JARA Jülich Aachen Research Alliance

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Monte Carlo Methods for Quantum Spin Models

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Outline

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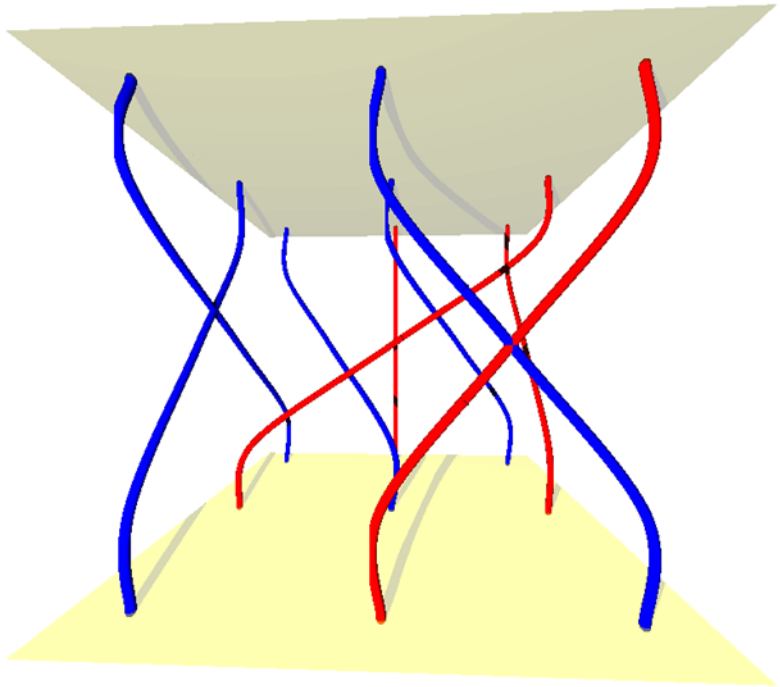
Overview
Review: classical Monte Carlo
World-line quantum Monte Carlo
Local and cluster updates (the loop algorithm)
Continuous-time formulation
Stochastic series expansion
Worms and directed loops
The sign problem



What can modern QMC algorithms do?

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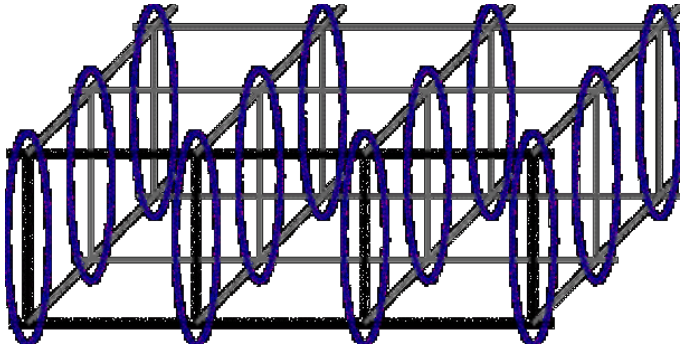
- Local updates (before 1994)
  - 200 spins
  - T/J=0.1
- Cluster algorithms (after 1995)
  - 2D quantum phase transition: 20’000 spins at T/J=0.005
  - 2D square lattice: 1’000’000 spins at T/J=0.2
- Extended ensemble methods (quantum Wang-Landau, parallel tempering)
  - Allow efficient simulations at 1st order (quantum) phase transitions
  - Determination of the free energy of a quantum system
- These algorithms allow
  - Accurate simulation of phase transitions in quantum systems
  - Quantitative modeling of many quantum magnets and bosonic systems

Example: quantum phase transition

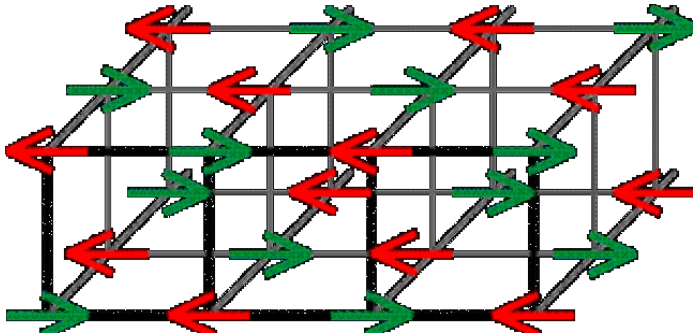
- Bilayer antiferromagnet

$$H = J \sum_{p=1}^{2} \sum_{<i,j>} \vec{S}_{i,p} \cdot \vec{S}_{j,p} + J_{\perp} \sum_{i} \vec{S}_{i,1} \cdot \vec{S}_{i,2}$$

$J << J_{\perp}$: spin gap, no long range order



$J >> J_{\perp}$: long range order



Quantum phase transition at $J_{\perp} / J \approx 2.522(2)$

Spin gap vanishes

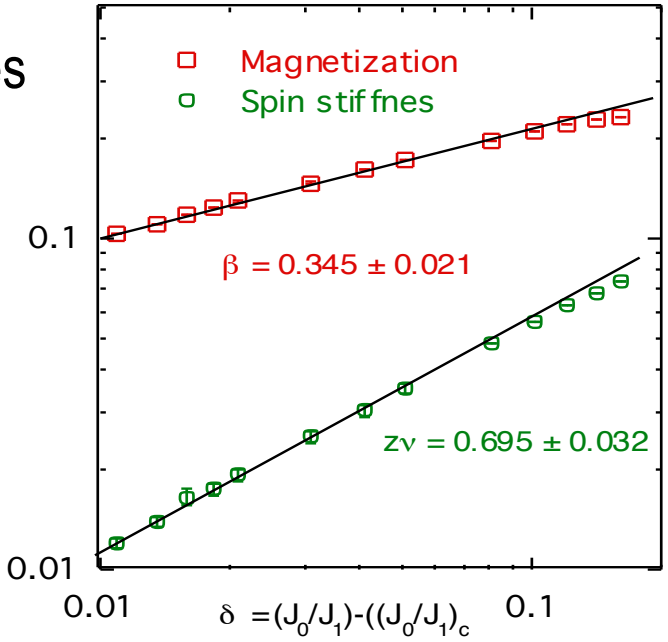
Magnetic order vanishes

Universal properties

Example: critical exponents

- 2D quantum phase transition in a quantum Heisenberg antiferromagnet
- Simulations of 20 000 spins at low temperatures
  Troyer, Imada and Ueda (1997)

Model	β	ν	η	z
QMC results no assumption	0.345 ± 0.025	0.685 ± 0.035	0.015 ± 0.020	1.018 ± 0.02
3D classical Heisenberg	0.3689 ± 0.0003	0.7112 ± 0.0005	0.0375 ± 0.0005	
Mean field	1/2	1	0	



- Wang, Beach Sandvik (2006): refined data analysis: $\nu = 0.7106(9)$
- More recent simulations with up to 1 million spins (Wessel et al., 2011).
- Consistent with classical 3D Heisenberg model exponents
- Can do quantum simulations with the same accuracy as classical

Review: classical Monte Carlo simulations

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- Want to calculate a thermal average

$$\langle A \rangle = \sum_c A_c e^{-\beta E_c} / Z \quad \text{with} \quad Z = \sum_c e^{-\beta E_c}$$

- Exponentially large number of configurations
  $\Rightarrow$ draw a representative statistical sample by importance sampling
  - Pick M configurations c_i with probability $p_{c_i} = e^{-\beta E_{c_i}} / Z$
  - Calculate statistical average $\langle A \rangle \approx \overline{A} = \frac{1}{M} \sum_{i=1}^{M} A_{c_i}$
  - Within a statistical error $\Delta A = \sqrt{(1 + 2\tau_A) \frac{\mathrm{Var}\, A}{M}}$

- Problem: we cannot calculate $p_{c_i} = e^{-\beta E_{c_i}} / Z$ since we do not know Z

Review: Markov chains and Metropolis

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- Metropolis algorithm builds a Markov chain

$$c_1 \rightarrow c_2 \rightarrow \ldots \rightarrow c_i \rightarrow c_{i+1} \rightarrow \ldots$$

- Transition probabilities $W_{x,y}$ for transition $x \rightarrow y$ need to fulfill
  - Ergodicity: any configuration reachable from any other

$$\forall x,y \; \exists n \; : \; \left(W^n\right)_{x,y} \neq 0$$

  - Detailed balance:

$$\frac{W_{x,y}}{W_{y,x}} = \frac{p_y}{p_x}$$

- Simple algorithm due to Metropolis et al (1953): $W_{x,y} = \min[1, p_y / p_x]$
- Needs only relative probabilities (energy differences) $p_y / p_x = e^{-\beta(E_y - E_x)}$

Metropolis Algorithm: 60th birthday

- General formulation of the method
- Application: 2D hard-spheres

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

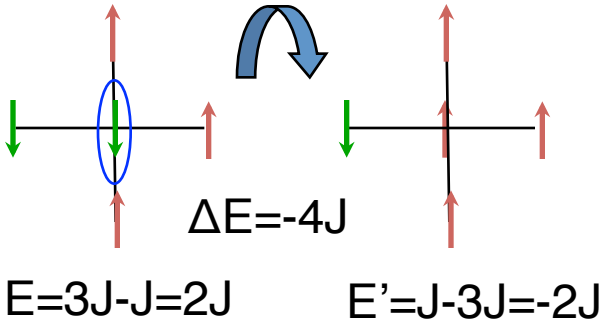
I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed,

II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† con-

Single spin-flip Metropolis algorithm



- Here is the algorithm:
  - Start with a random configuration *c*
  - Repeat the following many times:
    - Randomly pick a spin
    - Propose to flip that single spin, leading to a new configurations *c'*
    - Calculate the energy difference $\Delta E = E[c'] - E[c]$
    - If $\Delta E < 0$, the next configuration is *c'*
      If $\Delta E > 0$, accept *c'* with a probability $\exp(-\beta \Delta E)$, otherwise keep *c*
    - Measure all quantities of interest
- This algorithm is ergodic
- It fulfills detailed balance
- Before taking measurements, need to equilibrate (thermalization)

Quantum Monte Carlo

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- Not as "easy" as classical Monte Carlo

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_c e^{-\beta E_c}$$

- Calculating the energy eigenvalue E_c is equivalent to solving the problem

- Employ a mapping of the quantum partition function to an effective classical statistics problem

$$Z = \mathrm{Tr}\, e^{-\beta H} \equiv \sum_c p_c$$

- Different approaches
  - World-lines via Trotter-Suzuki formula
  - Path integrals (time-dependent perturbation theory in imaginary time)
  - Stochastic Series Expansion (high temperature expansion)
  - ...

- Sign problem if some $p_c < 0$ (thus try to avoid this)

- Then, need efficient updates for the effective classical problem

Hamiltonian of spin-1/2 models

- Example: two sites
  - Anisotropic exchange interactions J_{xy}, J_z
  - Magnetic field h

$$H_{XXZ} = J_{xy}(S_1^x S_2^x + S_1^y S_2^y) + J_z S_1^z S_2^z - h\left(S_1^z + S_2^z\right)$$

$$= \frac{J_{xy}}{2}(S_1^+ S_2^- + S_1^- S_2^+) + J_z S_1^z S_2^z - h\left(S_1^z + S_2^z\right)$$

  - Heisenberg model: $J_{xy} = J_z = J$

$$H = J\vec{S}_1\vec{S}_2 - h\left(S_1^z + S_2^z\right)$$

- Hamiltonian matrix in 2-site basis

$$\left\{ \left|\uparrow\uparrow\right\rangle, \left|\uparrow\downarrow\right\rangle, \left|\downarrow\uparrow\right\rangle, \left|\downarrow\downarrow\right\rangle \right\}$$

$$H_{XXZ} = \begin{pmatrix} \frac{J_z}{4} + h & 0 & 0 & 0 \\ 0 & -\frac{J_z}{4} & \frac{J_{xy}}{2} & 0 \\ 0 & \frac{J_{xy}}{2} & -\frac{J_z}{4} & 0 \\ 0 & 0 & 0 & \frac{J_z}{4} - h \end{pmatrix}$$

The world-line approach

- Representation based on mapping a quantum spin-1/2 system onto a classical Ising-like model

Progress of Theoretical Physics, Vol. 56, No. 5, November 1976

Relationship between d-Dimensional Quantal Spin Systems and $(d+1)$-Dimensional Ising Systems

——Equivalence, Critical Exponents and Systematic Approximants of the Partition Function and Spin Correlations——

Masuo SUZUKI

Department of Physics, University of Tokyo, Tokyo 113

(Received May 29, 1976)

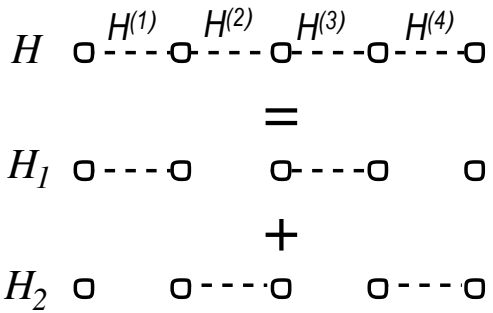
The partition function of a quantal spin system is expressed by that of the Ising model, on the basis of the generalized Trotter formula. Thereby the ground state of the d-dimensional Ising model with a transverse field is proven to be equivalent to the $(d+1)$-dimensional Ising model at finite temperatures. A general relationship is established between the two partition functions of a general quantal spin system and the corresponding Ising model with many-spin interactions, which yields some rigorous results on quantum systems. Some applications are given.

