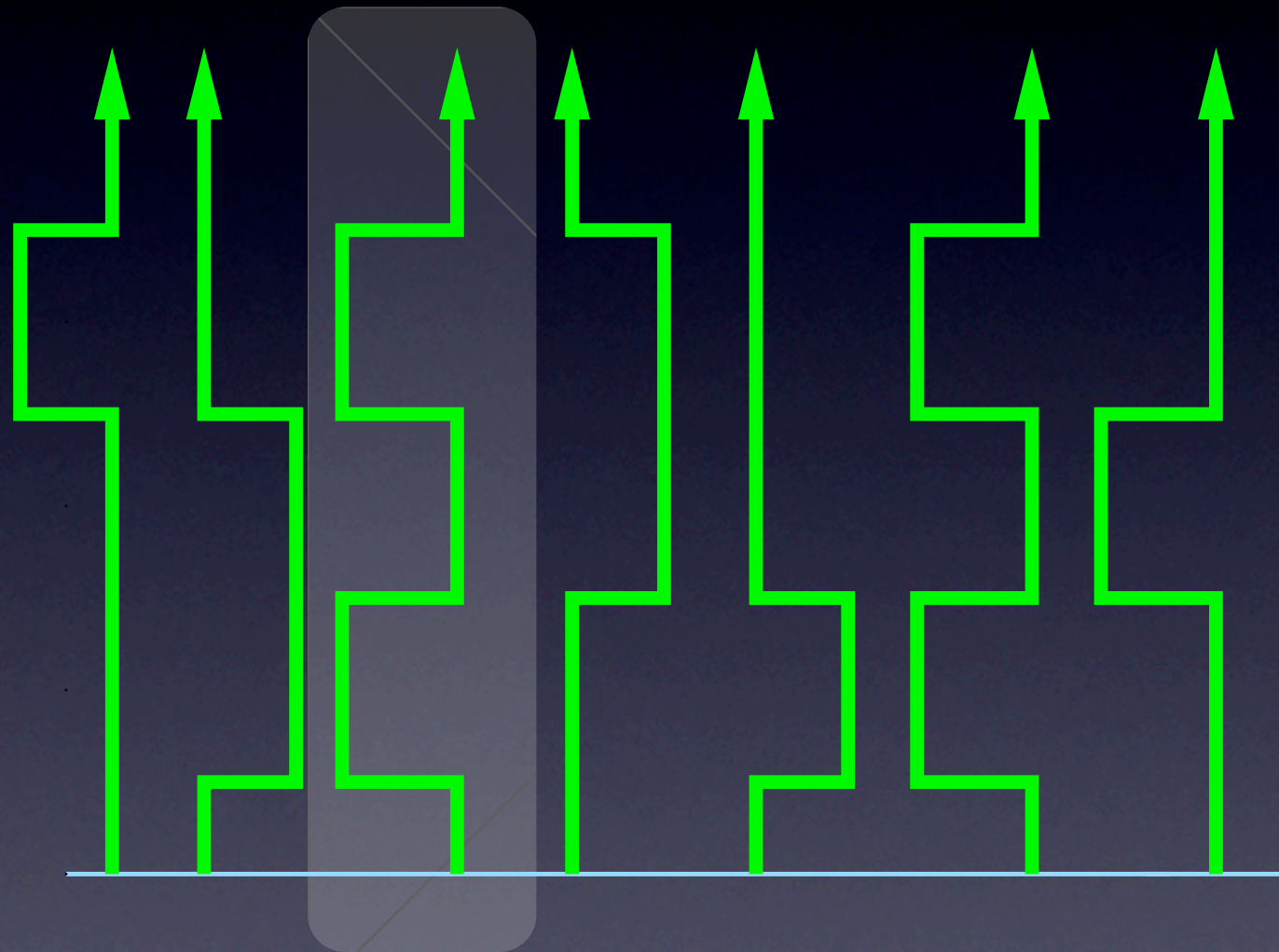
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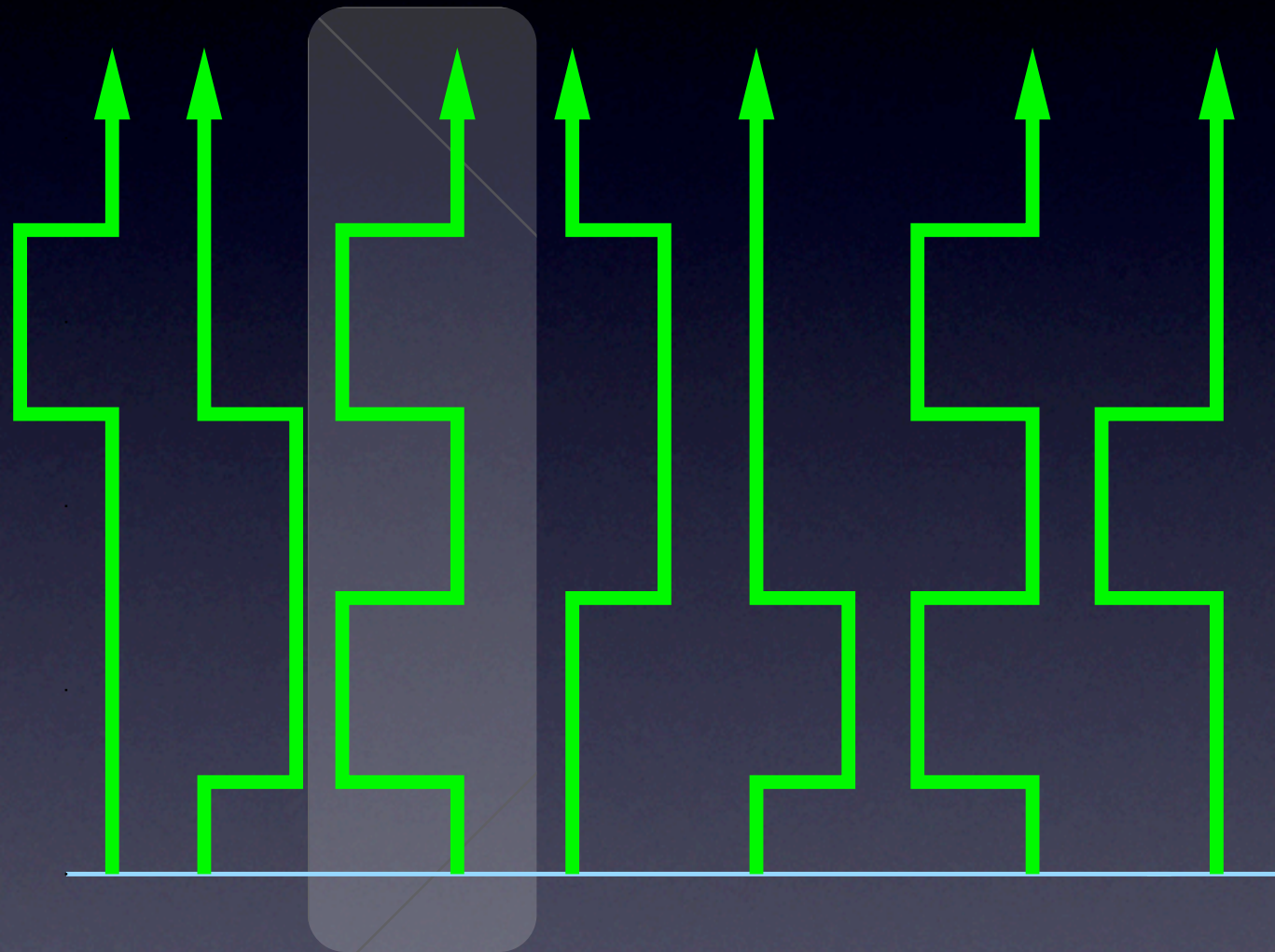
The “Continuous” time Heat Bath

1) Choose a site at random

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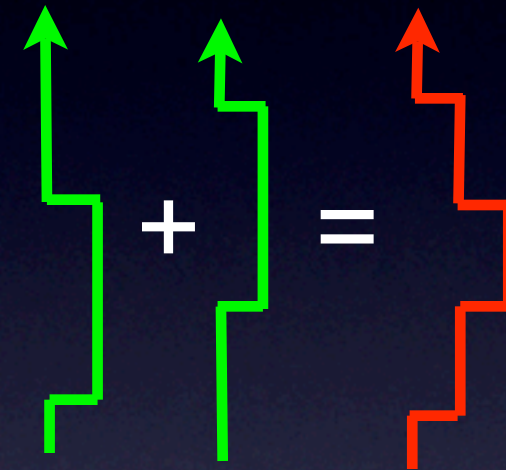


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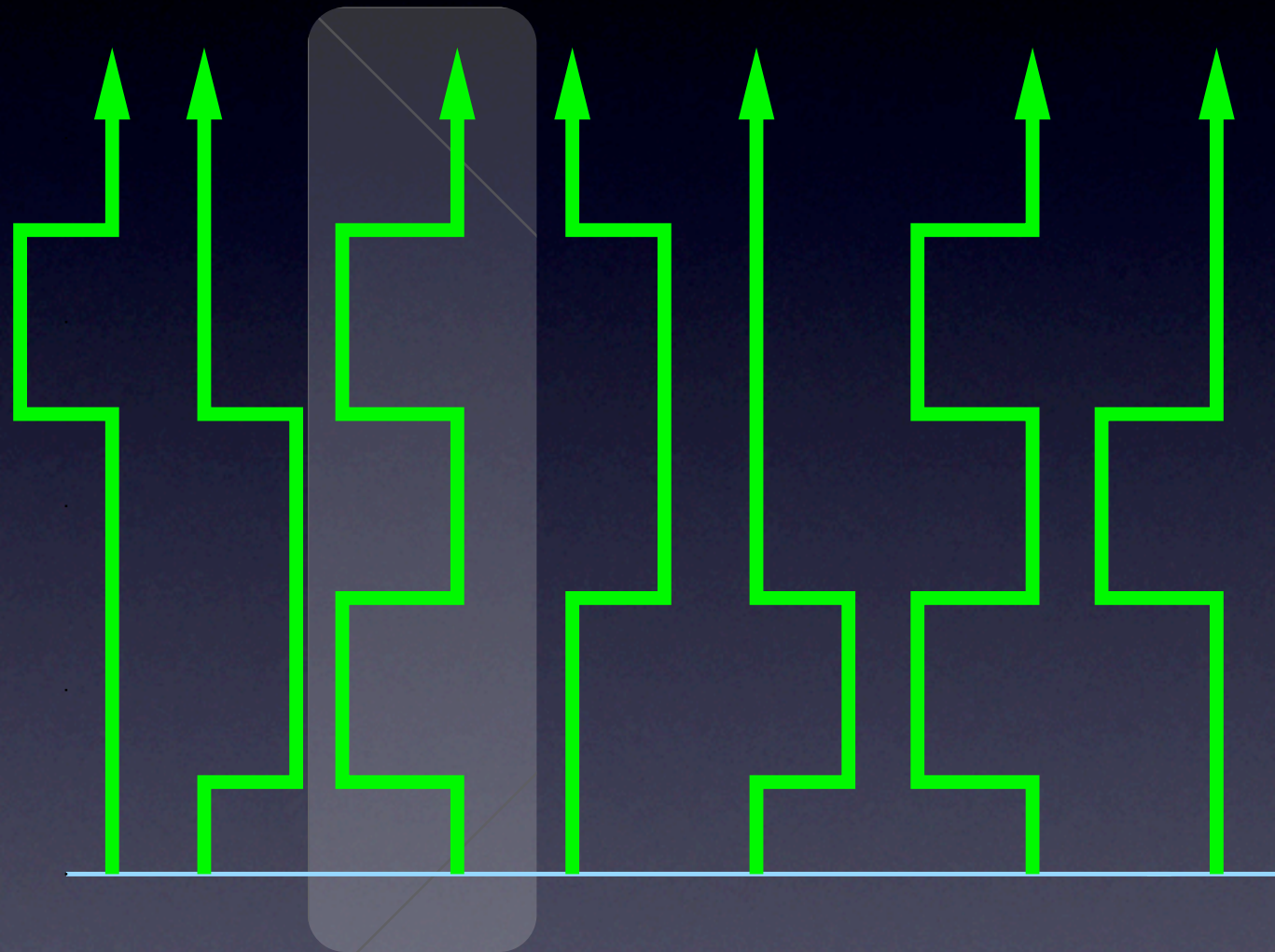
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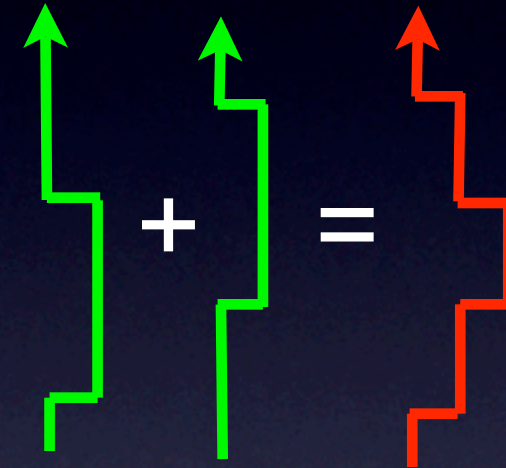
3) Choose the new path of the spin with Boltzmann probability

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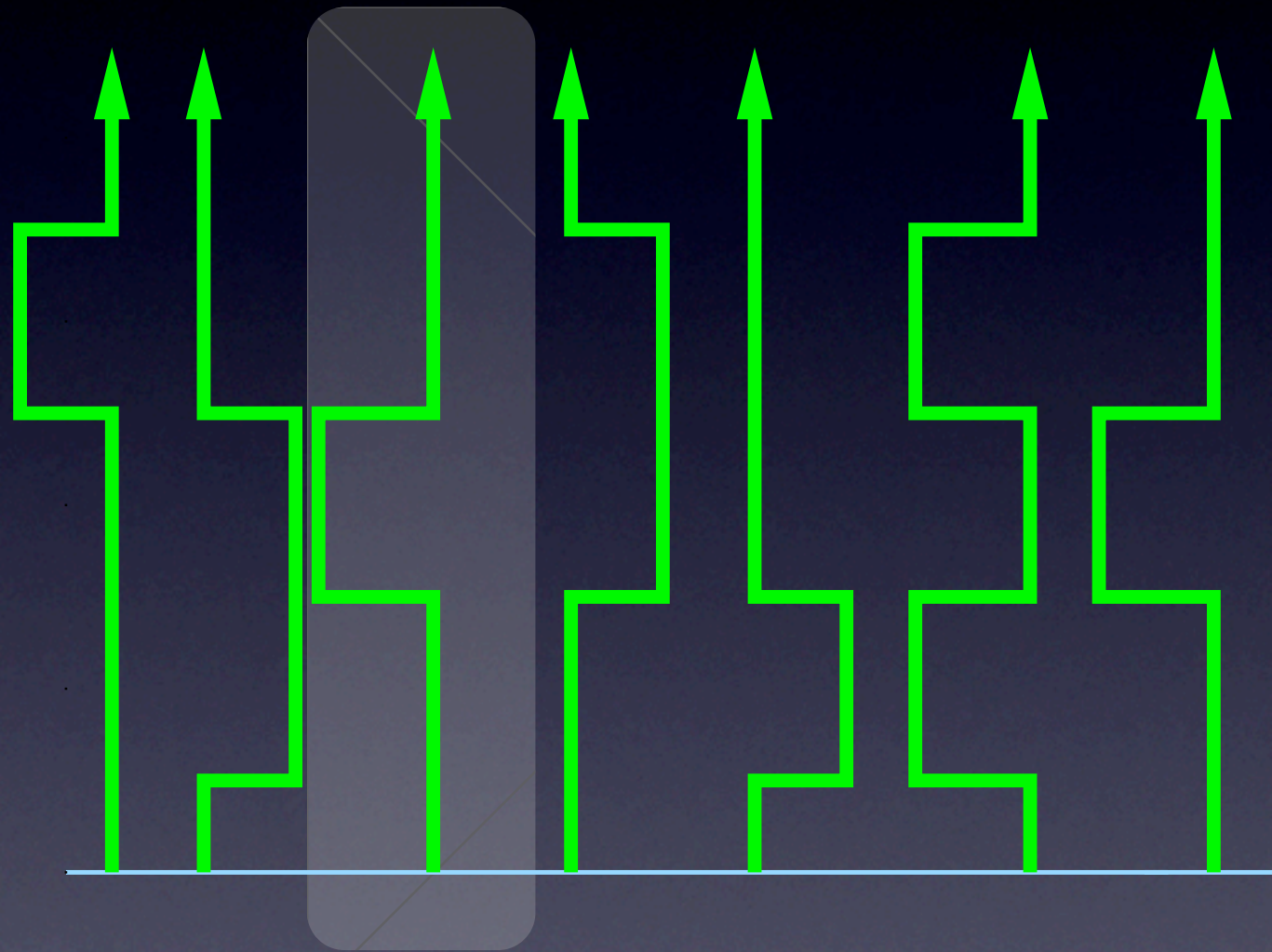
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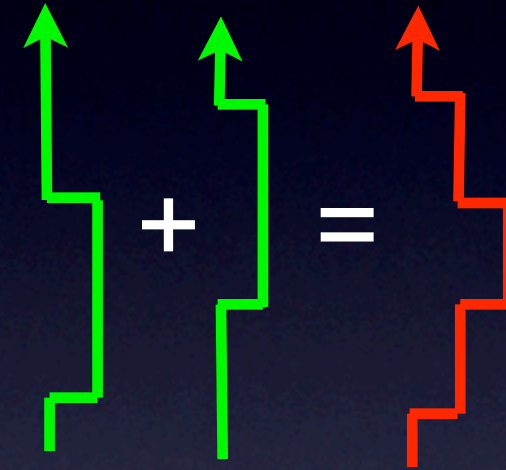
The difficulty is to generate a “world line of spin” given a “world line field”

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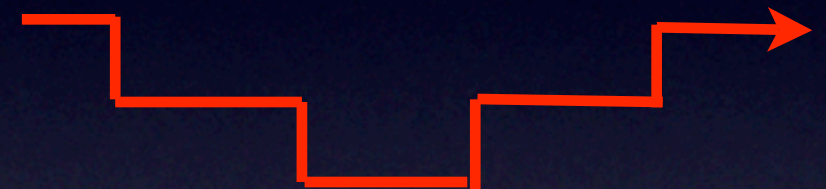


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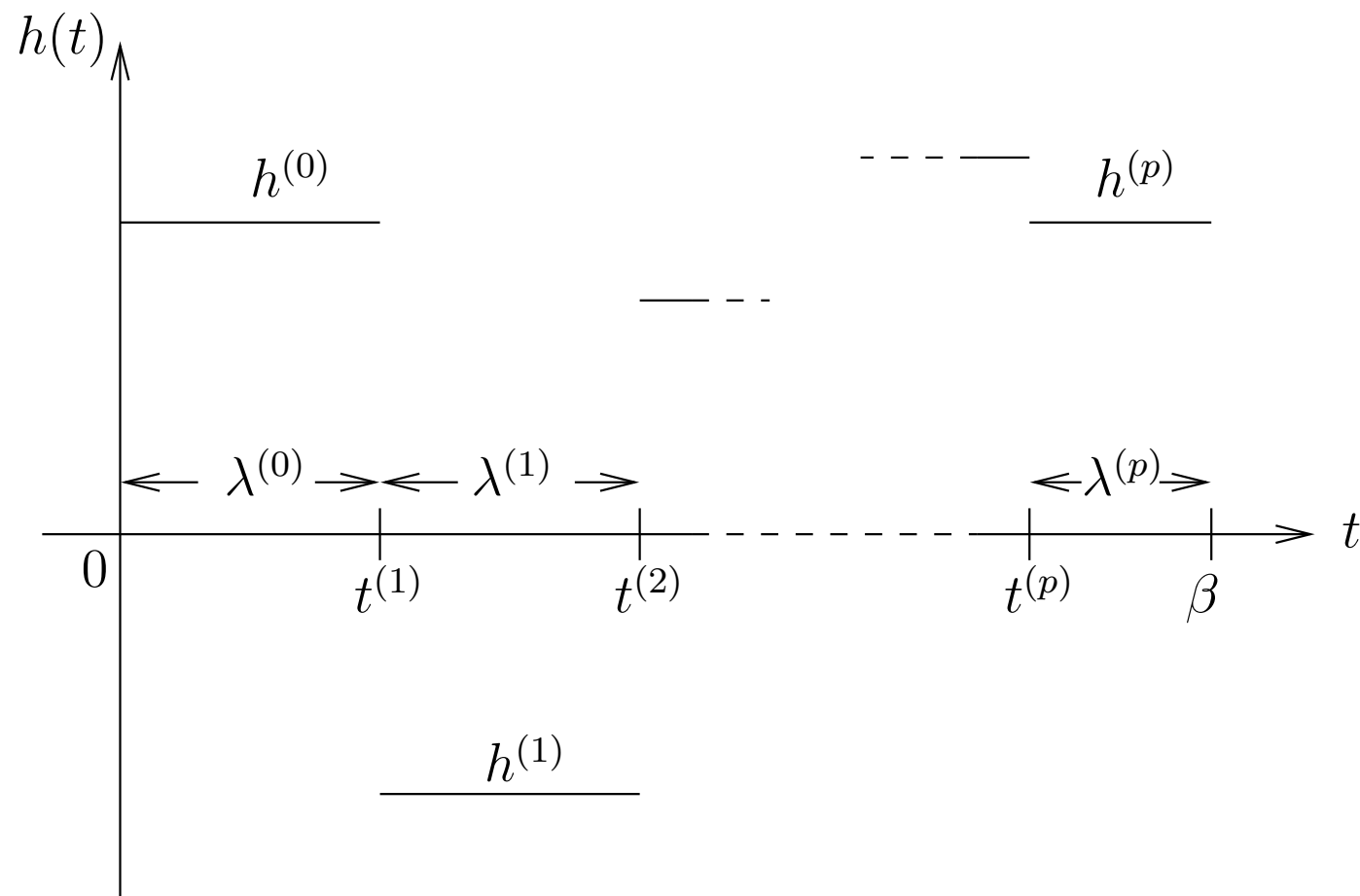
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Generating a new spin path in a heat bath way

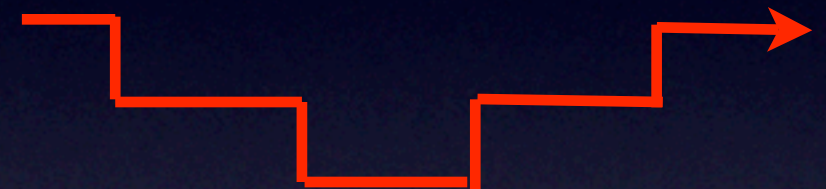
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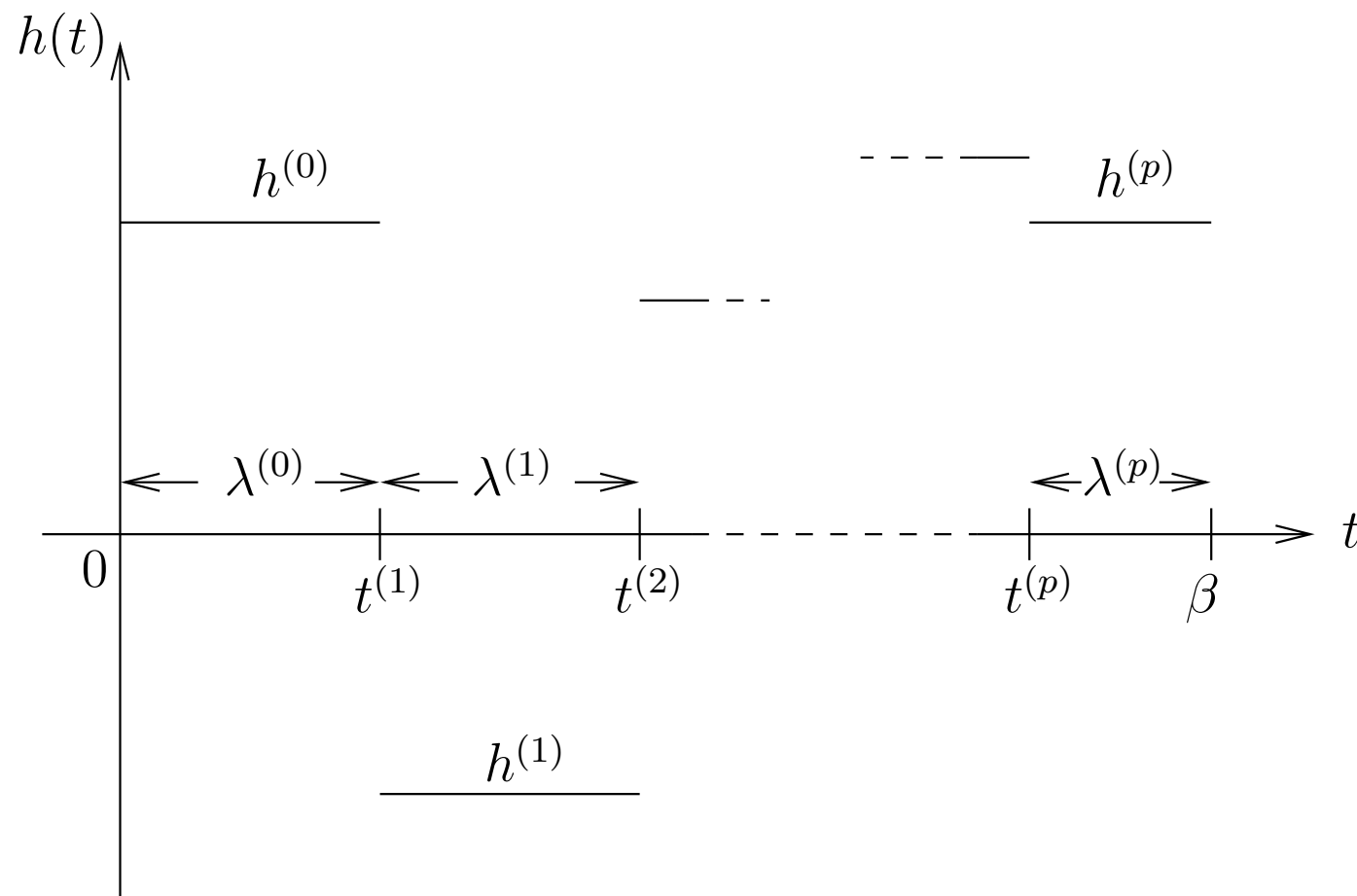
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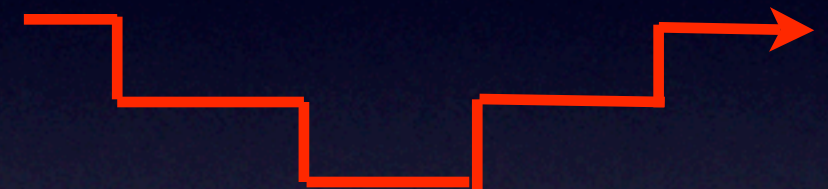
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Generating a new spin path in a heat bath way



How to generate the path
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- 1) How to generate a path
in a constant field ?
- 2) How to generate the path
in a piecewise constant field?