The Trotter-Suzuki decomposition

- Generic mapping of a quantum spin system onto a classical model
- Split Hamiltonian into two easily diagonalizable pieces

$$H = H_1 + H_2$$

$$e^{-\varepsilon H} = e^{-\varepsilon(H_1+H_2)} = e^{-\varepsilon H_1} e^{-\varepsilon H_2} + O(\varepsilon^2)$$



- Obtain a decomposition of the partition function

$$Z = \mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr}\, e^{-\beta(H_1+H_2)} = \lim_{M\to\infty} \mathrm{Tr}[(e^{-\Delta\tau(H_1+H_2)})^M] \quad (\Delta\tau = \beta/M)$$

$$= \mathrm{Tr}[(e^{-\Delta\tau H_1} e^{-\Delta\tau H_2})^M] + O(\Delta\tau^2)$$

- Insert sets of complete basis states between operators

$$= \sum_{i_1,\ldots,i_{2M}} \langle i_1 | e^{-\Delta\tau H_1} | i_{2M} \rangle \langle i_{2M} | e^{-\Delta\tau H_2} | i_{2M-1} \rangle \cdots \langle i_3 | e^{-\Delta\tau H_1} | i_2 \rangle \langle i_2 | e^{-\Delta\tau H_2} | i_1 \rangle$$

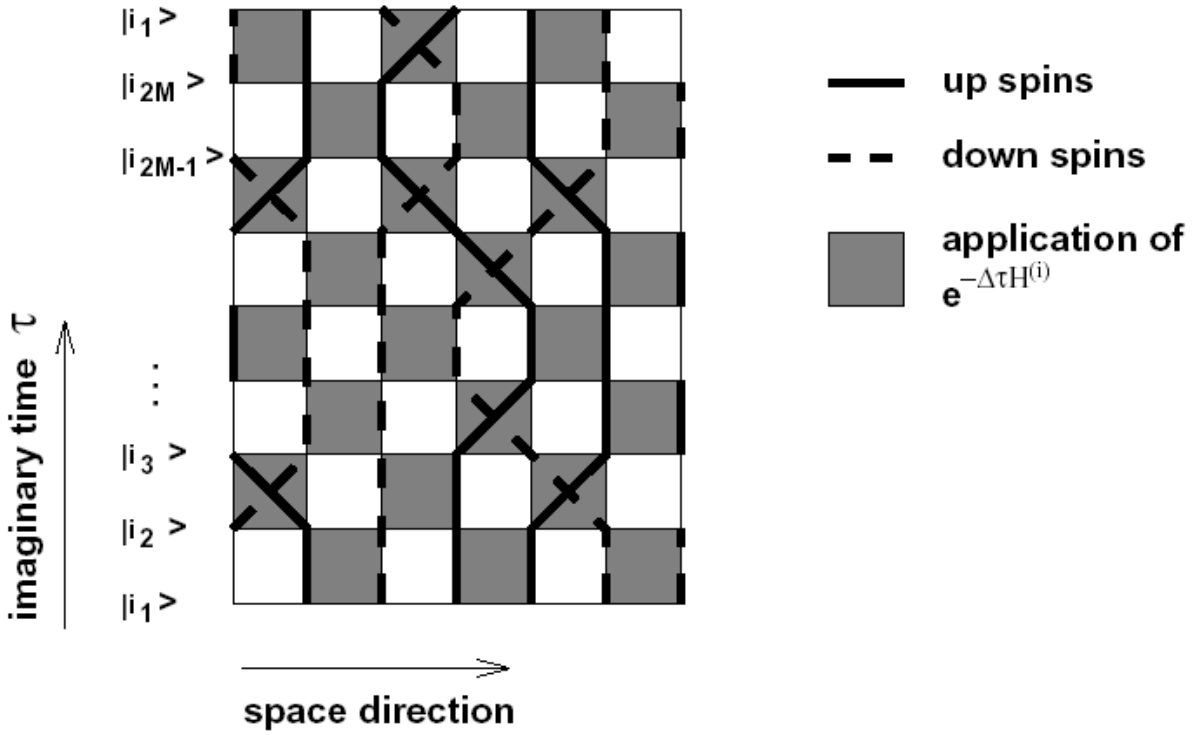
Example: Spin-1/2 Heisenberg model

Quantum problem in *d* dimensions maps onto a classical problem in *d+1*

- Expand the states $|i_\alpha\rangle$ in the S^z eigenbasis
- Effective Ising-model in d+1 dimensions with 2- and 4-sites interaction terms

$$Z = \sum_{i_1,\ldots,i_{2M}} \langle i_1 | e^{-\Delta\tau H_1} | i_{2M} \rangle \langle i_{2M} | e^{-\Delta\tau H_2} | i_{2M-1} \rangle \cdots \langle i_3 | e^{-\Delta\tau H_1} | i_2 \rangle \langle i_2 | e^{-\Delta\tau H_2} | i_1 \rangle$$

- Each of the matrix elements $\langle i_{j+1} | e^{-\Delta\tau H_{1,2}} | i_j \rangle$ corresponds to a row of shaded plaquettes and contribution to Z equals the product over those plaquettes



The weights for the Heisenberg model

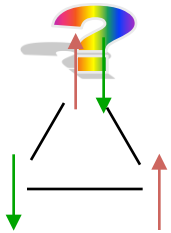
- The partition function becomes a sum of products of plaquette weights

$$Z = \sum_C W(C) = \sum_C \prod_{plaquettes\ p} w(C_p)$$

- Conservation of magnetization on each bond
- The only allowed plaquette-configurations are:

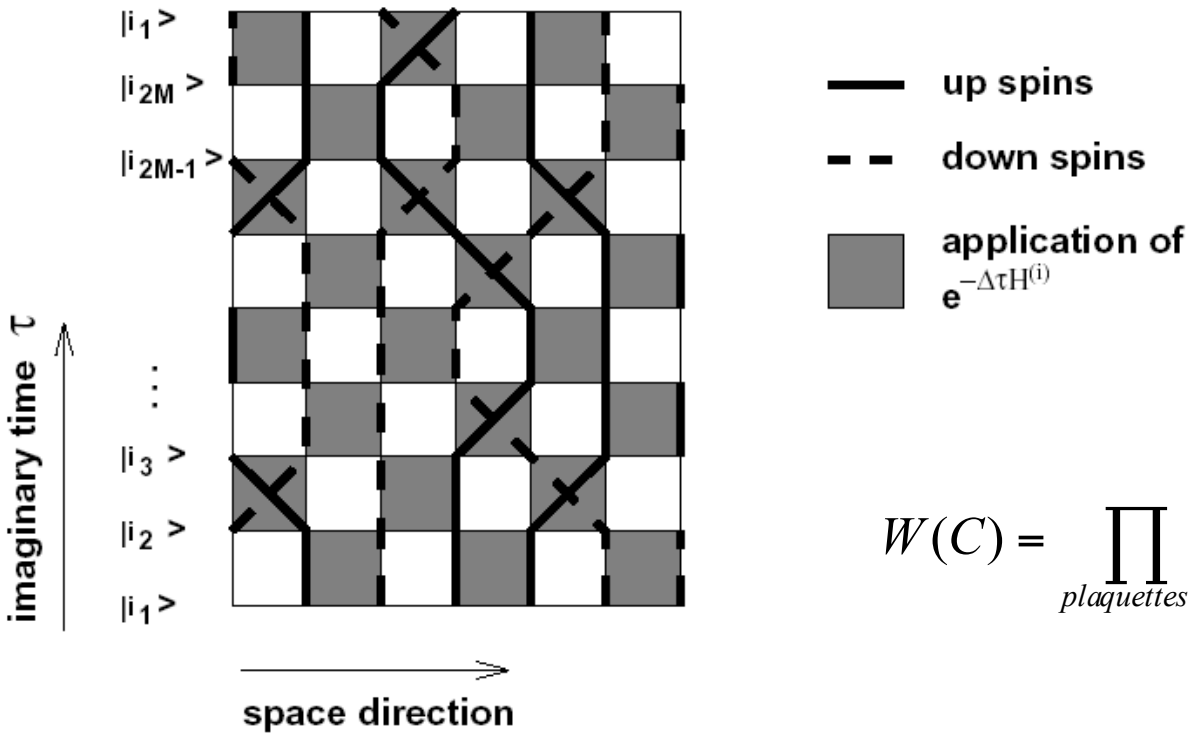
$\mathcal{C}_p$			
$w(\mathcal{C}_p)$	$e^{-\Delta\tau J/4}$	$e^{\Delta\tau J/4}\cosh(\Delta\tau J/2)$	$e^{\Delta\tau J/4}\sinh(-\Delta\tau J/2)$

- Ferromagnetic (J<0)
  - All weights are positive
- Antiferromagnetic on a bipartite lattice
  - trace requires an even number of spin-flip terms, so that overall sign vanish, and can be ignored
- Frustrated antiferromagnet:
  - we have a sign problem (see later)



World-lines

- Each valid configuration is represented by *continuous* world-lines



$$W(C) = \prod_{plaquettes\ p} w(C_p)$$

- Sampling over all (important) world-line configurations
  - According to the above weight
  - Try to generate a new configurations from a given one

Local updates

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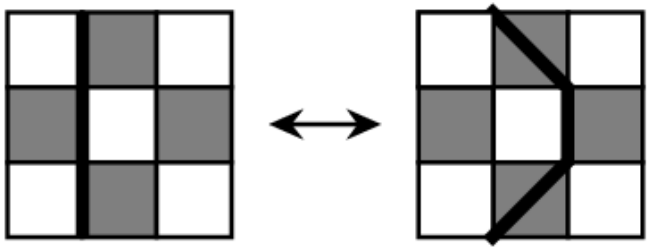
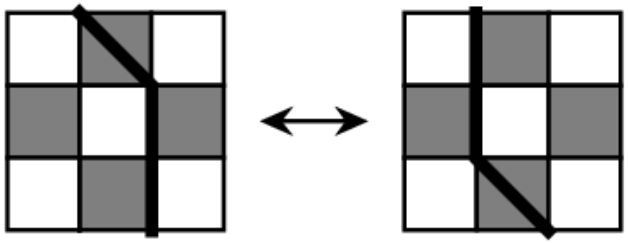
- Move the world-lines locally using Metropolis

  Acceptance probabilities given by the resulting plaquette weights

- Example moves:
  - Insert or remove two “kinks”



  - Shift a single “kink”



Beyond local updates

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- Problems with local updates:
  - Restricted to canonical ensemble
  - No change of magnetization (particle number), winding number
  - Critical slowing down near phase transitions
- Solution for classical Monte Carlo: cluster algorithms
  - R. H. Swendsen and J. S. Wang PRL (1987)
  - U. Wolff, PRL (1989)
- Try the same for the quantum case
  - Loop algorithm by H.G. Evertz, G. Lana and M. Marcu, PRL (1993)
  - Worm algorithm, operator loops, directed loops, ...