Generating a path in a constant field

*Define (and compute) the propagators
in constant field h for a time λ :*

$$e^{\lambda(h\sigma_z + \lambda\Gamma\sigma_x)} = \begin{pmatrix} W_{u,u} & W_{u,d} \\ W_{d,u} & W_{d,d} \end{pmatrix}$$

$$W(s \rightarrow s', h, \lambda) = \begin{cases} \cosh(\lambda\sqrt{\Gamma^2 + h^2}) + s\frac{h}{\sqrt{\Gamma^2 + h^2}} \sinh(\lambda\sqrt{\Gamma^2 + h^2}) & \text{if } s = s' \\ \frac{\Gamma}{\sqrt{\Gamma^2 + h^2}} \sinh(\lambda\sqrt{\Gamma^2 + h^2}) & \text{if } s = -s' \end{cases}$$

A useful recursion

$$\begin{aligned}
 & \text{Diagram 1: } \sigma \text{ --- } \text{dashed arc} \text{ --- } \sigma = \text{straight line} + \int du \text{Diagram 2: } u \\
 & \text{Diagram 3: } \sigma \text{ --- } \text{dashed arc} \text{ --- } -\sigma = \int du \text{Diagram 4: } u
 \end{aligned}$$

$$W(s \rightarrow s, h, \lambda) = e^{sh\lambda} + \Gamma \int_0^\lambda du e^{shu} W(-s \rightarrow s, h, \lambda - u) ,$$

$$W(s \rightarrow -s, h, \lambda) = \Gamma \int_0^\lambda du e^{shu} W(-s \rightarrow -s, h, \lambda - u) .$$

A simple recursive algorithm

$$\begin{array}{c} + \\ - \end{array} \quad \text{-----} \quad \begin{array}{c} + \\ - \end{array}$$

$$\begin{array}{l} \sigma \text{ --- } \text{dashed} \text{ --- } \sigma = \text{---} + \int du \text{ --- } \text{dashed} \\ \sigma \text{ --- } \text{dashed} \text{ --- } -\sigma = \int du \text{ --- } \text{dashed} \end{array}$$

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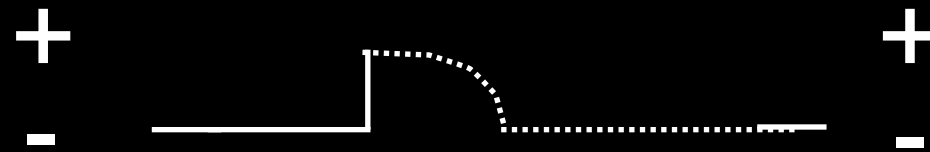
$$\begin{array}{c} + \\ - \end{array} \quad \text{-----} \quad \begin{array}{c} + \\ - \end{array}$$

- if $s = s'$:
- with probability $e^{sh\lambda} / W(s \rightarrow s, h, \lambda)$,
set $\sigma(t) = \sigma$ on the whole time interval
 - otherwise, draw a random variable $u \in [0, \lambda]$
with density proportional to $e^{shu} W(-s \rightarrow s, h, \lambda - u)$
and set $s(t) = \sigma$ up to time u

$$\begin{array}{l} \sigma \text{---} \text{dashed dip} \text{---} \sigma = \text{---} \sigma \text{---} + \int du \text{---} \sigma \text{---} \text{dashed fluctuation} \\ \sigma \text{---} \text{dashed curve} \text{---} -\sigma = \int du \text{---} \sigma \text{---} \text{dashed fluctuation} \end{array}$$

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A simple recursive algorithm

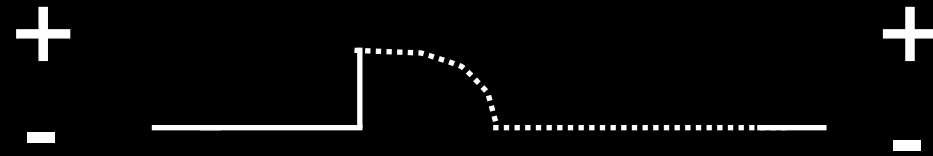


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A diagram showing the decomposition of a path into a constant path and a path with a step up. The first part shows a path starting at σ , dipping down, and returning to σ . This is equal to a constant path at σ plus an integral over du of a path that starts at σ , steps down to u , and then returns to σ . The second part shows a path starting at σ , dipping down to $-\sigma$, and returning to σ . This is equal to an integral over du of a path that starts at σ , steps down to u , and then returns to σ .

$$W(s \rightarrow s, h, \lambda) = e^{sh\lambda} + \Gamma \int_0^\lambda du e^{shu} W(-s \rightarrow s, h, \lambda - u) ,$$

A simple recursive algorithm



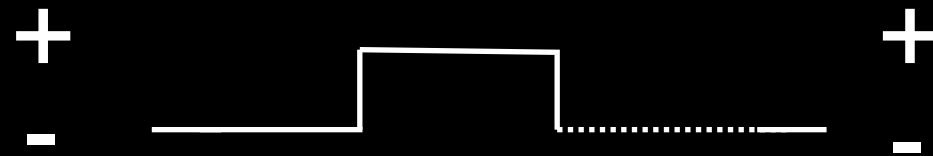
If $s = -s'$: – draw a random number with
density proportional to $e^{shu} W(-s \rightarrow -s, h, \lambda - u)$

- set $\sigma(t) = \sigma$ up to time u
- call the previous procedure to generate the remaining trajectory

Diagram showing the decomposition of a path from σ to σ into a direct path and a path through $- \sigma$. The first equation shows a path from σ to σ as a sum of a direct path and an integral over u of a path from σ to $- \sigma$ and then back to σ . The second equation shows a path from σ to $- \sigma$ as an integral over u of a path from σ to $- \sigma$ and then back to σ .

$$W(s \rightarrow -s, h, \lambda) = \Gamma \int_0^\lambda du e^{shu} W(-s \rightarrow -s, h, \lambda - u) .$$

A simple recursive algorithm



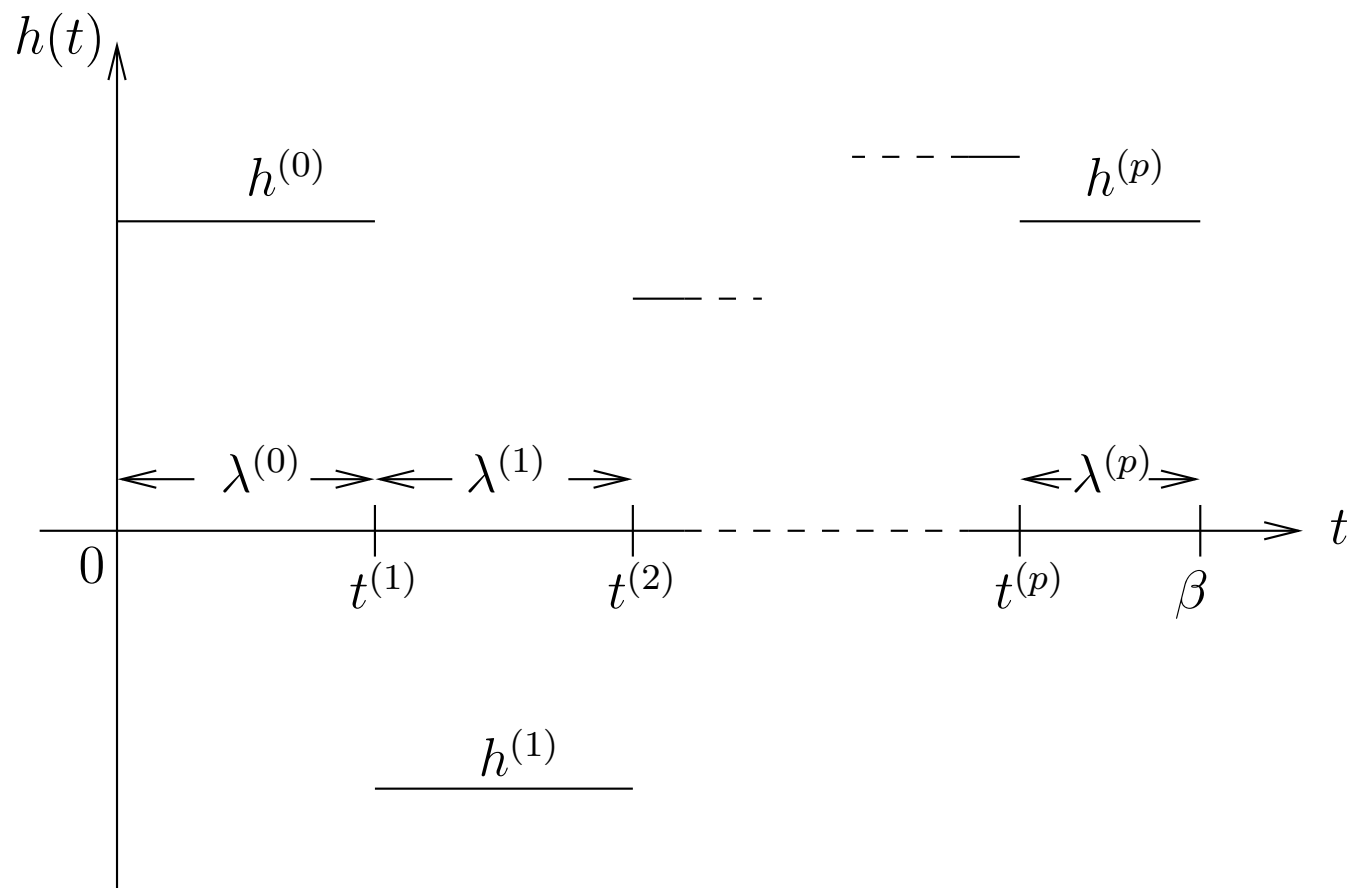
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$$\begin{aligned} \sigma \text{ (solid) } \rightarrow \sigma \text{ (solid)} &= \text{constant} + \int du \text{ (solid) } \rightarrow \sigma \text{ (solid) } \\ \sigma \text{ (solid) } \rightarrow -\sigma \text{ (solid)} &= \int du \text{ (solid) } \rightarrow -\sigma \text{ (solid)} \end{aligned}$$

$$W(s \rightarrow -s, h, \lambda) = \Gamma \int_0^\lambda du e^{shu} W(-s \rightarrow -s, h, \lambda - u) .$$

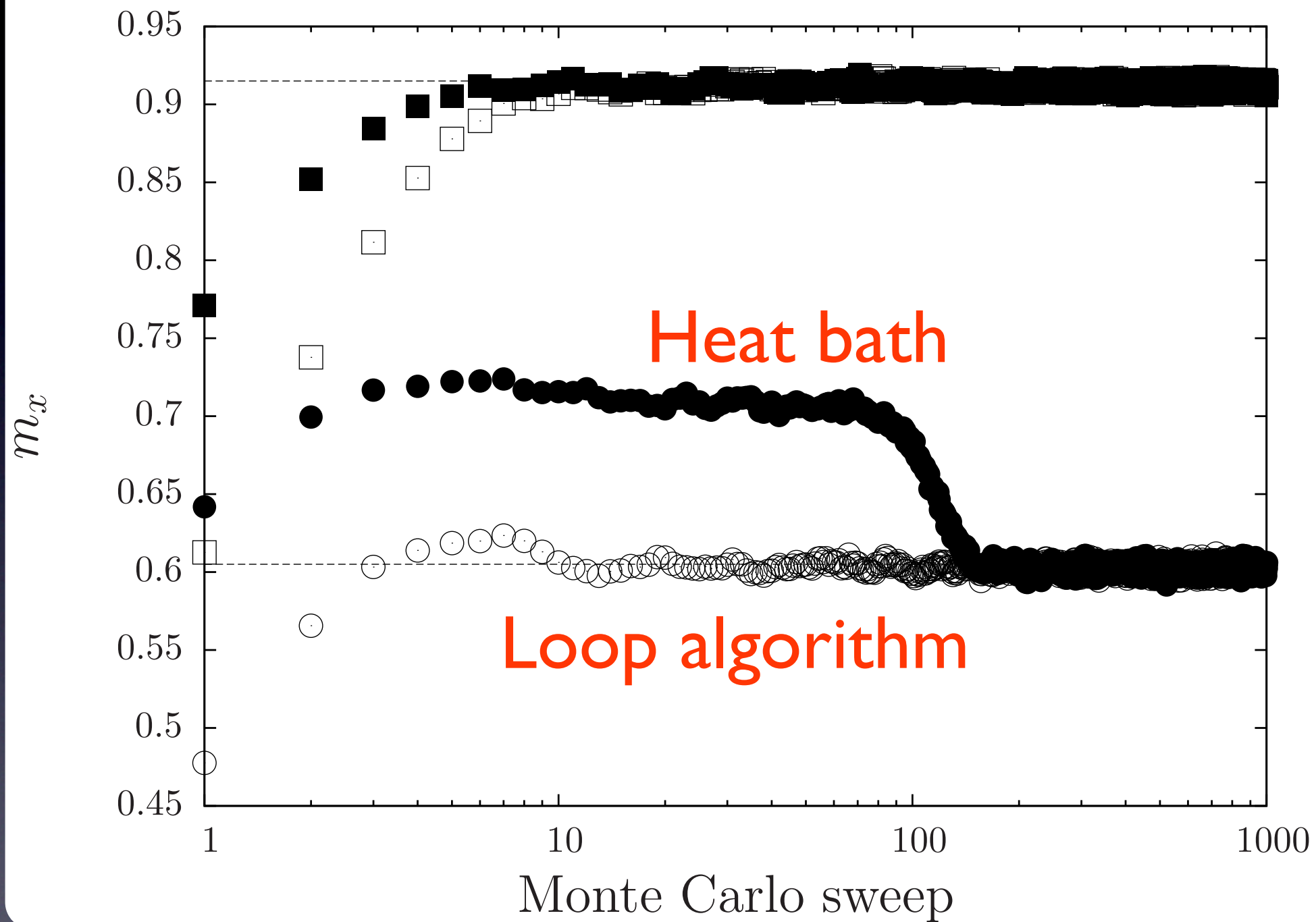
Generating a path in a constant piecewise field



We need to know the spin orientation at time $t(1), t(2) \dots$ in order to apply the “constant field algorithm”

$$P(s_1, \dots, s_p | \mathbf{h}) = \prod_{i=0}^p W(s_i \rightarrow s_{i+1}, h^{(i)}, \lambda^{(i)})$$

Some results



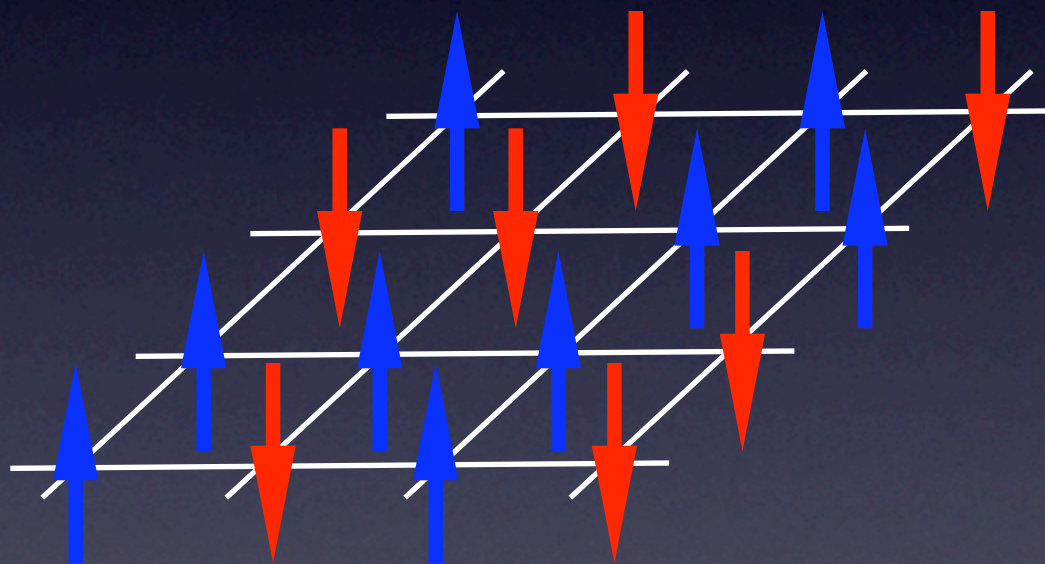
Comparison with the best available algorithm
(Loop Algorithm, Rieger-Kawashima 98')
on a regular random graph

Overview

- Heat bath for classical and quantum spins
- Cavity Method for classical and quantum spins
- Conclusions and perspectives

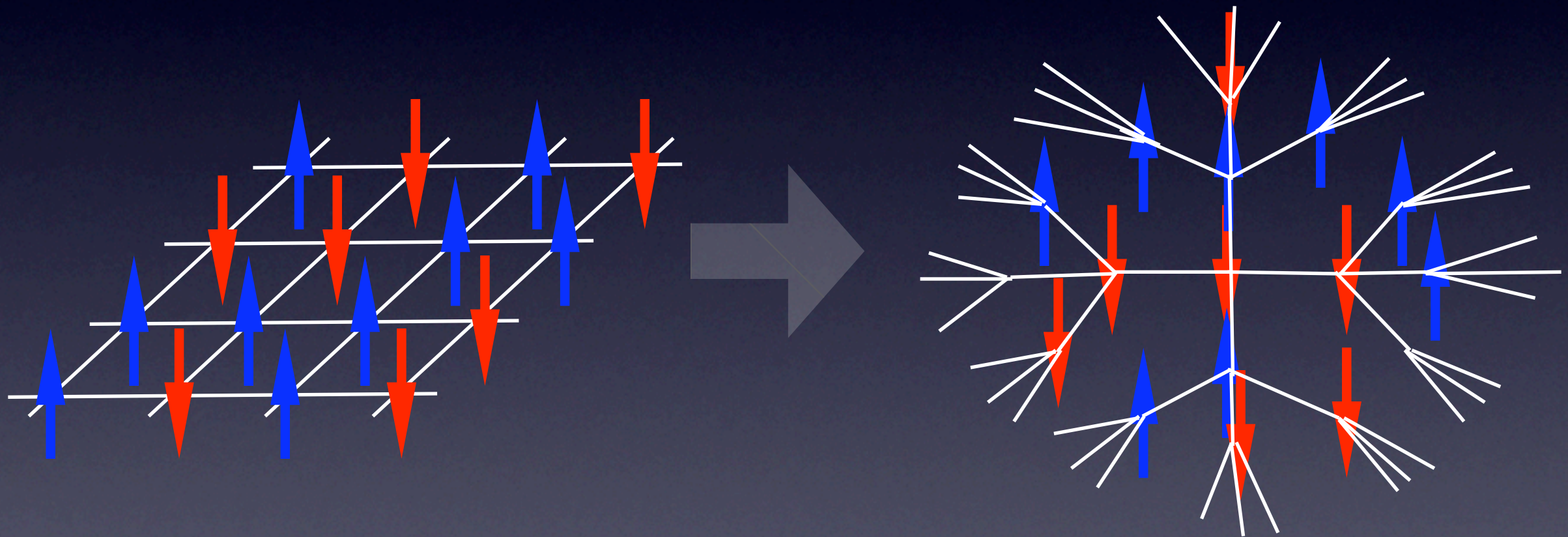
Bethe-Peierls Approximation

(Replica-Symmetric cavity method)



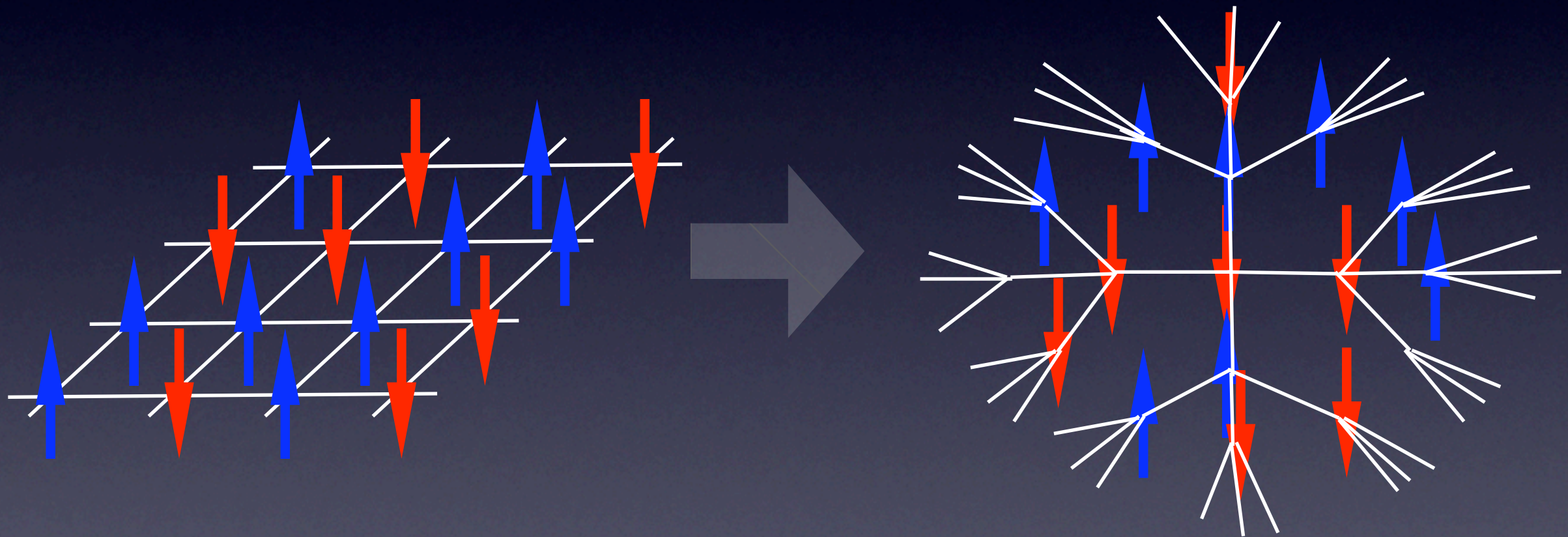
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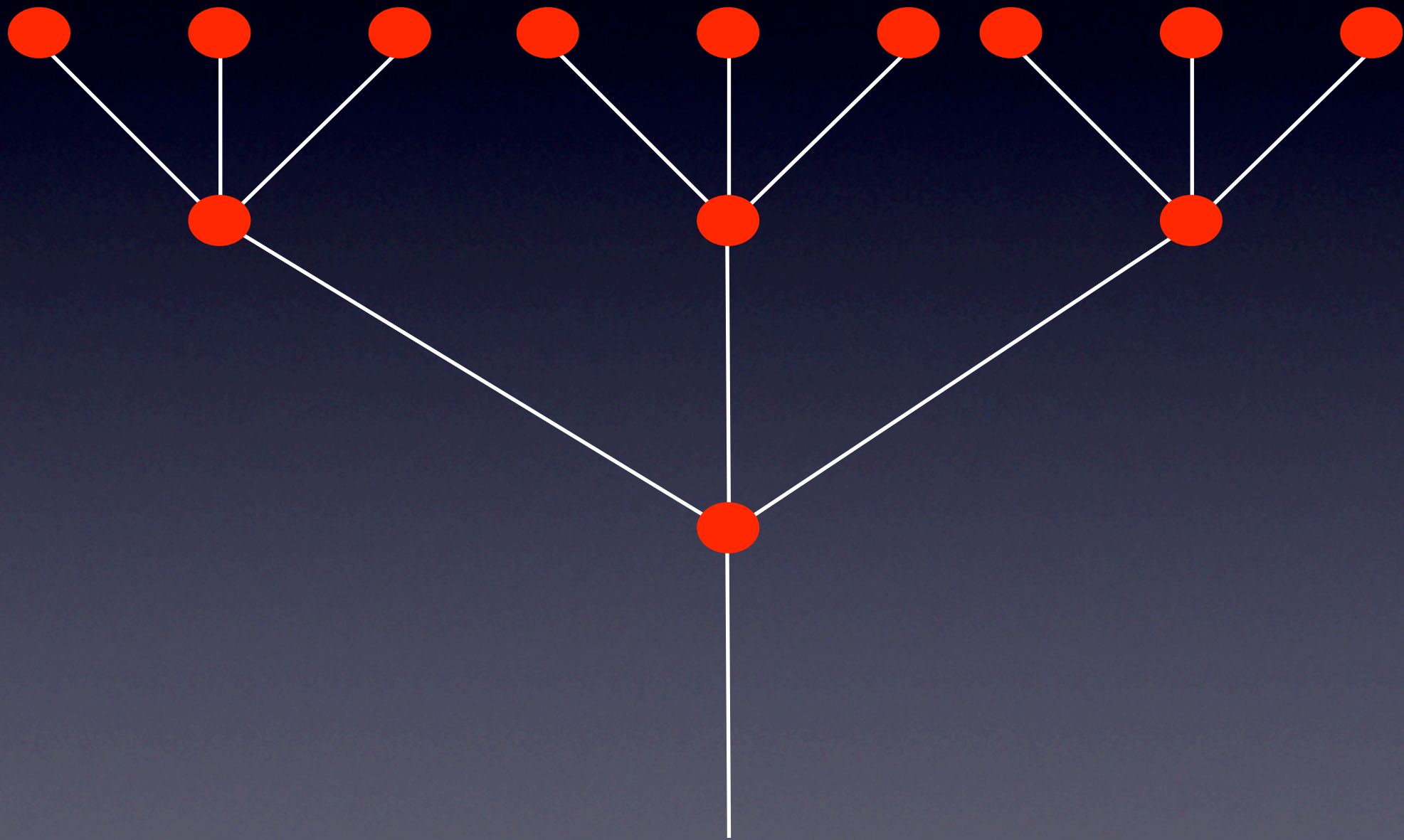
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Solve the model on a tree with the same connectivity