Cluster-updates in classical Monte Carlo

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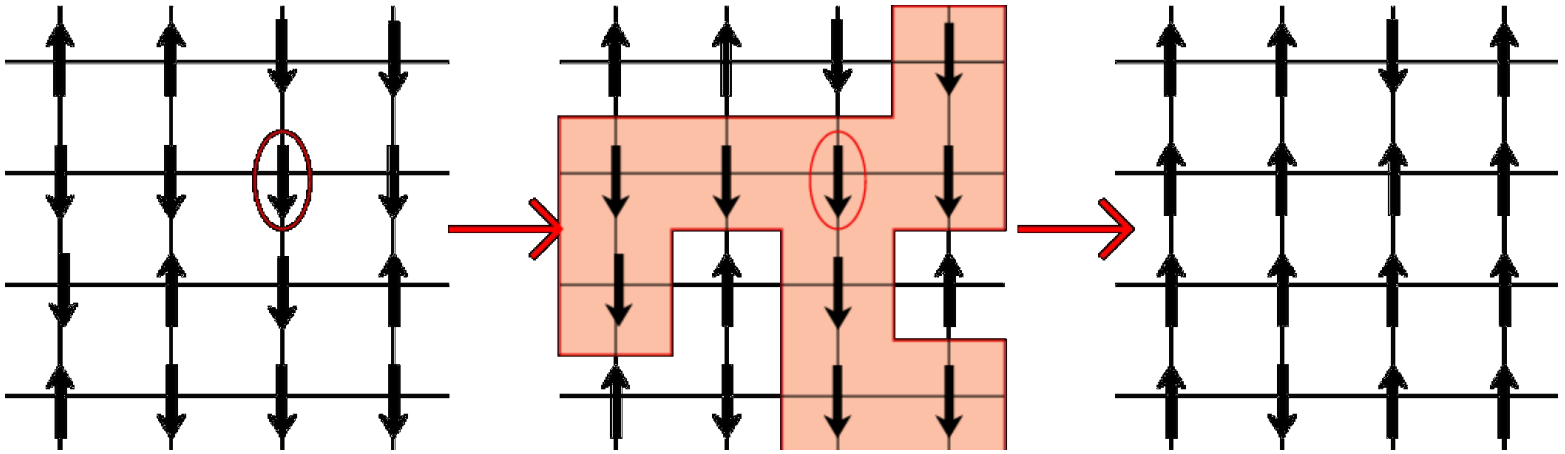
- Ask for each spin: "do we want to flip it against a neighbor?"
  - antiparallel: yes
  - parallel: costs energy
    - Accept with $P = \exp(-2\beta J)$
    - Otherwise: also flip neighbor! $P = 1 - \exp(-2\beta J)$
    - Repeat for all flipped spins => cluster updates



- No more severe critical slowing down!

Cluster algorithms: Formal description

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Extend the phase space (Kandel-Domany framework)

– From configurations C to configurations + graphs (C,G)

$$Z = \sum_C W(C) = \sum_C \sum_G W(C,G) \text{ with } W(C) = \sum_G W(C,G)$$

Ising model:
C: spins
G: clusters

Choose graph weights independent of configuration

$$W(C,G) = \Delta(C,G)V(G) \text{ where } \Delta(C,G) = \begin{cases} 1 & \text{graph } G \text{ allowed for } C \\ 0 & \text{otherwise} \end{cases}$$

Perform updates

2. Discard configuration

4. Discard graph

$$C_i \rightarrow (C_i,G) \rightarrow G \rightarrow (C_{i+1},G) \rightarrow C_{i+1}$$

1. Pick a graph G with $P[G] = \frac{V(G)}{W(C)}$

3. Pick any allowed new configuration

Detailed balance is then assured

Cluster algorithms: The Ising model

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- We need to find $\Delta(C,G)$ and $V(G)$ that fulfill
  - Do this on the local (bond) level

$$W(C) = \sum_G W(C,G) = \sum_G \Delta(C,G) V(G)$$

$\Delta(C,G)$	**o-o**	**o o**	$W(C)$
$\uparrow\uparrow, \downarrow\downarrow$	1	1	$e^{+\beta J}$
$\uparrow\downarrow, \downarrow\uparrow$	0	1	$e^{-\beta J}$
$V(G)$	$e^{+\beta J} - e^{-\beta J}$	$e^{-\beta J}$	

- This means for:

$$C_i \rightarrow (C_i, G) \rightarrow G$$

  - Parallel spins: pick connected graph **o-o** with

$$P(\ \textbf{o-o}\ ) = \frac{e^{+\beta J} - e^{-\beta J}}{e^{+\beta J}} = 1 - e^{-2\beta J}$$

  - Antiparallel spins: always pick open graph **o o**

- And for:

$$G \rightarrow (C_{i+1}, G) \rightarrow C_{i+1}$$

  - Configuration must be allowed $\Rightarrow$ connected spins must be parallel

$\Rightarrow$ connected spins flipped as one cluster

The loop algorithm

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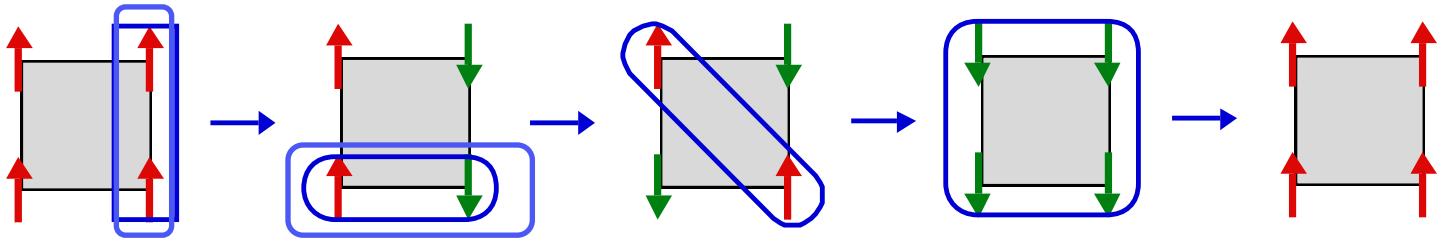
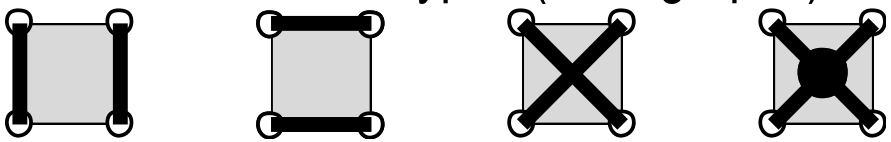
- Classical Swendsen-Wang cluster algorithm for the Ising model
  - two choices on each bond: connected or disconnected

  - all connected spins are flipped together

- Loop algorithm is a generalization to quantum systems
  - world lines must not be broken
  - always 2 or 4 spins on a plaquette must be flipped together



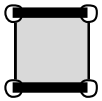
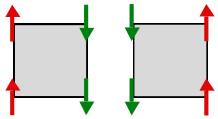
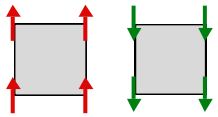
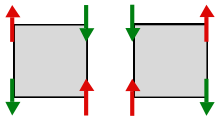
  - four different connection types (local graphs)



Local graphs - Heisenberg limit

$$H_{\text{Heisenberg}} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$W(C) = \sum_G W(C,G) = \sum_G \Delta(C,G) V(G)$$

$\Delta(C,G)$			$W(C)$
	1	1	$1+ (J/4)\,\Delta\tau$
	1	0	$1-(J/4)\,\Delta\tau$
	0	1	$(J/2)\,\Delta\tau$
$V(G)$	$1-(J/4)\,\Delta\tau$	$(J/2)\,\Delta\tau$	

- Here, we give the expression in the small $\Delta\tau/J$ limit, relevant for later discussion
- Connected spins form a cluster and have to be flipped together

Global loop update

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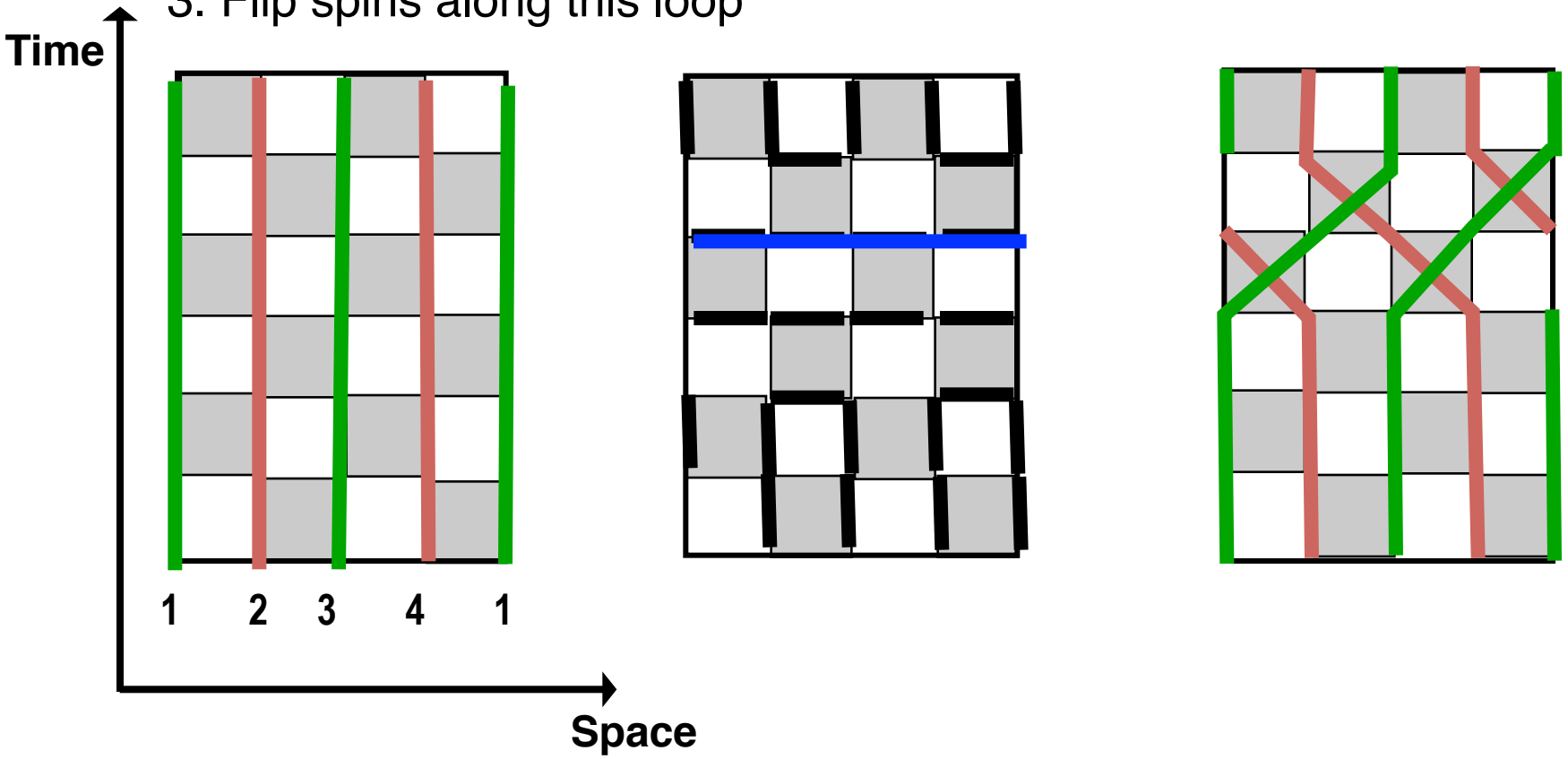
Example of a single loop flip

1. Choose breakups on each plaquette
2. Pick a loop
3. Flip spins along this loop

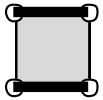
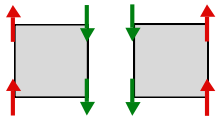
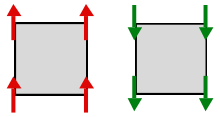
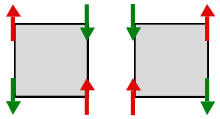


Easy plane antiferromagnet

$$H_{XXZ} = \frac{J_{xz}}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z$$

with $0 \le J_z \le J_{xy}$

$$W(C) = \sum_G W(C,G) = \sum_G \Delta(C,G) V(G)$$

$\Delta(C,G)$				$W(C)$
	1	1	0	$1+ (J_z/4)\ \Delta\tau$
	1	0	0	$1-(J_z/4)\ \Delta\tau$
	0	1	1	$(J_{xy}/2)\ \Delta\tau$
$V(G)$	$1-(J_z/4)\Delta\tau$	$(J_z/2)\ \Delta\tau$	$(J_{xy}- J_z)/2\ \Delta\tau$	

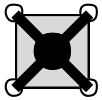
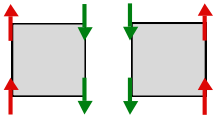
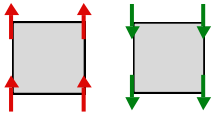
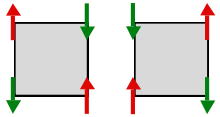
- Connected spins form a cluster and have to be flipped together

Ising-like ferromagnet

$$H_{XXZ} = -\frac{J_{xz}}{2}\sum_{\langle i,j\rangle}(S_i^+ S_j^- + S_i^- S_j^+) - J_z \sum_{\langle i,j\rangle} S_i^z S_j^z$$

with $0 \le J_{xy} \le J_z$

$$W(C) = \sum_G W(C,G) = \sum_G \Delta(C,G) V(G)$$

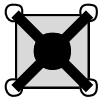
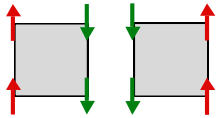
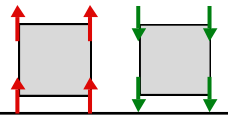
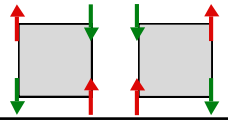
$\Delta(C,G)$				$W(C)$
	1	0	0	$1 - (J_z/4)\,\Delta\tau$
	1	1	1	$1 + (J_z/4)\,\Delta\tau$
	0	1	0	$(J_{xy}/2)\,\Delta\tau$
$V(G)$	$1-(J_z/4)\Delta\tau$	$(J_{xy}/2)\,\Delta\tau$	$(J_z-J_{xy})/2\,\Delta\tau$	

- Now 4-spin freezing graph is needed for $J_{xy} \neq J_z$
  - Connects (freezes) loops

The Ising limit

$$H_{\text{Ising}} = -J\sum_{\langle i,j\rangle} S_i^z S_j^z = -\frac{J}{4}\sum_{\langle i,j\rangle}\sigma_i\sigma_j$$

$$W(C) = \sum_G W(C,G) = \sum_G \Delta(C,G)V(G)$$

$\Delta(C,G)$			$W(C)$
	1	0	1- $(J/4)\,\Delta\tau$
	1	1	1+ $(J/4)\,\Delta\tau$
	0	0	0
$V(G)$	1-$(J/4)\,\Delta\tau$	$(J/2)\,\Delta\tau$	

$$(\Delta\tau = \beta / M)$$

- Two spins are frozen, if there is any freezing graph along the world line

  We recover the Swendsen Wang algorithm: probability for no freezing

$$P_{\text{no freezing}} = \lim_{M\to\infty}(1-(\beta/M)J/2)^M = \exp(-\beta J/2) = \exp(-2\beta J_{classical})$$

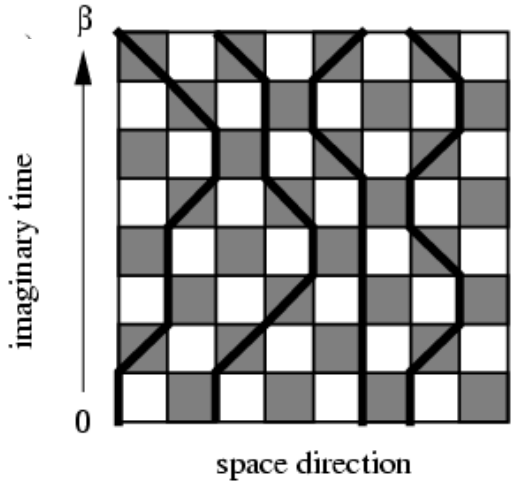
The continuous time limit

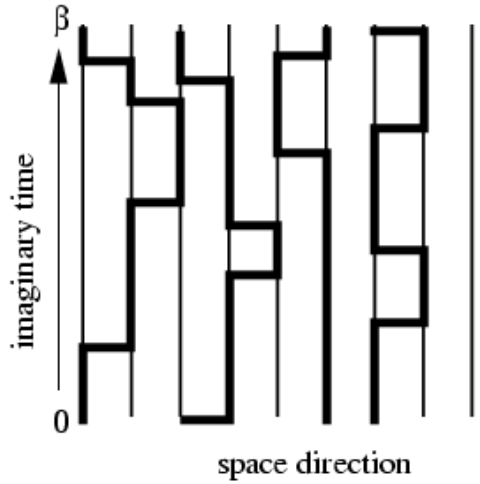
- Systematic error due to finite value of $\Delta\tau$ ("Trotter error")
  - Need to perform an extrapolation to $\Delta\tau \to 0$ from simulations with different values of $\Delta\tau$ (or Trotter number *M*) $(\Delta\tau = \beta / M)$
- The limit $\Delta\tau \to 0$ can be taken in the construction of the algorithm! (Prokof'ev , Svistunov, Tupitsyn, 1996; Beard, Wiese, 1996)
  - Number of changes

$$N_c = M\frac{\Delta\tau J}{2} \to \frac{\beta J}{2}$$

stays finite as

$$\Delta\tau \to 0$$

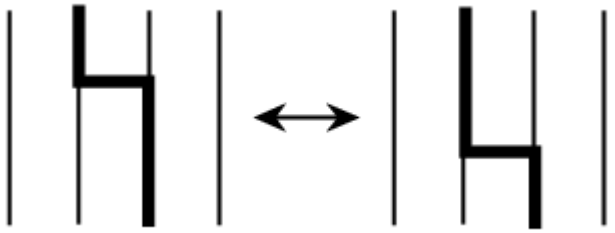




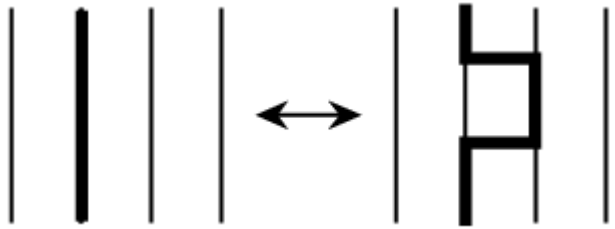
- Different computational approach:
  - Discrete time: store configuration at all time steps
  - Continuous time: store times at which configuration *changes (kinks)*

Local updates in continuous time

- Shift a kink



- Insert or remove two kinks (kink-antikink pair creation process)



$$P = 1 \qquad P = (\Delta\tau\, J/2)^2 \to 0$$

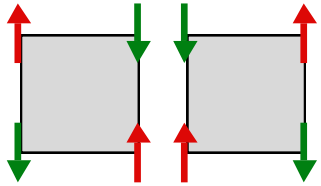
– Vanishing acceptance rate: $P_{\to} = \min[1, (\Delta\tau\, J/2)^2] \to 0$

– Solution: Integrate over all possible insertion within a finite time window

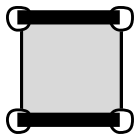
$$P_{\to} = \int_0^{\Lambda}\int_{\tau_1}^{\Lambda} (J/2)^2 d\tau_2 d\tau_1 \to \frac{\Lambda^2 J^2}{8} \neq 0$$

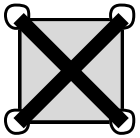
Cluster updates in the continuum limit

- How do we deal with the vanishing $\Delta\tau$ terms in continuous time?
- First example: the exchange process



  - Possible graph connections:





  - Graph weights:

$$\frac{J_z}{2}\Delta\tau \qquad \frac{J_{xy}-J_z}{2}\Delta\tau$$

  - Probability to pick graph: (divide weight by sum)

$$\frac{J_z}{J_{xy}} \qquad \frac{J_{xy}-J_z}{J_{xy}}$$

- The infinitesimal $\Delta\tau$ terms cancel out
  - Randomly pick one of the graphs (with appropriate probabilities) for each exchange process (kink)

Cluster updates in the continuum limit

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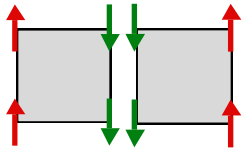
- How do we deal with the vanishing $\Delta\tau$ terms in continuous time?
- Second example: the "decay" process



  - Possible graph connections:

  - Graph weights:

$$1-\frac{J_z}{4}\Delta\tau \qquad \frac{J_z}{2}\Delta\tau$$

  - Probability to pick graph: (divide weight by sum)

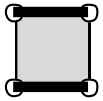
$$1-\frac{J_z}{2}\Delta\tau \qquad \frac{J_z}{2}\Delta\tau$$

- The infinitesimal $\Delta\tau$ terms remain
  - How can we deal with them?
  - Infinitesimal acceptance rate at infinitely many time steps?

Cluster updates in the continuum limit

- How do we deal with the vanishing $\Delta\tau$ terms in continuous time?
- Probabilities:

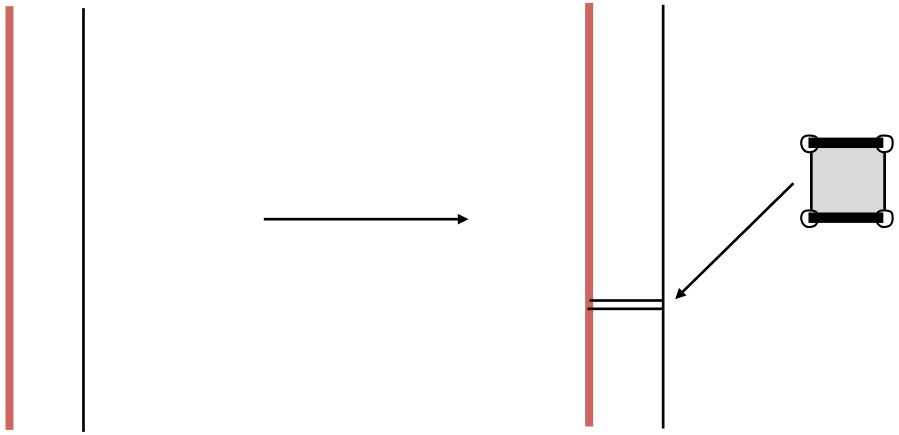
$$1-\frac{J_z}{2}\Delta\tau$$



$$\frac{J_z}{2}\Delta\tau$$

- Solution: reinterpret the  graph as a "decay process" with a decay constant $J_z/2$
  - Graph is  except at certain "decay times" determined like in the radioactive decay by an exponential distribution using

$$\tau = -\frac{2}{J_z}\ln(1-r) \quad \text{with} \quad r \in [0,1]$$



Loop updates in continuum time

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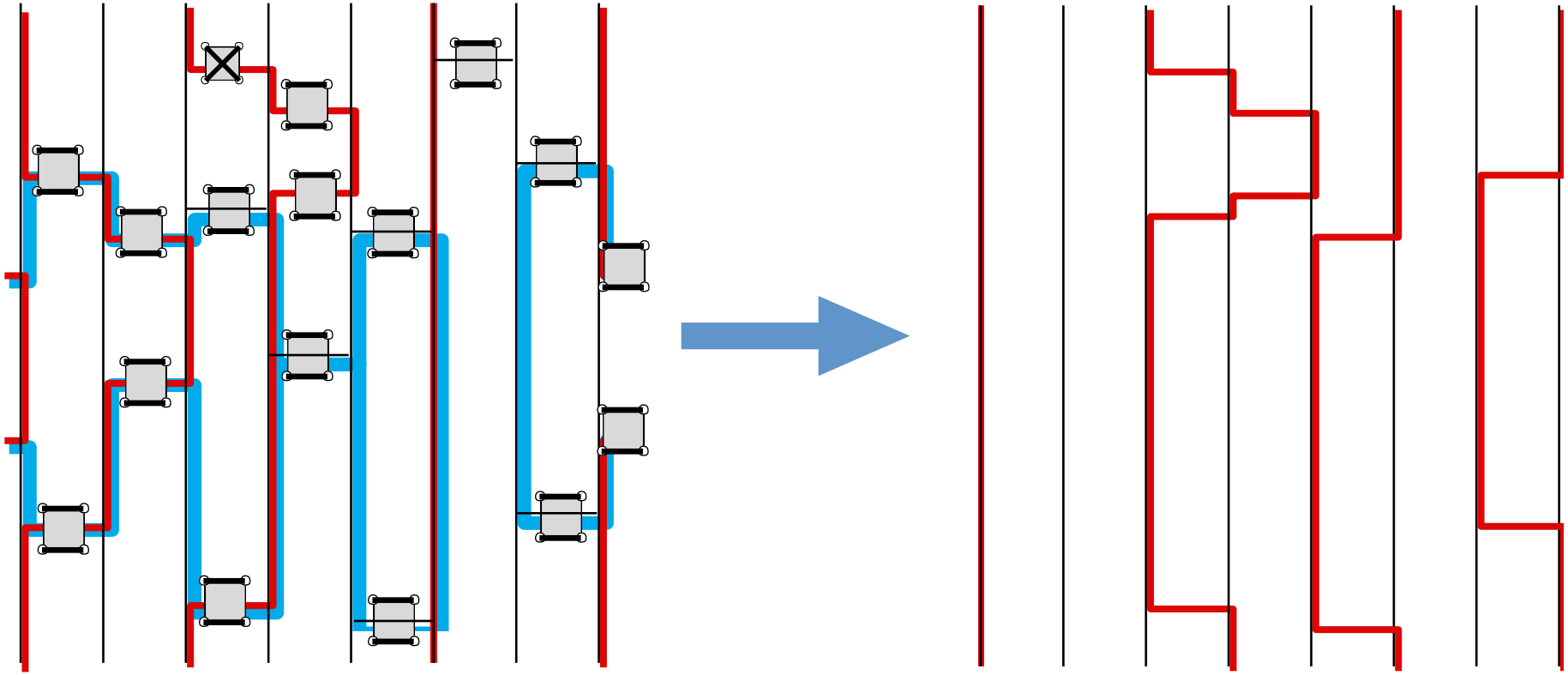
1. Define “breakups” (graphs) for exchange processes
2. Insert “decay” graphs
3. Build and flip one or more loops