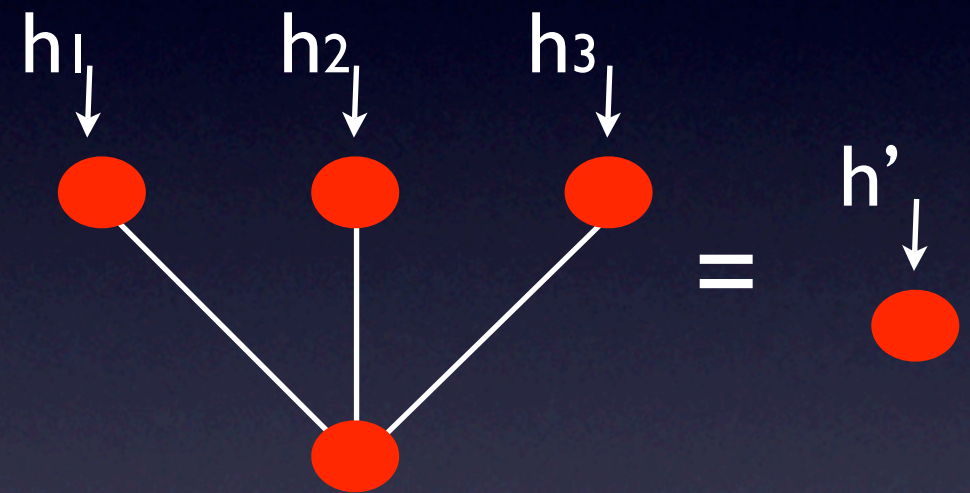
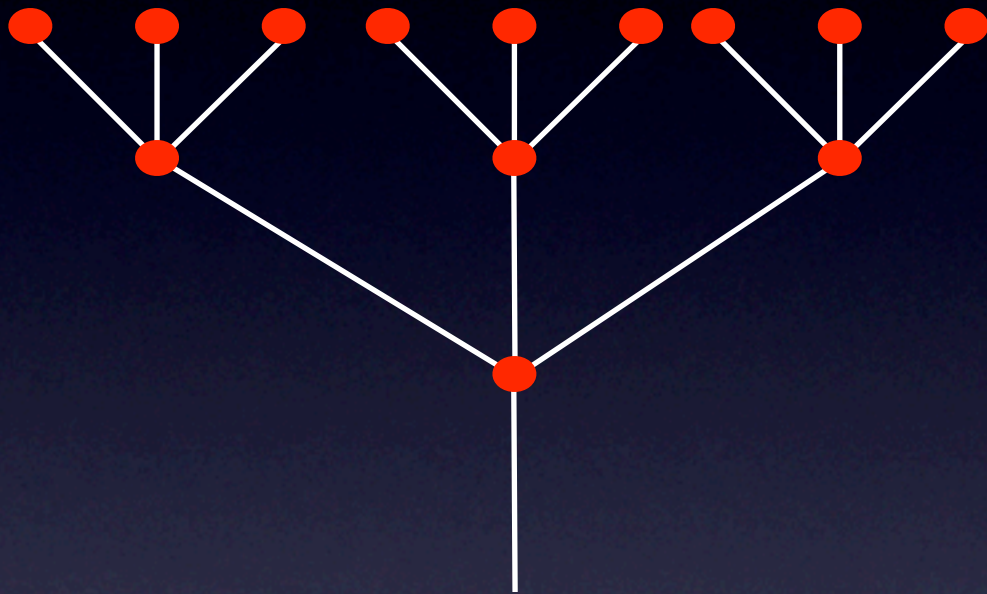
Classical Bethe-Peierls Approximation

The Cavity Method: solving by recursion



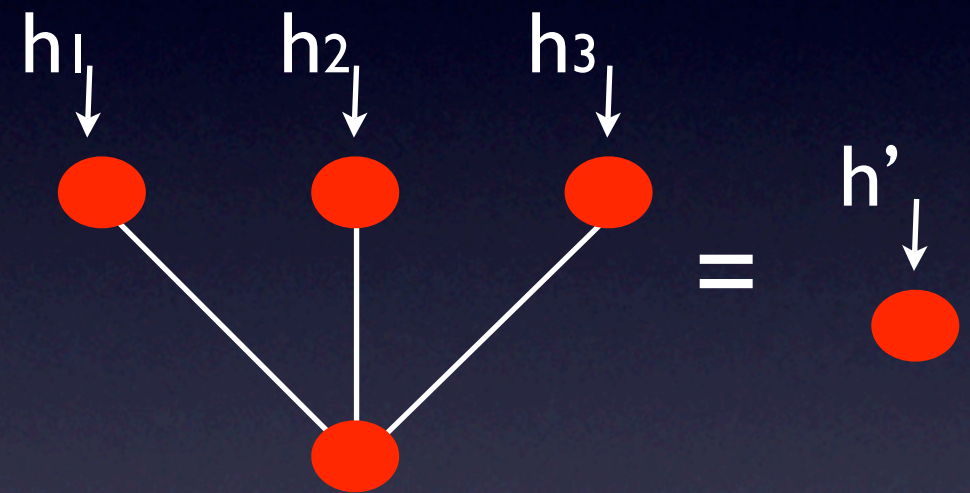
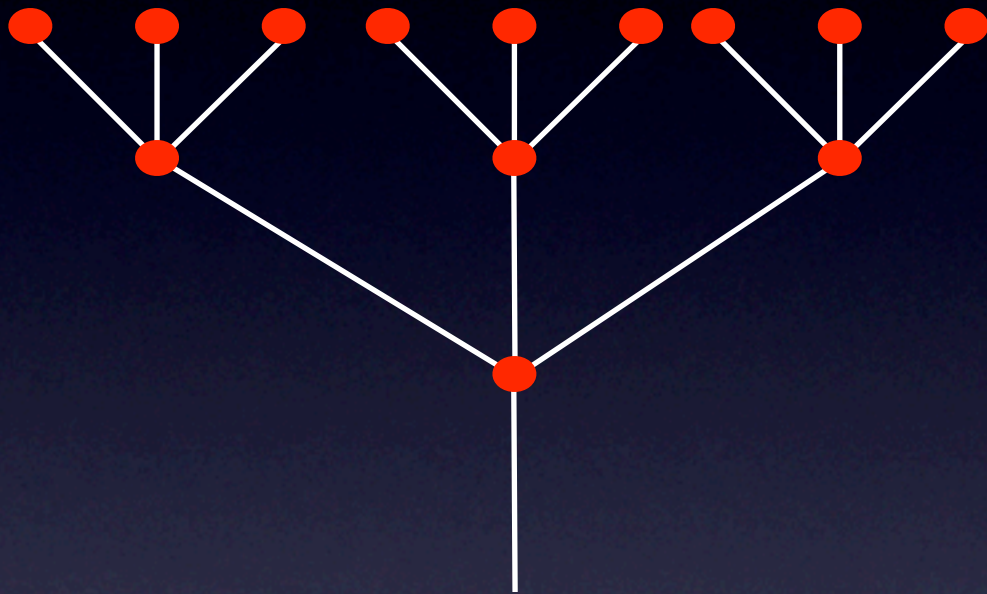
Classical Bethe-Peierls Approximation

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Classical Bethe-Peierls Approximation

The Cavity Method: solving by recursion



$$h' = \sum_{i=1}^3 \frac{1}{\beta} \tanh^{-1} (\tanh \beta h_i \tanh \beta J)$$

Classical Bethe-Peierls Approximation

The Cavity Method: solving by recursion

Classical Bethe-Peierls Approximation

The Cavity Method: solving by recursion

Fixed Point

$$h = \frac{c-1}{\beta} \tanh^{-1} (\tanh \beta h \tanh \beta J)$$

BP

! d=no transition

$$\beta(2d)=0.346$$

$$\beta(3d)=0.203$$

$$\beta(4d)=0.144$$

$$\beta(5d)=0.112$$

Monte-Carlo

! d=no transition

$$\beta(2d)=0.44$$

$$\beta(3d)=0.221$$

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Classical Bethe-Peierls Approximation

The Cavity Method: solving by recursion

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Good quantitative approximation !

Monte-Carlo

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One field is enough for Ising spins

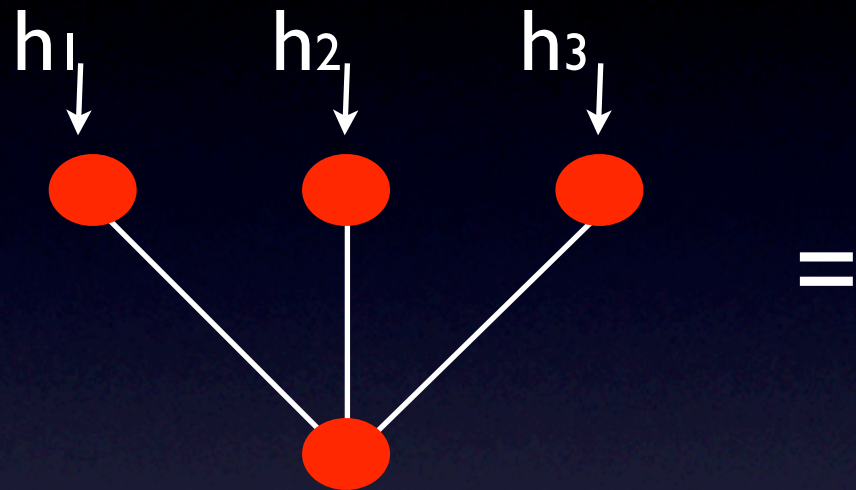
$$p_{up} = \frac{e^{\beta h}}{Z}$$



$$p_{down} = \frac{e^{-\beta h}}{Z}$$




One field is enough for Ising spins




=

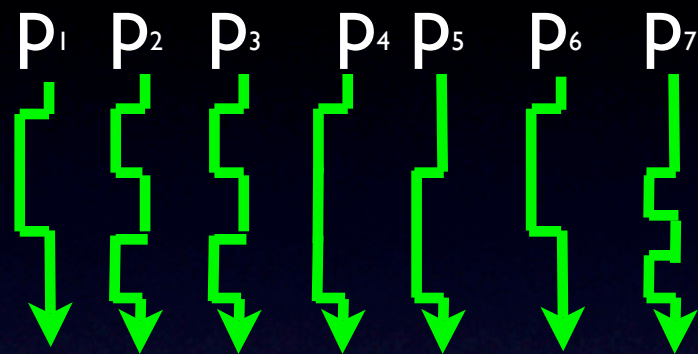


$$p_{up} = \frac{e^{\beta h}}{Z}$$
A thick blue arrow pointing upwards, positioned below the equation for p_{up} .

$$h' = \sum_{i=1}^3 \frac{1}{\beta} \tanh^{-1} (\tanh \beta h_i \tanh \beta J)$$

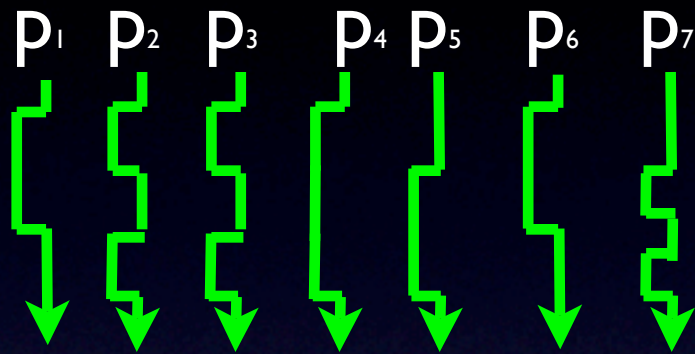
$$p_{down} = \frac{e^{-\beta h}}{Z}$$
A thick red arrow pointing downwards, positioned below the equation for p_{down} .

But not for quantum spins !!!!



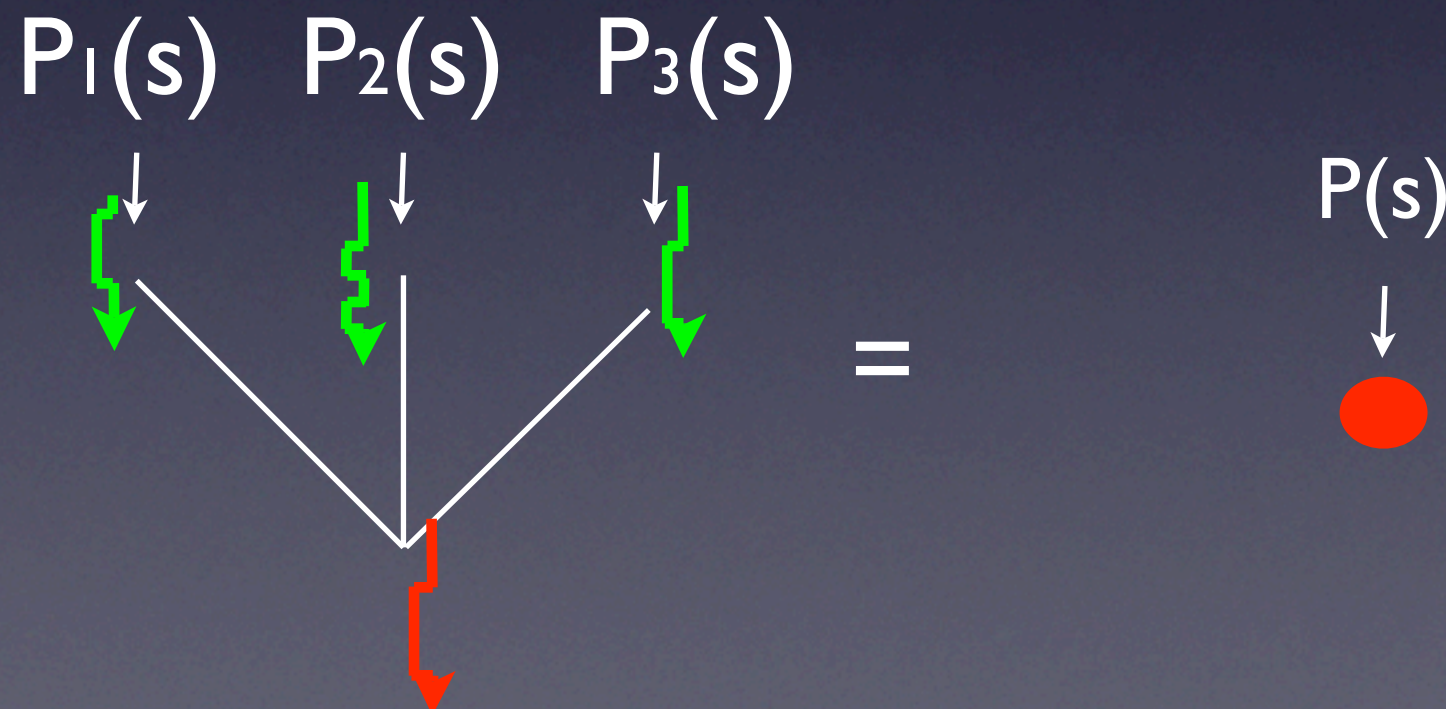
The probability distribution $P(s)$
is a quite complicated object !