Path integral representation

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- Based on the perturbation expansion of the path integral

Exact quantum Monte Carlo process for the statistics of discrete systems

N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn
Kurchatov Institute Russian Science Center, 123182 Moscow, Russia

(Submitted 20 November 1996)
Pis'ma Zh. Éksp. Teor. Fiz. **64**, No. 12, 853–858 (25 December 1996)

We propose an exact Monte Carlo approach for the statistics of discrete quantum systems that does not employ the standard partition of the imaginary time into a mesh and does not contain small parameters. The method operates with discrete objects — kinks, describing virtual transitions at different moments in time. The global statistics of the kinks is reproduced by exact local procedures, the main one being based on the known solution for an asymmetric two-level system. © *1996 American Institute of Physics.* [S0021-3640(96)00824-9]

PACS numbers: 46.10.+2, 0270.Lq, 03.20.+i

- Equivalent to continuous time representation
- Discrete local objects (kinks, changes in word-line configuration)
- Local updates of kinks using Metropolis
- Improved update scheme using worm update (Prokofev et al., 1997)

Path integral representation

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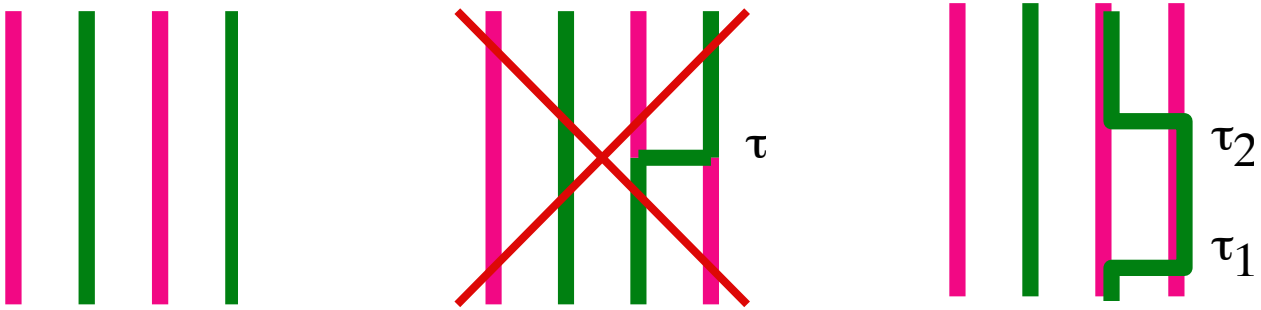
Perturbation expansion:

$$H = H_0 + V, \quad H_0 = \sum_{<i,j>} J_{ij}^z S_i^z S_j^z - \sum_i h S_i^z, \quad V = \sum_{<i,j>} J_{ij}^{xy} (S_i^x S_j^x + S_i^y S_j^y)$$

$$Z = \mathrm{Tr}(e^{-\beta H}) = \mathrm{Tr}(e^{-\beta H_0} \mathrm{T} e^{-\int_0^\beta d\tau V(\tau)}), \qquad V(\tau) = e^{\tau H_0} V e^{-\tau H_0}$$

$$Z = \mathrm{Tr}(e^{-\beta H_0} (1 - \int_0^\beta d\tau V(\tau) + \int_0^\beta d\tau_2 \int_0^{\tau_2} d\tau_1 V(\tau_2) V(\tau_1) + \ldots))$$

Each term represented by a world line configuration



Stochastic series expansion (SSE)

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- Based on a high temperature series expansion of the partition function

PHYSICAL REVIEW B VOLUME 43, NUMBER 7 1 MARCH 1991

Quantum Monte Carlo simulation method for spin systems

Anders W. Sandvik* and Juhani Kurkijärvi
Department of Physics, Åbo Akademi, Porthansgatan 3-5, SF-20500 Åbo, Finland
(Received 29 June 1990)

A quantum Monte Carlo simulation scheme for spin systems is presented. The method is a generalization of Handscomb's method but applicable to any length of the spin, i.e., when the spin traces cannot be evaluated analytically. The Monte Carlo sampling is extended to the space of spin vectors in addition to the usual operator-index sequences. An important technical point is that the index sequences are augmented with the aid of unit operators to a constant, self-consistently determined length. The scheme is applied to the one-dimensional antiferromagnetic spin-S Heisenberg model. Results at low temperatures are reported for $S=1$ and $S=\frac{3}{2}$ and system sizes up to $N=64$. The computed magnetic structure factor in the $S=1$ chain is in agreement with earlier ground-state calculations. For $S=\frac{3}{2}$ we find the exponent $\overline{\gamma}=0.49\pm0.04$ for the divergence of the antiferromagnetic structure factor. Further, the susceptibility as a function of the wave number is computed. For $S=1$ the staggered susceptibility $\chi(\pi)$ at $T=0$ is found to take the value 20.0 ± 1.5 in units such that $\chi(q)\rightarrow T^{-1}$ at high temperatures (with the temperature scale defined by $k_B=1$). For $S=\frac{3}{2}$ we obtain the exponent $\gamma=1.45\pm0.05$ for the divergence of the staggered susceptibility.

- Original formulation based on local updates using Metropolis
- Cluster updates using the operator loop update (Sandvik 1999)
- Improved updates using directed loops
  (Syljuåsen and Sandvik 2002; Alet, Wessel, Troyer 2005)

Hamiltonian decomposition

- Break up the Hamiltonian into offdiagonal and diagonal bond terms

$$H = \sum_{\langle i,j \rangle} H^o_{(i,j)} + H^d_{(i,j)}$$

- Example: Heisenberg antiferromagnet

$$H_{XXZ} = \frac{J_{xy}}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z - h \sum_i S_1^z$$

convert site terms into bond terms

$$= \frac{J_{xy}}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z - \frac{h}{z} \sum_{\langle i,j \rangle} \left(S_i^z + S_j^z \right)$$

$$= \sum_{\langle i,j \rangle} H^o_{(i,j)} + \sum_{\langle i,j \rangle} H^d_{(i,j)}$$

split into diagonal and offdiagonal bond terms

with $$H^o_{(i,j)} = \frac{J_{xy}}{2} (S_i^+ S_j^- + S_i^- S_j^+)$$

$$H^d_{(i,j)} = J_z S_i^z S_j^z - \frac{h}{z} \left(S_i^z + S_j^z \right)$$

High temperature series expansion

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- Expansion in inverse temperature

$$Z = \mathrm{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \mathrm{Tr}(-H^n)$$

$$= \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{|\alpha\rangle} \sum_{(b_1,\ldots,b_n)} \langle \alpha | \prod_{i=1}^{n} (-H_{b_i}) | \alpha \rangle$$

- Using the bond Hamiltonians

$$H_{b_i} \in \bigcup_{\langle i,j \rangle} \left\{ H^d_{(i,j)}, H^o_{(i,j)} \right\}$$

Ensuring positive weights

- SSE expansion:

$$Z = \sum_{n=0}^{\infty} \sum_{|\alpha\rangle} \sum_{(b_1,\ldots,b_n)} \frac{\beta^n}{n!} \langle \alpha | \prod_{i=1}^{n} (-H_{b_i}) | \alpha \rangle$$

$$= \sum_{n=0}^{\infty} \sum_{|\alpha\rangle} \sum_{(b_1,\ldots,b_n)} W\left(|\alpha\rangle, (b_1,\ldots,b_n)\right)$$

- Negative matrix elements are the bond weights
  - Need to make all matrix elements non-positive
  - Diagonal matrix elements: subtract an energy shift
    - Does not change the physics

$$H^d_{(i,j)} = J_z S^z_i S^z_j - \frac{h}{z}\left(S^z_i + S^z_j\right) - C \qquad C \geq \left|\frac{J_z}{4}\right| + |h|$$

Positivity of off-diagonal bond weights

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- Energy shift will not help with off-diagonal matrix elements

$$H^{o}_{(i,j)} = \frac{J_{xy}}{2}(S^{+}_{i}S^{-}_{j} + S^{-}_{i}S^{+}_{j})$$

- Ferromagnet ($J_{xy} < 0$)
  - no problem on any lattice(!)
- Antiferromagnet on a bipartite lattice
  - no problem as well: need an EVEN number of exchange terms to recover starting state: sign of allowed configurations is positive!
- Frustrated antiferromagnet:
  - we have a sign problem, similar to the world-line approach!

Fixed length operator strings

- SSE sampling requires variable length n operator strings

$$Z = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{|\alpha\rangle} \sum_{(b_1,\ldots,b_n)} \langle \alpha | \prod_{i=1}^{n} (-H_{b_i}) | \alpha \rangle \qquad H_{b_i} \in \bigcup_{\langle i,j \rangle} \left\{ H^d_{(i,j)}, H^o_{(i,j)} \right\}$$

- Extend operator string to fixed length Λ by adding extra unit operators:

$$H_{id} = -1$$

n: number of non-unit operators

$$Z = \sum_{n=0}^{\Lambda} \sum_{|\alpha\rangle} \sum_{(b_1,\ldots,b_\Lambda)} \frac{(\Lambda - n)! \beta^n}{\Lambda!} \langle \alpha | \prod_{i=1}^{\Lambda} (-H_{b_i}) | \alpha \rangle \qquad H_{b_i} \in \{H_{id}\} \cup \bigcup_{\langle i,j \rangle} \left\{ H^d_{(i,j)}, H^o_{(i,j)} \right\}$$

- Ensure Λ large enough during thermalization
  - Such that e.g. $n_{\max} < \frac{4}{3}\Lambda$ $\qquad n_{\max} > \langle n \rangle \propto \beta V$

The SSE configuration space

- Each SSE configuration is given by a initial state and a fixed length operator string

$$Z = \sum_{|\alpha\rangle} \sum_{S_\Lambda} \frac{(\Lambda - n)!\beta^n}{\Lambda!} \langle \alpha | \prod_{i=1}^{\Lambda} (-H_{b_i}) | \alpha \rangle$$

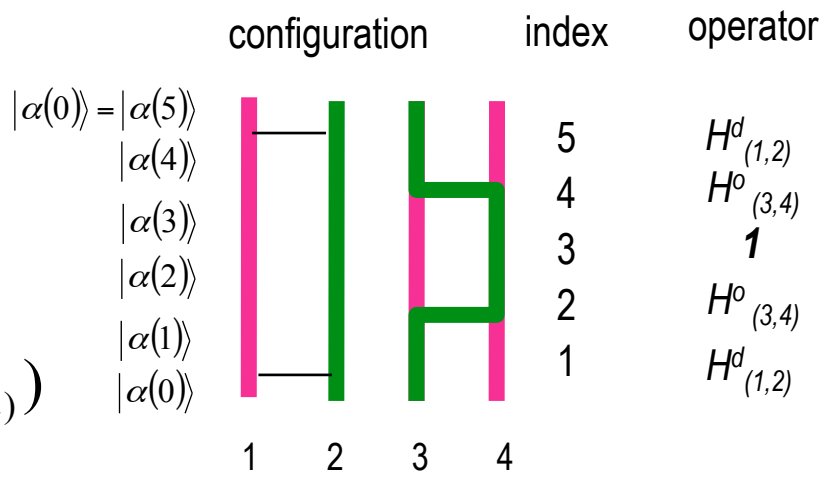
- Example for a four site problem:

$\Lambda = 5$

$n = 4$

$|\alpha\rangle = |\downarrow\uparrow\uparrow\downarrow\rangle$

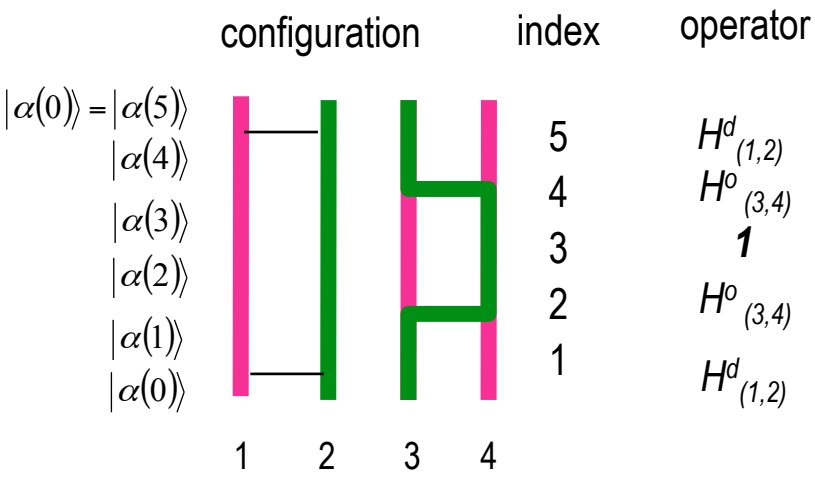
$S_\Lambda = (H^d_{(1,2)}, H^o_{(3,4)}, 1, H^o_{(3,4)}, H^d_{(1,2)})$



- Now we need efficient update schemes

Measurements in SSE

- Some observables are very simple:
  - Energy: $E = \langle H \rangle = -\frac{1}{\beta}\langle n \rangle$
  - Specific Heat: $C_V = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle$
  - Uniform Susceptibility: $\chi = \beta \left\langle \langle \alpha | \sum_i S_i^z | \alpha \rangle^2 \right\rangle$



- Some look a bit more involved:
  - Equal time diagonal correlations:

$$\langle D_1 D_2 \rangle = \left\langle \frac{1}{n+1} \sum_{p=0}^{n} d_2[p] d_1[p] \right\rangle, \quad \text{where} \quad d_i[p] = \langle \alpha(p) | D_i | \alpha(p) \rangle$$

  - Imaginary time depended diagonal correlations:

$$\langle D_1(\tau) D_2(0) \rangle = \left\langle \sum_{\Delta p=0}^{n} \binom{n}{\Delta p} \left(\frac{\tau}{\beta}\right)^{\Delta p} \left(1 - \frac{\tau}{\beta}\right)^{n-\Delta p} C_{12}(\Delta p) \right\rangle, \quad C_{12}(\Delta p) = \frac{1}{n+1} \sum_{p=0}^{n} d_1[p+\Delta p] d_2[p]$$

Comparing path integrals and SSE

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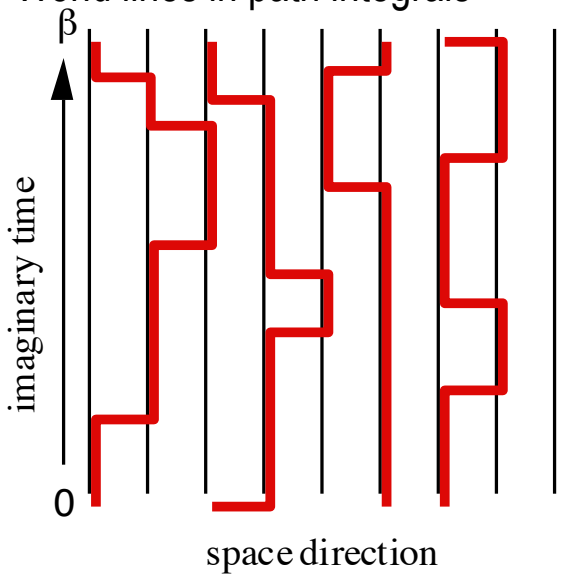
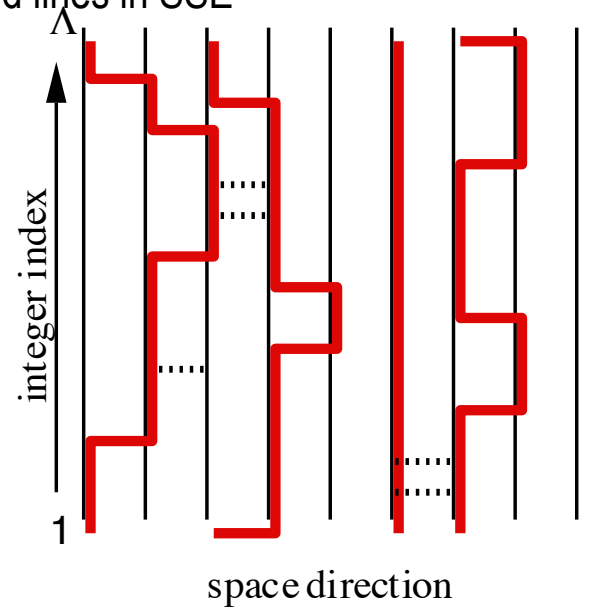
- World lines in path integrals



- Advantage
  - Diagonal terms treated exactly
- Disadvantage
  - Continuous imaginary time

- World lines in SSE



- Disadvantage
  - Perturbation also in diagonal terms
- Advantage
  - Integer index instead of time

Diagonal updates

- Recall the weight of a configuration:

$$Z = \sum_{|\alpha\rangle} \sum_{S_\Lambda} \frac{(\Lambda - n)!\beta^n}{\Lambda!} \langle \alpha | \prod_{i=1}^{\Lambda} (-H_{b_i}) | \alpha \rangle$$

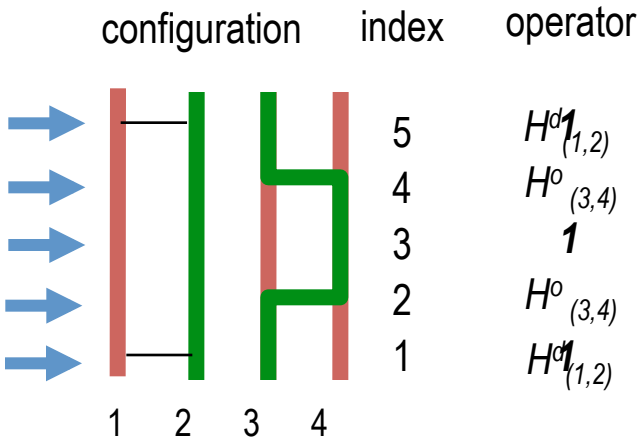
- Walk through operator string
  - Propose to insert diagonal operators instead of unit operators

$$P[1 \to H^d_{(i,j)}] = \min\left(1, \frac{\beta N_{bonds} \langle \alpha | H^d_{(i,j)} | \alpha \rangle}{\Lambda - n}\right)$$

  - Propose to remove diagonal operators

$$P[H^d_{(i,j)} \to 1] = \min\left(1, \frac{\Lambda - n + 1}{\beta N_{bonds} \langle \alpha | H^d_{(i,j)} | \alpha \rangle}\right)$$

- Changes the expansion order
- Does not touch the off-diagonal operators nor the state vector



Offdiagonal updates

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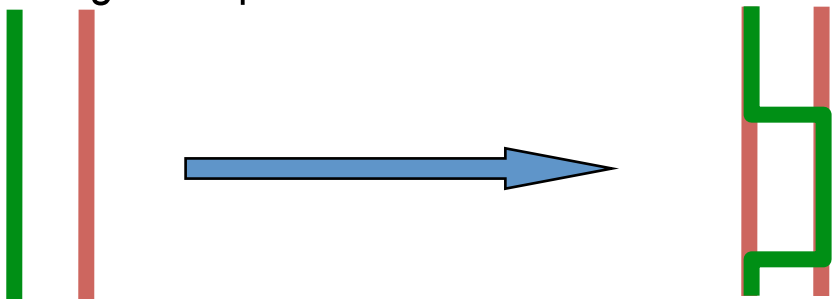
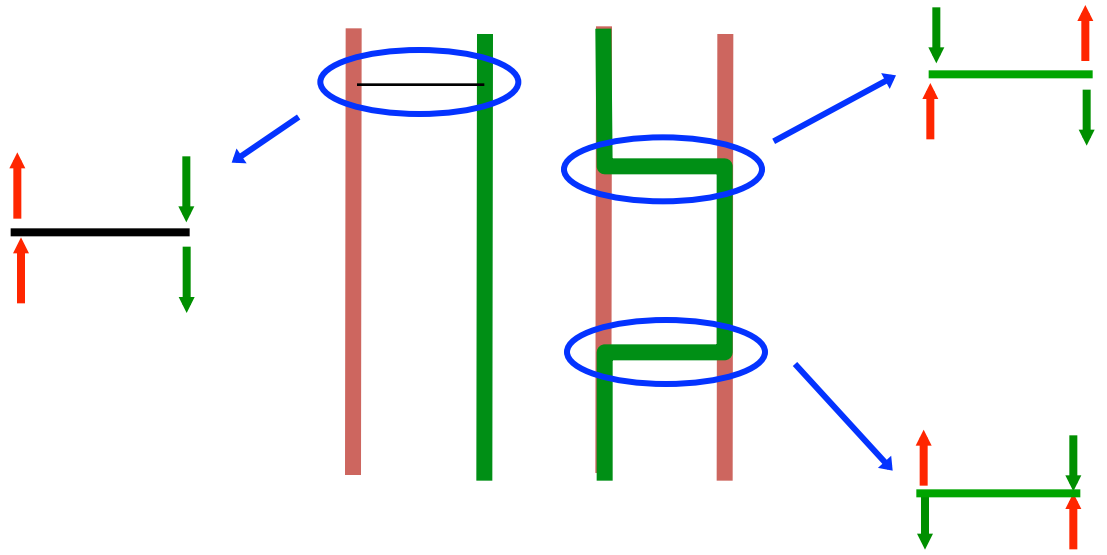
- Local changes using Metropolis



- Problems
  - Critical slowing down
  - No change of magnetization, particle number, winding number
- Solutions:
  - Loop algorithm
  - Operator loop algorithm
  - Directed loop algorithm

The SSE vertex list

- Consider only the non-unity operators
- Each defines a vertex with 4 legs
- All together form a quadruplely-linked list (vertex-list)
  - Contains the full configuration information
  - Conveniently represented as a vector data-structure



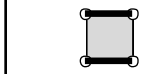
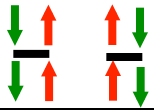
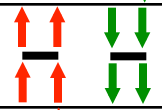
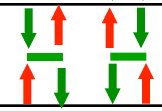
- Updates performed using this data structure

Loop update in SSE

- Select breakups for each vertex similar to loop algorithm
- Example: XXZ easy-plane antiferromagnet:

$$H_{XXZ} = \frac{J_{xz}}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z \quad (0 \le J_z \le J_{xy})$$

$$W(C) = \sum_G W(C,G) = \sum_G \Delta(C,G) V(G)$$

$\Delta(C,G)$			$W(C)$
	1	0	$J_z/2$
	0	0	0
	1	1	$J_{xy}/2$
$W(G)$	$J_z/2$	$(J_{xy}- J_z)/2$	

- Connected spins form a cluster and have to be flipped together
- For the Heisenberg model, the loop construction becomes deterministic ()!