But not for quantum spins !!!!

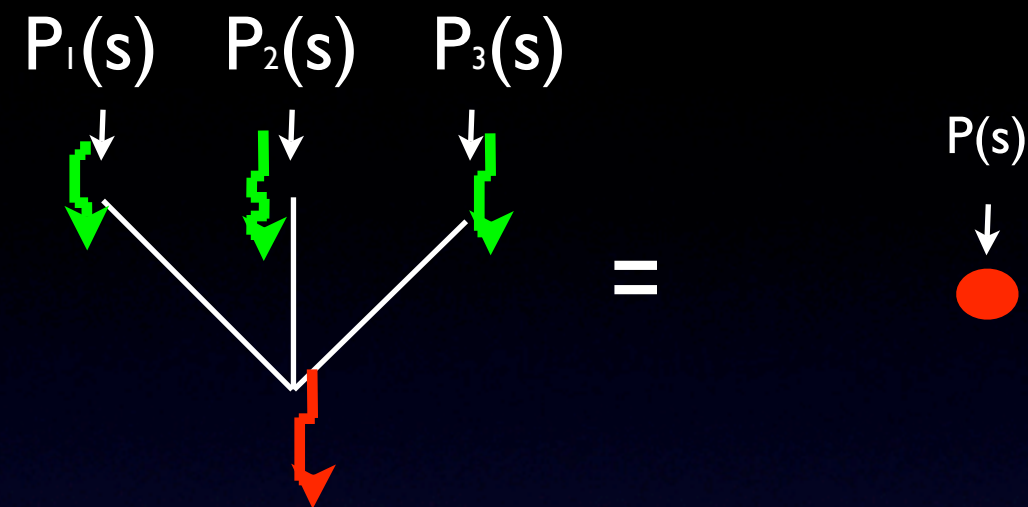


The probability distribution $P(s)$ is a quite complicated object !

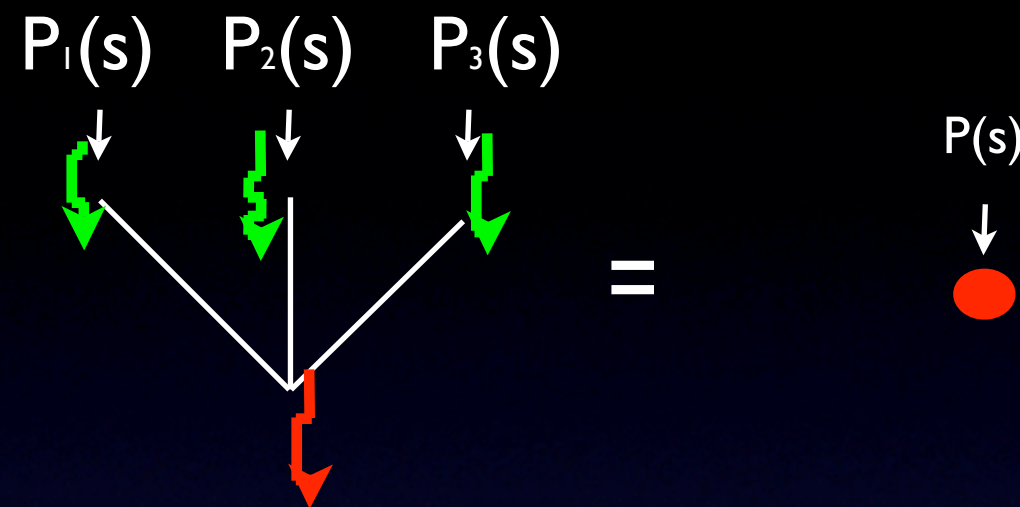
Need for a recursion for $P(s)$!



Structure of the recurrence equation

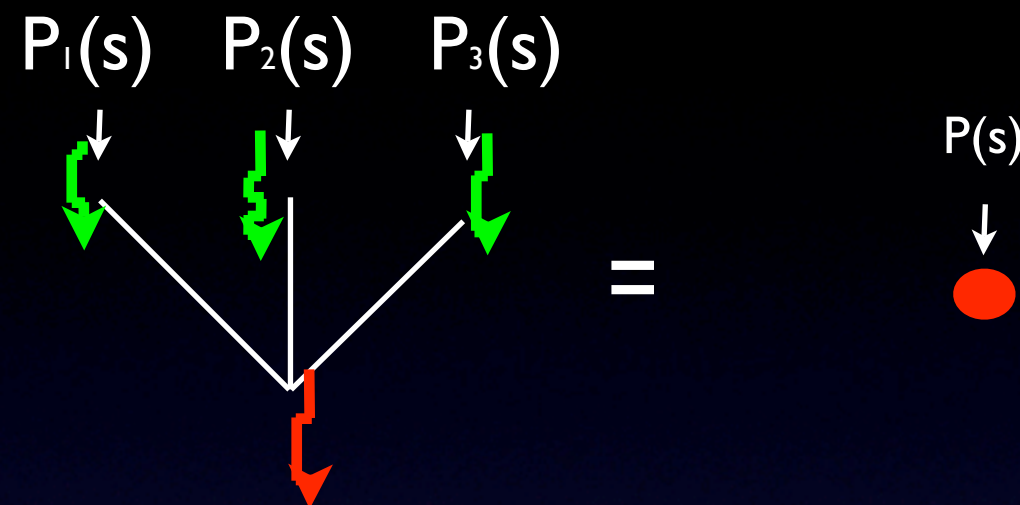


Structure of the recurrence equation



$$P(s) = \sum_{s_1, s_2, s_3} P_1(s_1) P_2(s_2) P_3(s_3) e^{\beta(s_1 + s_2 + s_3)s} \frac{\omega(s)}{Z}$$

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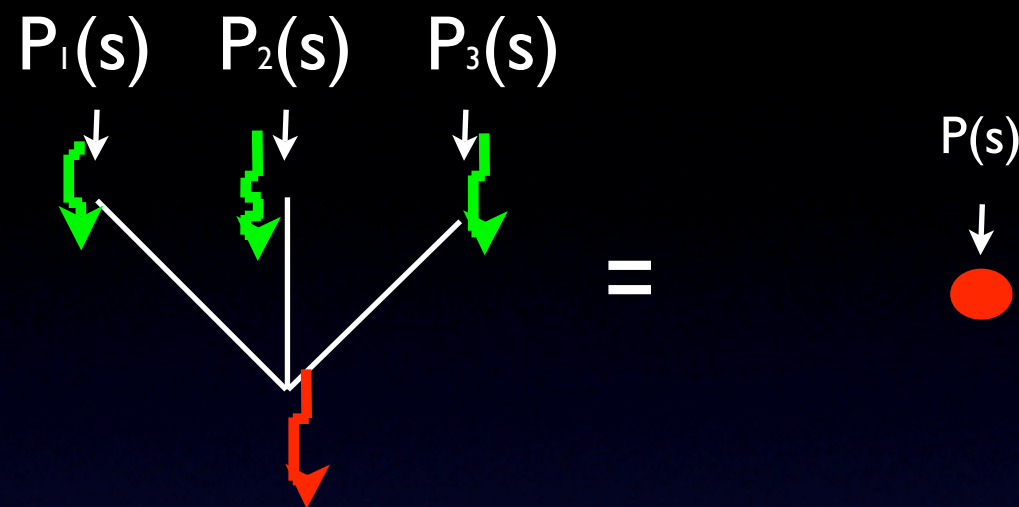


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Define the probability distribution
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$$\longrightarrow p(s|\mathbf{h}) = \frac{1}{Z(\mathbf{h})} \omega(s) e^{\beta \mathbf{h} s}$$

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Note $\mathbf{h} = s_1 + s_2 + s_3$ and rewrite the recursion as

$$P(s) = \sum_{s_1, s_2, s_3} P_1(s_1) P_2(s_2) P_3(s_3) p(s|s_1 + s_2 + s_3) \frac{Z(s_1 + s_2 + s_3)}{Z}$$

Solving the problem with Population Dynamics

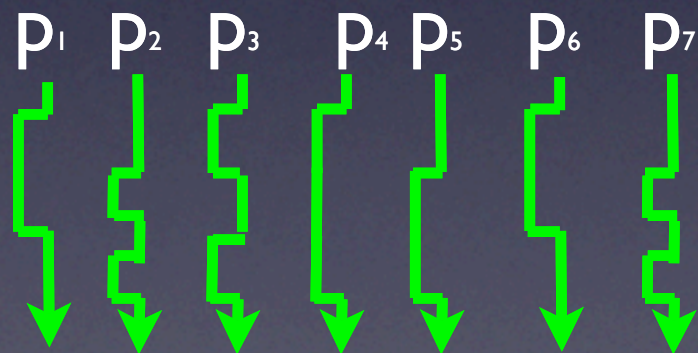
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Use the “population” representation :

$$P(s) = \sum_{i=1}^{\mathcal{N}} p_i \delta(s - \sigma_i)$$

Example for a population of 7 elements



Solving the problem with Population Dynamics

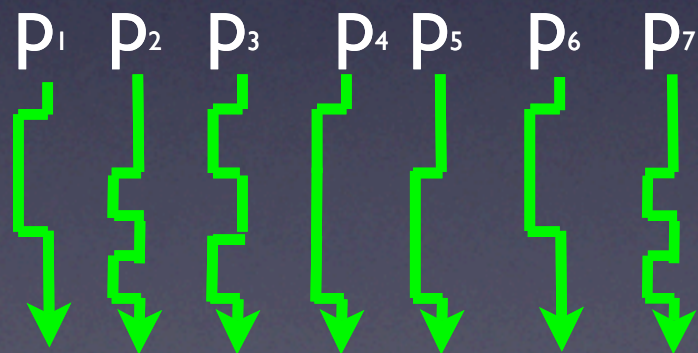
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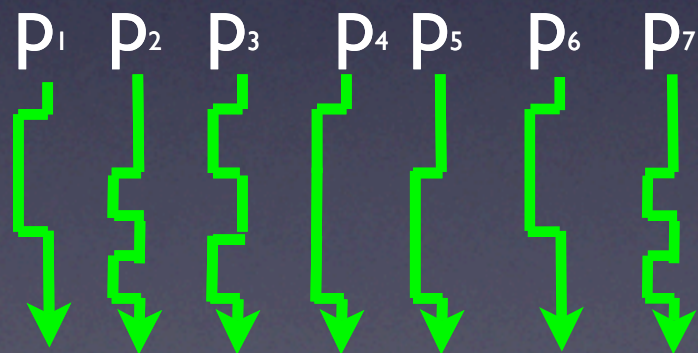
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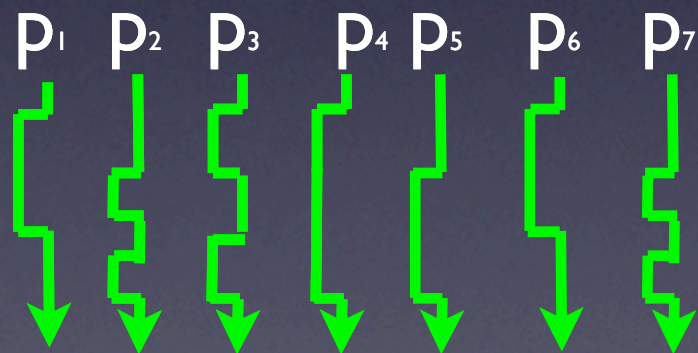
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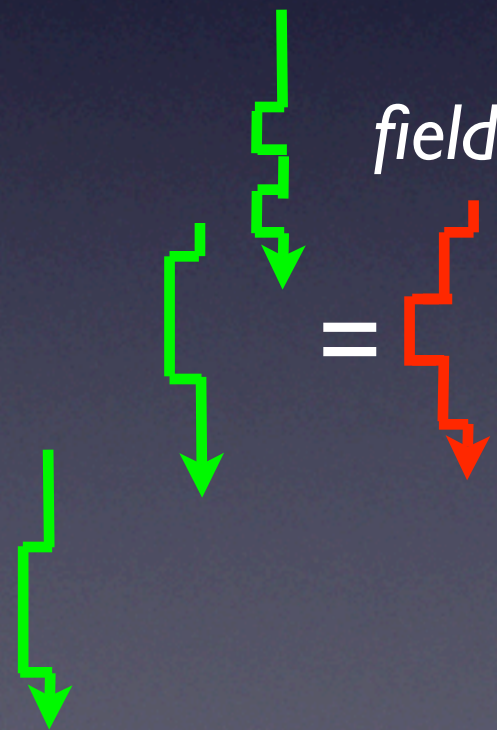
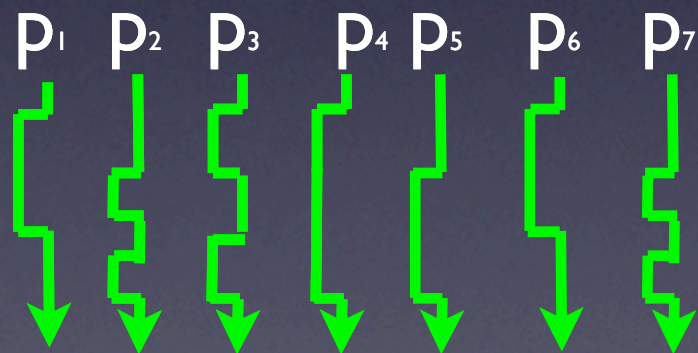
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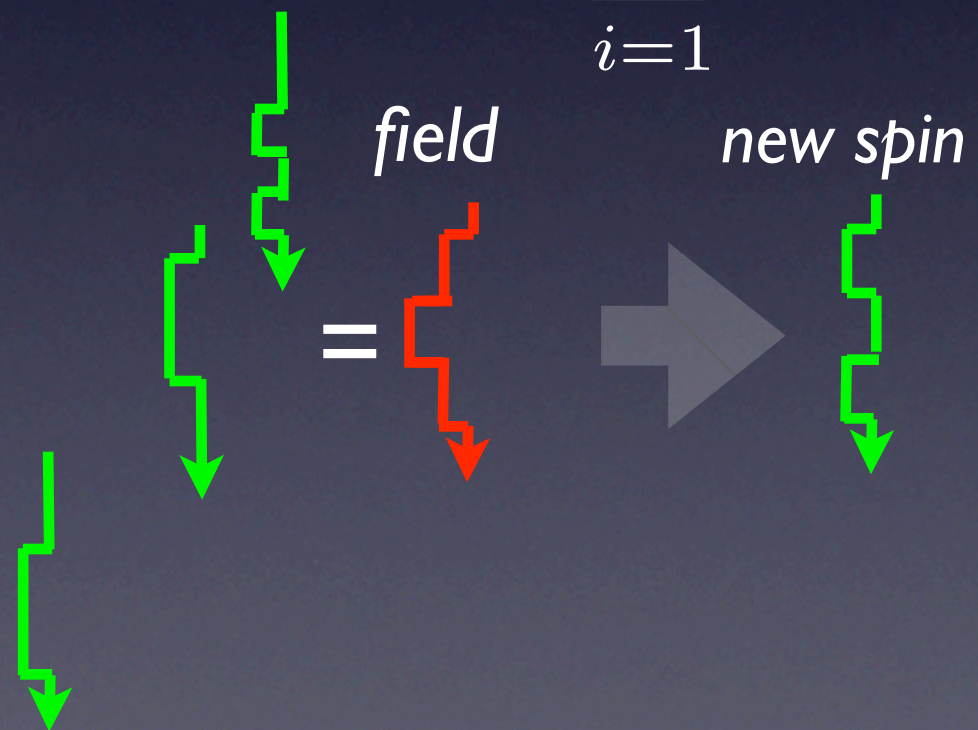
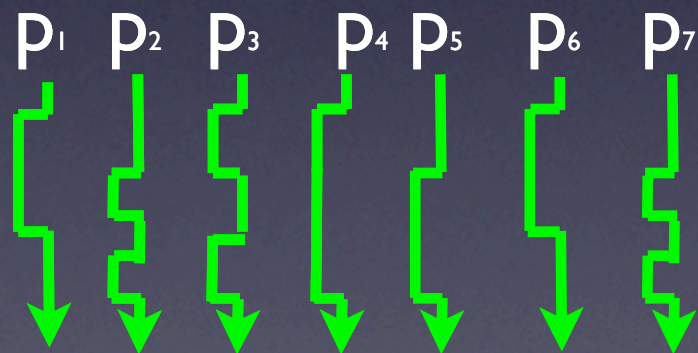
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Example for a population of 7 elements