Loop updates in SSE

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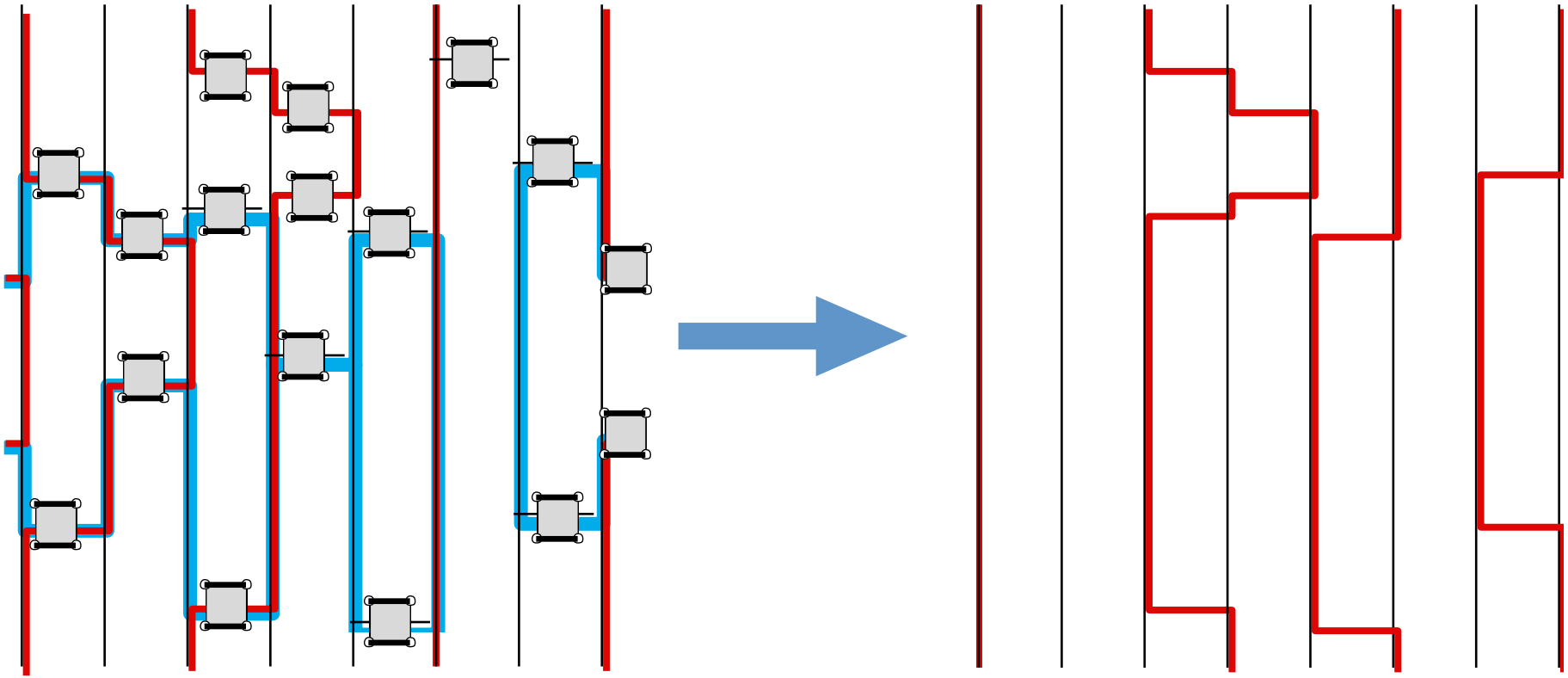
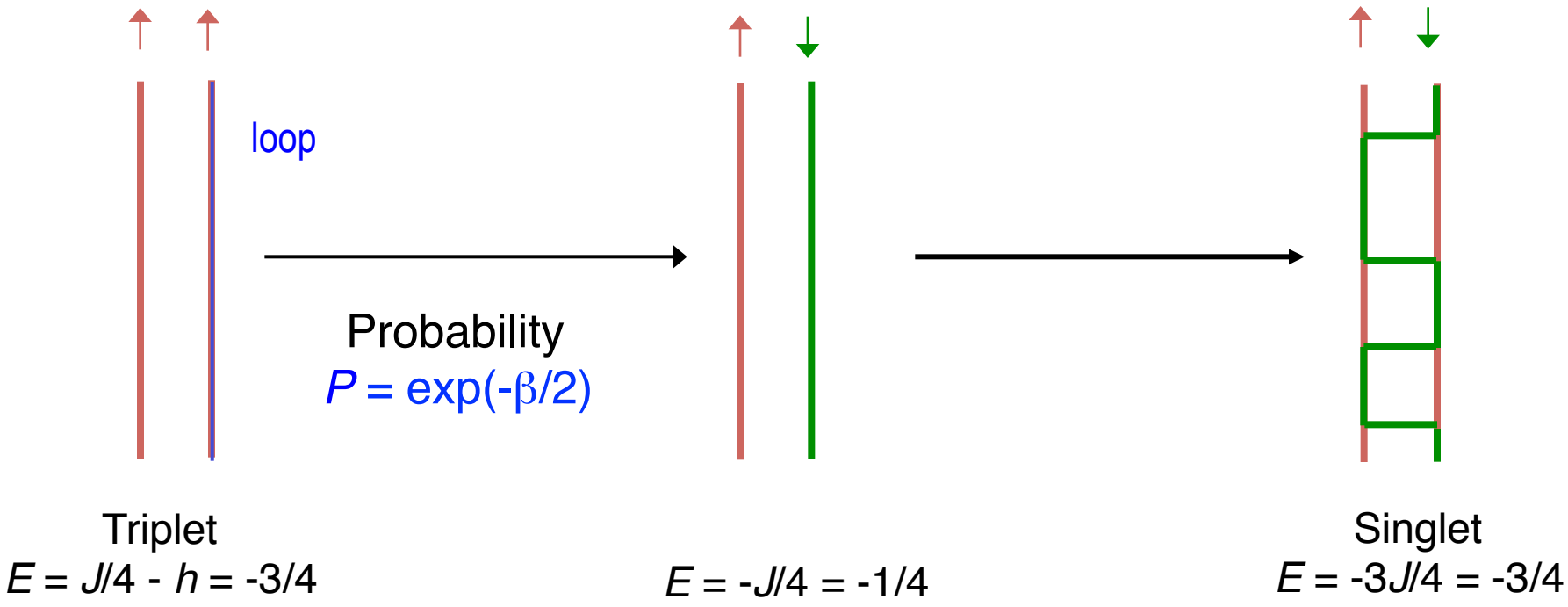
1. Insert/remove diagonal operators
2. Decide “breakups” at each vertex
3. Build and flip one or more loops

Similarity to path integrals: an exact mapping exists



Loop algorithm in a magnetic field

- Loop algorithm requires spin inversion symmetry
  - Magnetic field implemented by a-posteriori acceptance (flip) rate
- Example: spin dimer at $J = h = 1$

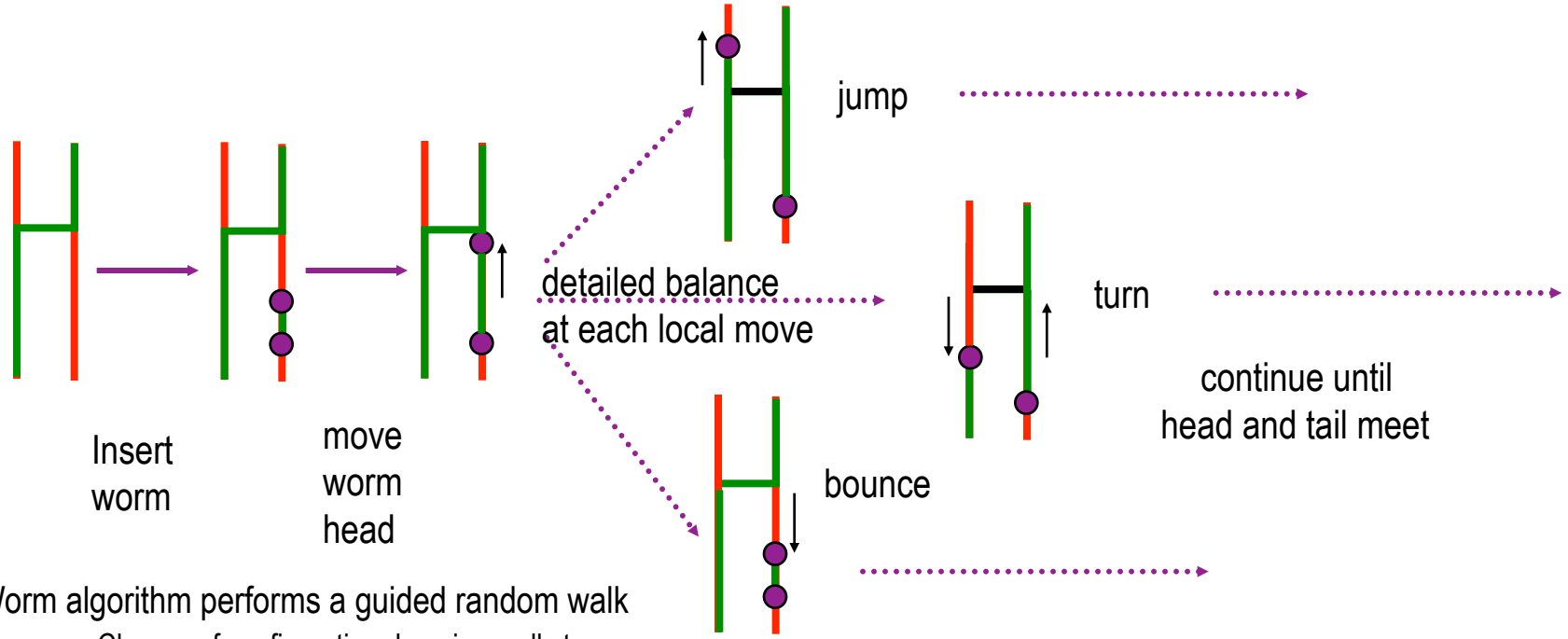


Loop algorithm must go through high energy intermediate state

Exponential slowdown

Worm and operator loop updates

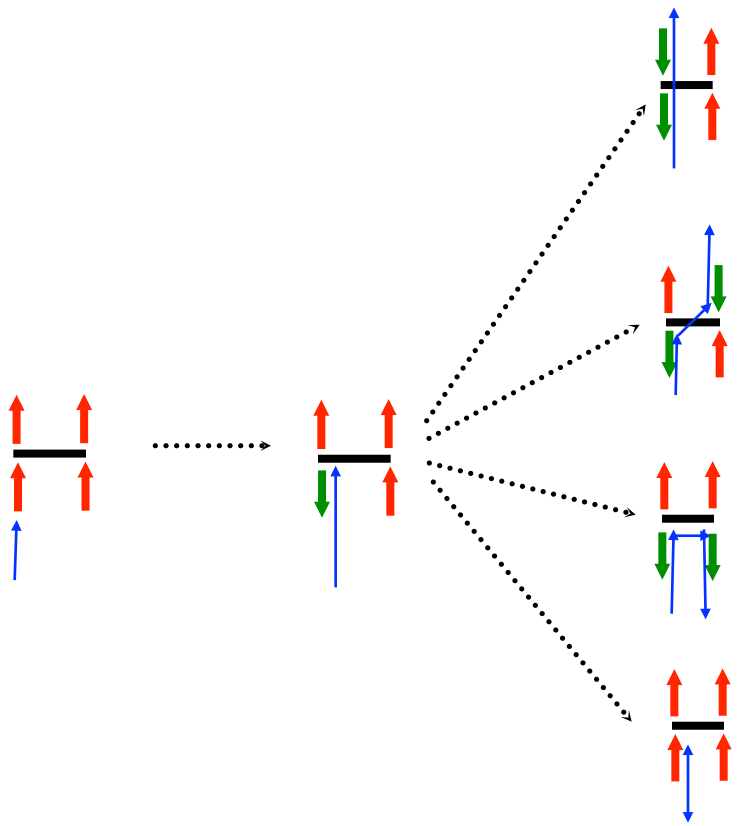
- Prokof'ev et al. 1997 (path integrals), Sandvik 1999 (SSE)
- Insert pair of spin rising/lowering operators (world line discontinuities)
  - move these operators (worm head/tail) using local moves
  - when head and tail meet ⇒ have created a loop, update is finished



- Worm algorithm performs a guided random walk
  - Change of configuration done in small steps

Operator loop update in SSE

- Instead of following a pre-chosen path given by graphs we pick randomly
  - E.g. using heat bath method



	weight		*probability*
	$\frac{J_z}{4} + C$	*"straight"*	$\frac{J_z/4 + C}{2C + J_{xy}/2 + h/z}$
	$\frac{J_{xy}}{2}$	*"jump"*	$\frac{J_{xy}/2}{2C + J_{xy}/2 + h/z}$
	0	*"turn"*	0
	$-\frac{J_z}{4} + \frac{h}{z} + C$	*"bounce"*	$\frac{-J_z/4 + h + C}{2C + J_{xy}/2 + h/z}$

Operator loop algorithm in a magnetic field

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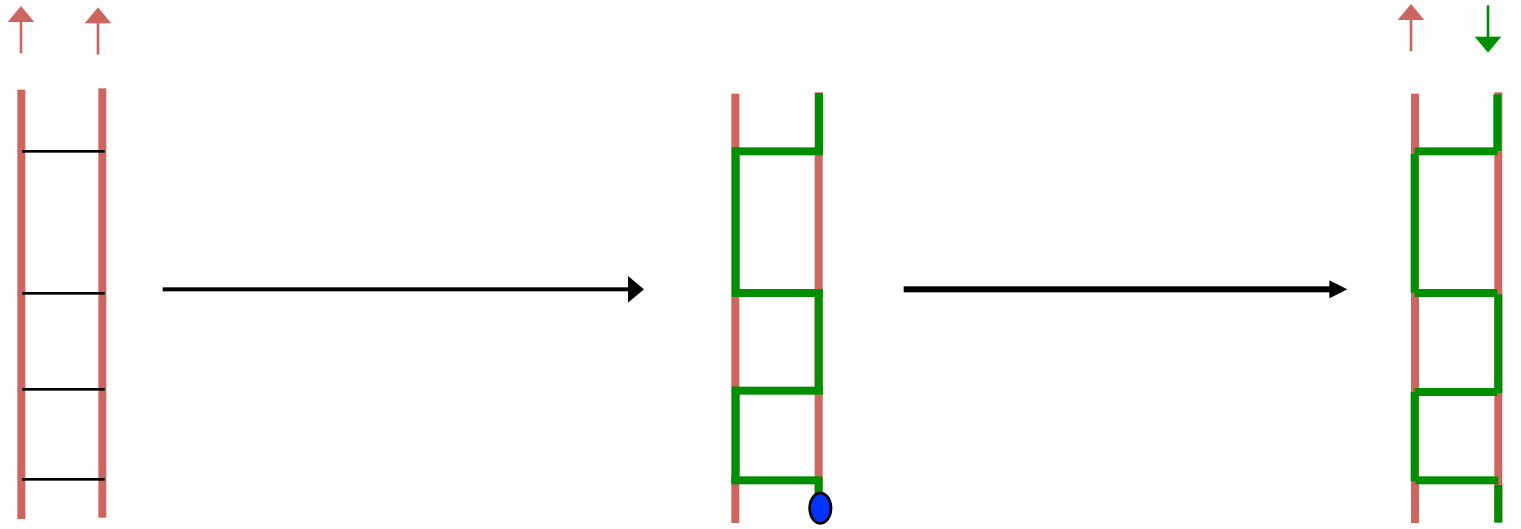
- Example: spin dimer at $J = h = 1$