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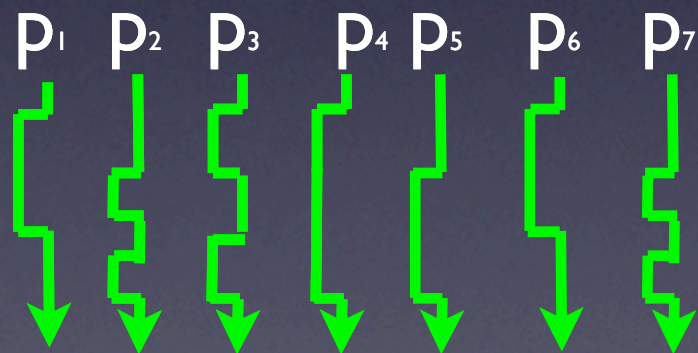
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Example for a population of 7 elements



new population



Solving the problem with Population Dynamics

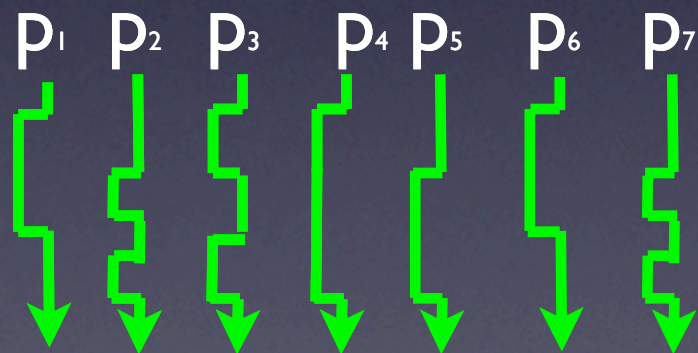
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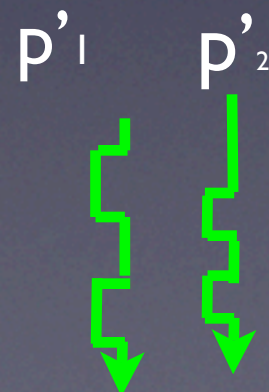
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Example for a population of 7 elements



new population



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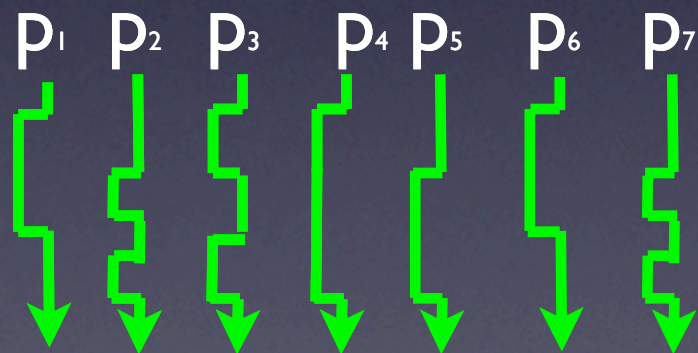
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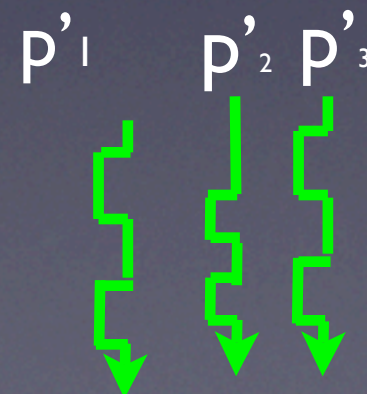
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Example for a population of 7 elements



new population



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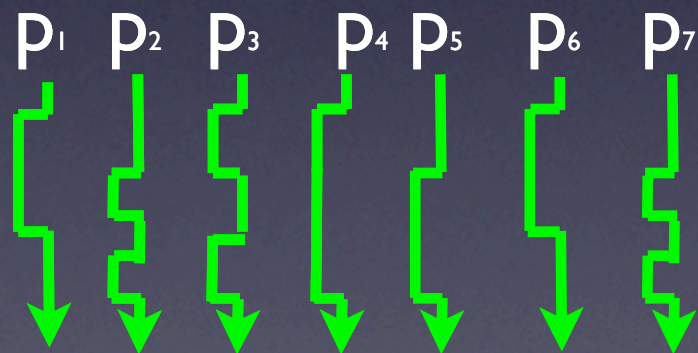
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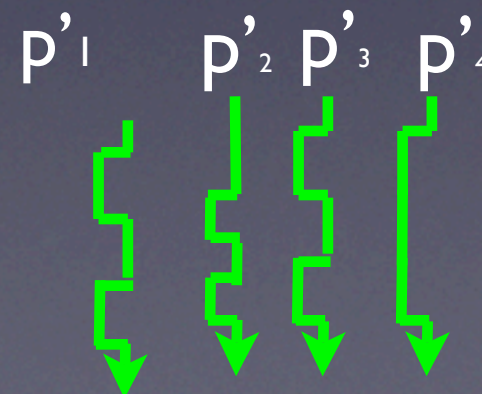
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Example for a population of 7 elements



new population



Solving the problem with Population Dynamics

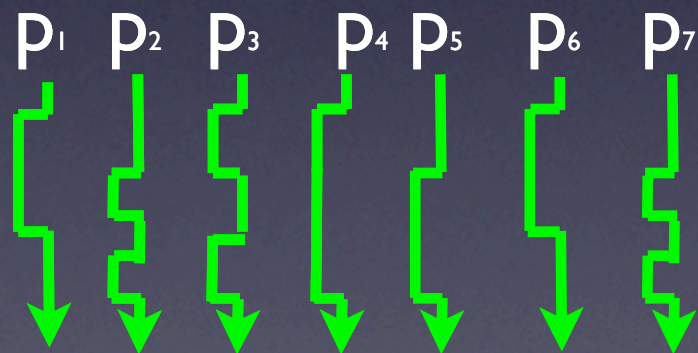
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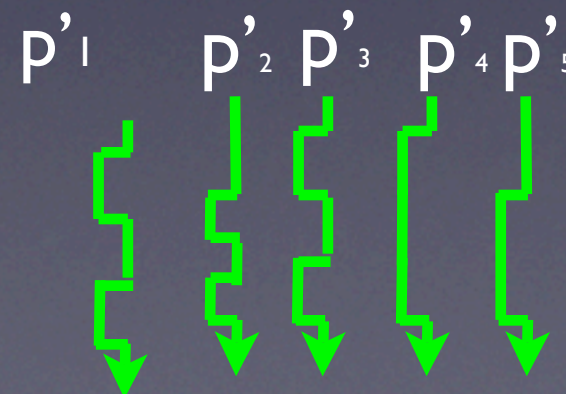
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Example for a population of 7 elements



new population



Solving the problem with Population Dynamics

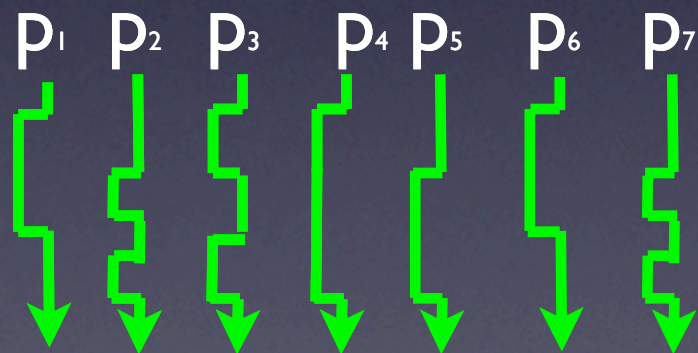
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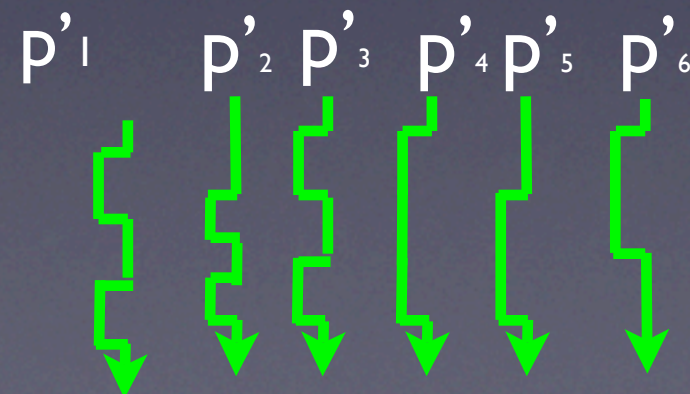
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Example for a population of 7 elements



new population



Solving the problem with Population Dynamics

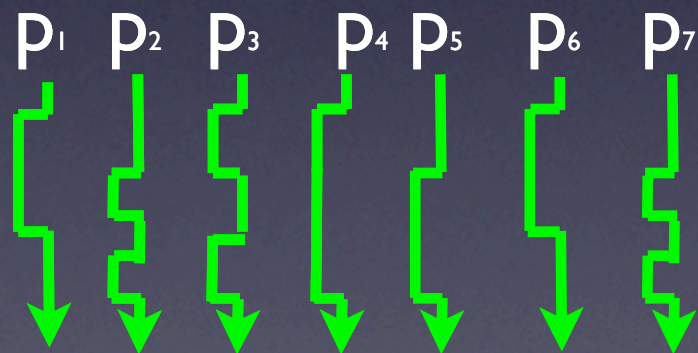
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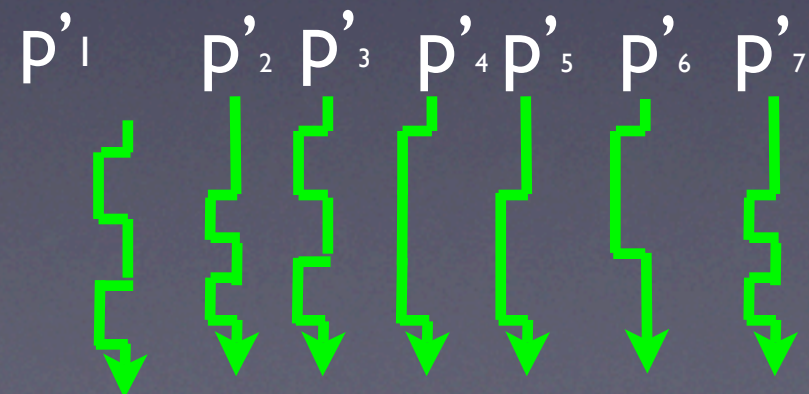
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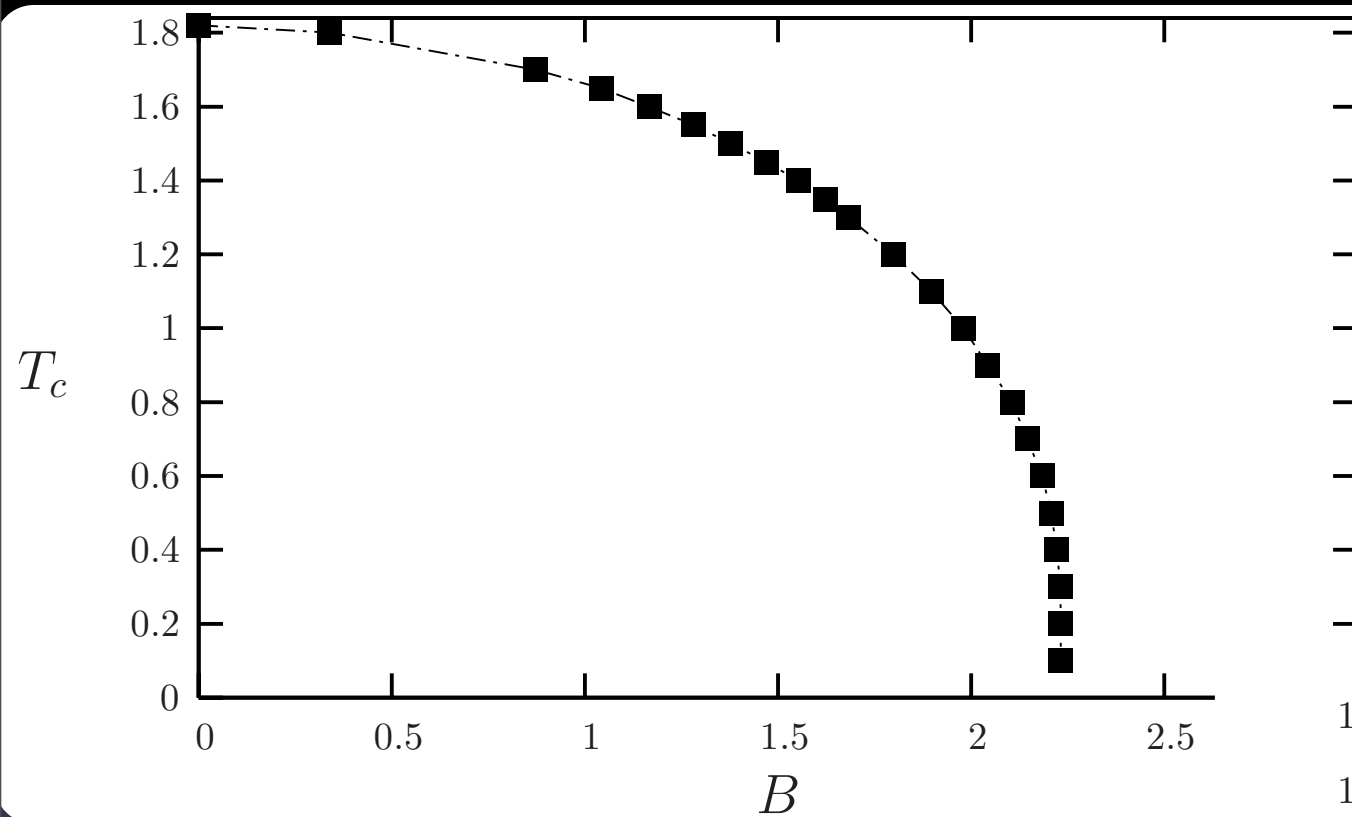


new population

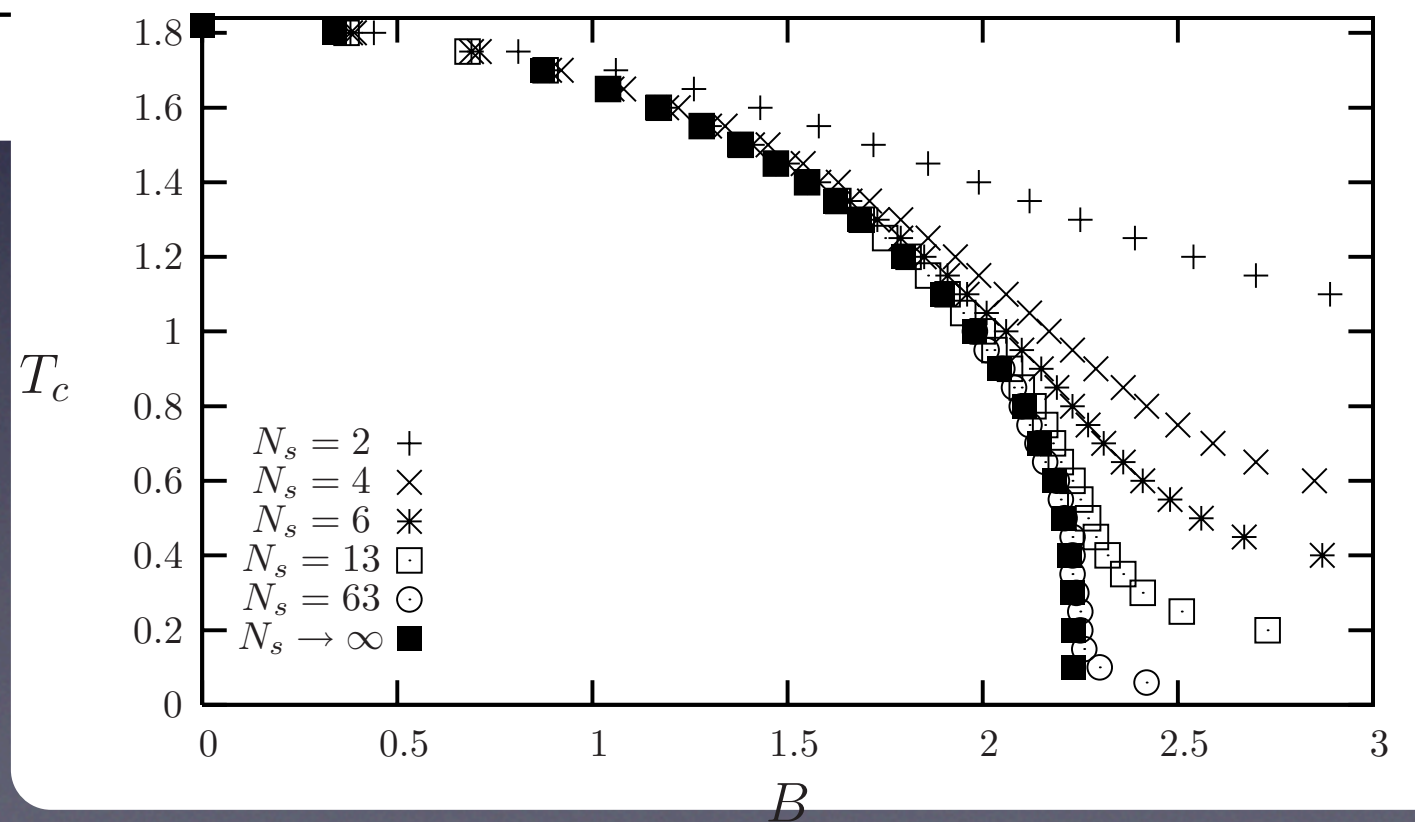


Some Results

Ising ferromagnet in transverse field on a random 3-regular graph

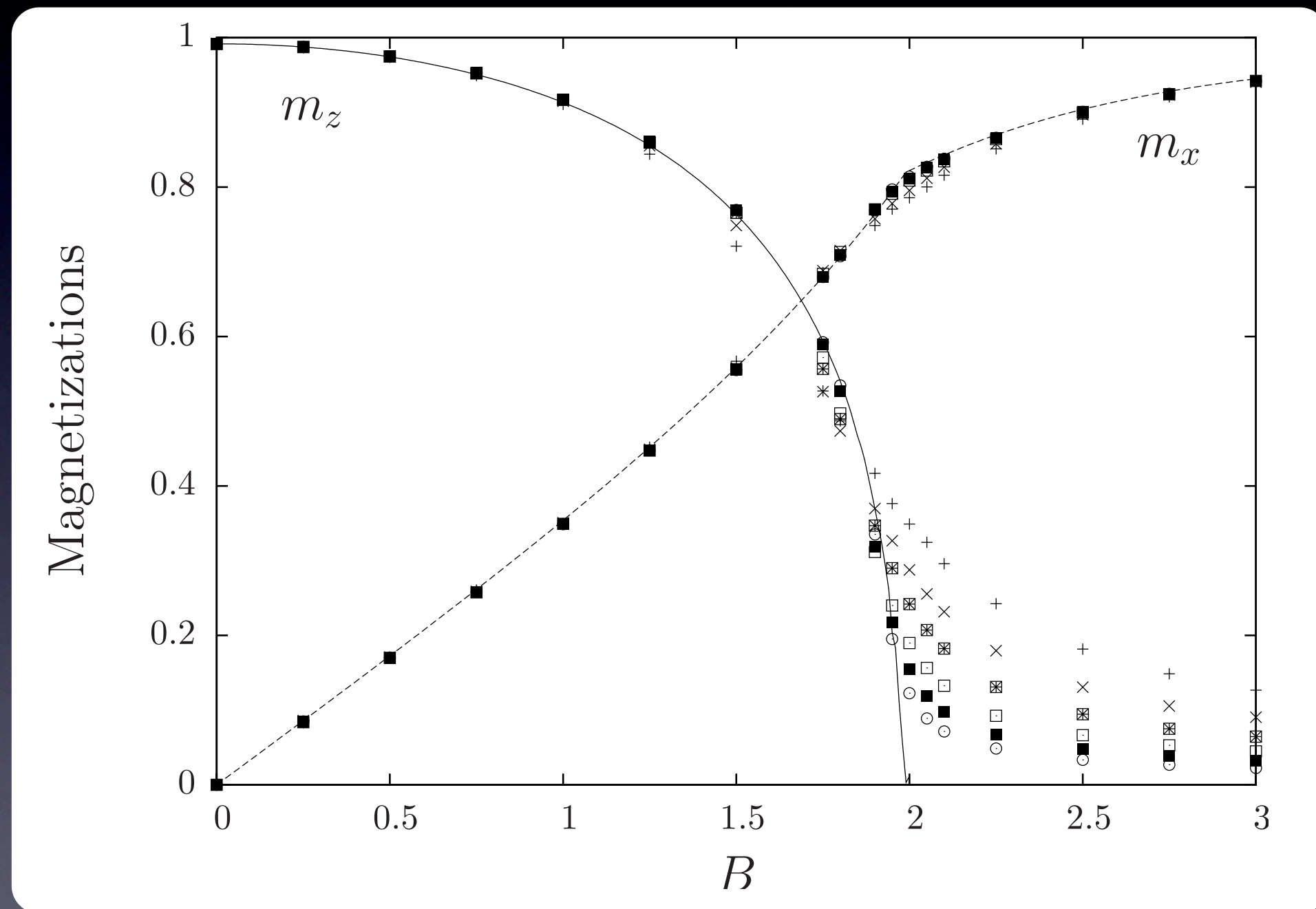


Versus ➡



Some Results

Ising ferromagnet in transverse field on a random 3-regular graph



$$T=1$$

Conclusions...

- A heat bath method for generic quantum spin-1/2 models in transverse field
- Allows to formulate a quantum version of the cavity method to solve the same models on trees (or more generally on random graphs)

... and perspectives

- Simulation of quantum spin-1/2 problem where no loop algorithm is known (Quantum Spin Glasses, Quantum Constraint Satisfaction Problems....)
- Application of the quantum cavity method to the same models on trees/random graphs
- Application to particles systems (Bosonic Hubbard model) e.g. to study glassy phases of cold atoms in disordered potentials
- Application to dynamics of classical models?

Thanks to my collaborators...

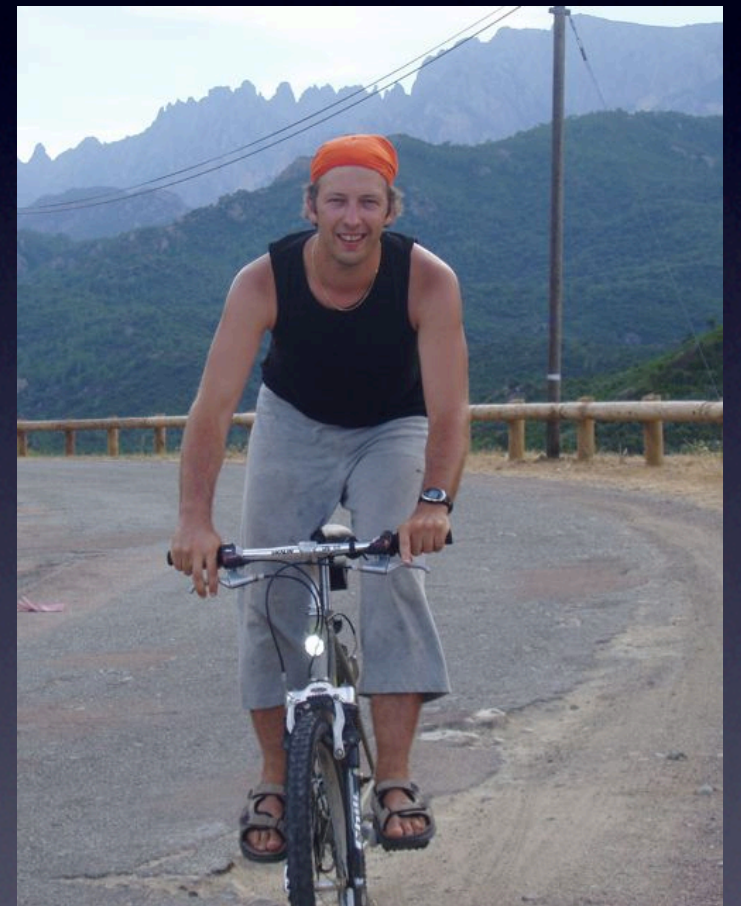
Guilhem Semerjian



Alberto Rosso



Florent Krzakala



...and to you for your attention!