  1. perform diagonal updates
  2. insert “worm”
  3. move “worm”
  4. annihilate “worm”

$$H_{\text{dimer}} = J\vec{S}_1\vec{S}_{2-h} - h\left(S_1^z + S_2^z\right)$$



Triplet
$E = J/4 - h = -3/4$

No high energy intermediate state

Efficient update in presence of a magnetic field

Singlet
$E = -3J/4 = -3/4$

Directed loop scheme - idea

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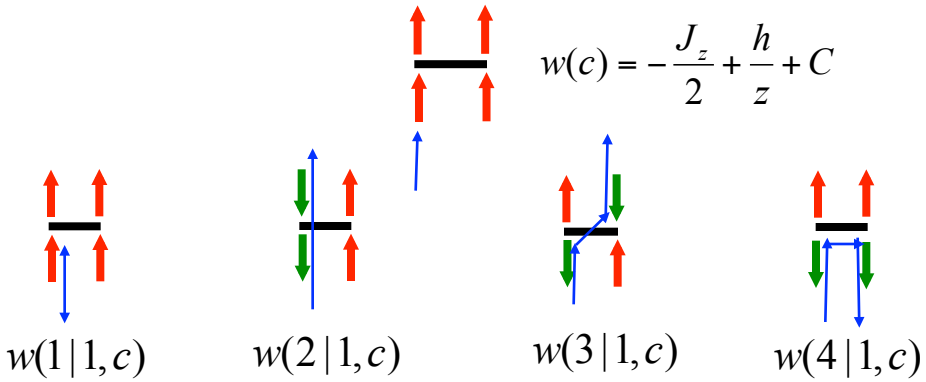
- Bounces are bad
  - since they undo the last change
- If bounce path can be eliminated $\Rightarrow$ loop algorithm possible
  - Loop algorithm as a limit for some models
  - Even becomes deterministic for isotropic models
- Bounce path can be minimized
  - In models where there is no loop algorithm
    - Directed loops scheme
    - O.F. Syljuåsen and A.W. Sandvik, PRE (2002)
    - O.F. Syljuåsen , PRE (2003)
  - Give worm "head" and "tail" an operator matrix element
    - Minimizes bounces further
    - F. Alet, S. Wessel and M. Troyer, PRE (2005)

Directed loop scheme - setup

- Consider exit leg *e*, given an incoming leg *i* at a vertex in configuration *c:*
  - Assign this path a weight $w(e \mid i,c)$
  - The sum over all paths must equal the vertex weight: $\sum_e w(e \mid i,c) = w(c)$



  - Choose exit leg *e* with probability $P(e \mid i,c) = \frac{w(e \mid i,c)}{w(c)}$ leading to configuration c_e

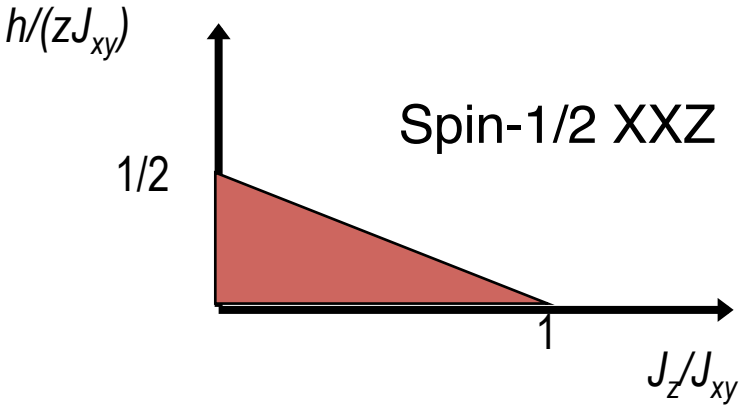
- Consider the reversed path $w(i \mid e,c_e)$, leading back to c

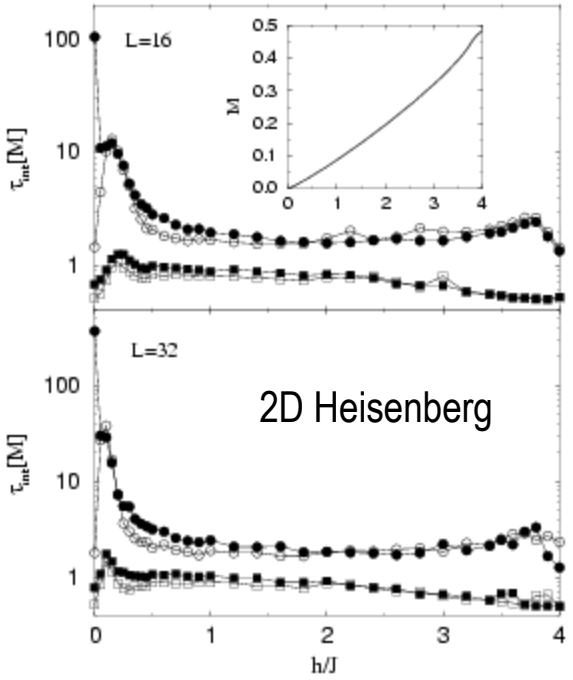
  - If $w(e \mid i,c) = w(i \mid e,c_e)$ is always fulfilled, then we obtain

Local detailed balance $P(e \mid i,c)w(c) = P(i \mid e,c_e)w(c_e)$

Directed loop scheme - solutions

- Heat-bath solution is always possible: $w(e \mid i,c) = \dfrac{w(c)w(c_e)}{w(c_1)+w(c_2)+w(c_3)+w(c_4)}$
  - However, contains large bounces
- Optimize the path weight factors
  - eliminate or minimize all bounces
  - i.e. all $w(i \mid i,c)$ should be zero or small
- Can be done analytically in many cases
- Numerically using linear programming
- Obtain large bounce-free regions





- Even outside the bounce-free region: reduction of autocorrelation times

Summary: the loop algorithm

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- A generalization of cluster algorithm idea to quantum systems
  - Essentially solves problem of critical slowing down
- Generalizations from spin-1/2 case presented
  - Higher spin models
  - SU(N) models
  - Biquadratic interactions
  - Long ranged interactions
  - Boson and fermion models (1D)
- Implementation choices
  - Discrete or continuous time
  - Single / multi loop implementations
  - SSE or path integrals

Summary: worm and directed loops

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- Relax loop-building rules
  - A partial loop (“worm”) performs a random walk on the space-time lattice
  - Detailed balance fulfilled at each step
  - Once “head” and “tail” meet a loop is finished
- Relationship to loop algorithms
  - Can recover loop algorithm if pre-defined path choices (“breakups”) possible
  - Loop algorithm performs a self-avoiding random walk
- Implementation choices
  - Worm algorithm in path integrals
  - Directed loop algorithm in SSE

BUT: Frustrated quantum Magnets

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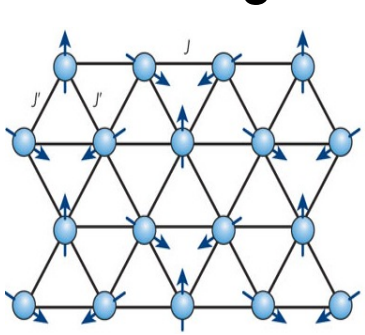
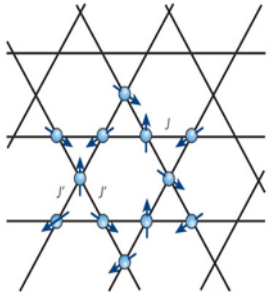
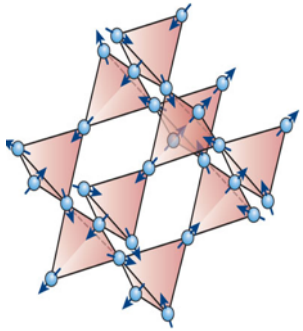
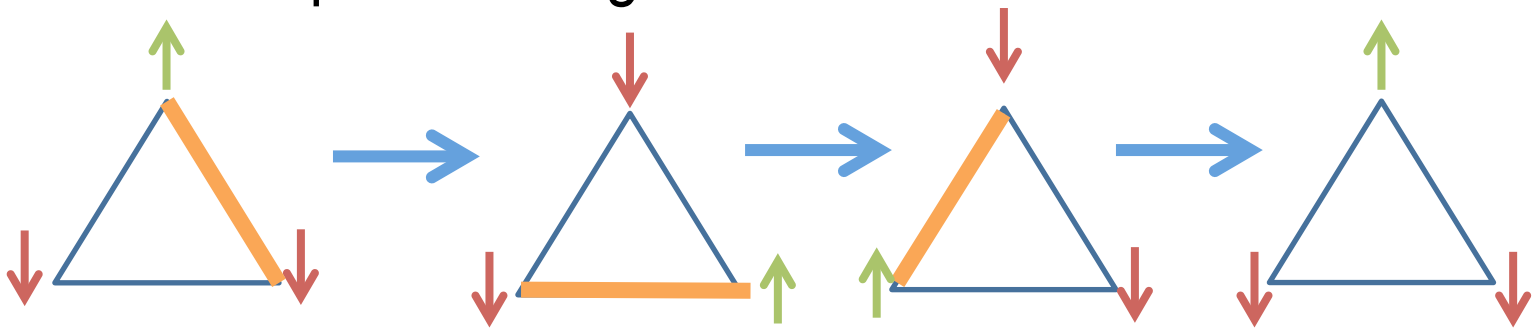
- We obtain non-positive weights e.g. for the antiferromagnetic Heisenberg model on non-bipartite lattices:







- Can return to starting configuration with an odd number of spin exchange terms:



The sign problem

The *negative sign* problem

- In mapping of quantum to classical system

$$\langle A \rangle = \frac{\mathrm{Tr}\left[A \exp(-\beta H)\right]}{\mathrm{Tr}\left[\exp(-\beta H)\right]} = \frac{\sum_i A_i p_i}{\sum_i p_i}$$

- "Sign problem" if some of the $p_i < 0$
  - Cannot interpret p_i as probabilities
  - Appears in simulation of fermions and frustrated magnets
- "Way out": Perform simulations using $|p_i|$ and measure the sign:

$$\langle A \rangle = \frac{\sum_i A_i p_i}{\sum_i p_i} = \frac{\sum_i A_i \,\mathrm{sgn}\, p_i |p_i| \Big/ \sum_i |p_i|}{\sum_i \mathrm{sgn}\, p_i |p_i| \Big/ \sum_i |p_i|} \equiv \frac{\langle A\, Sign \rangle_{|p|}}{\langle Sign \rangle_{|p|}}$$

  - Sampling according to $Z_{|p|} = \sum_i |p_i|$

The negative sign *problem*

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- The average sign becomes very small:

$$\langle Sign \rangle_{|p|} = \frac{1}{Z_{|p|}} \sum_i \operatorname{sgn} p_i |p_i| = \frac{Z}{Z_{|p|}} = e^{-\beta V \Delta f}$$

  - Both in system size and inverse temperature
  - This is the origin of the sign problem!

- The error of the sign:

$$\frac{\Delta Sign}{\langle Sign \rangle_{|p|}} = \frac{\sqrt{\langle Sign^2 \rangle_{|p|} - \langle Sign \rangle_{|p|}^2}}{\sqrt{N} \langle Sign \rangle_{|p|}} \approx \frac{\sqrt{\langle 1 \rangle_{|p|}}}{\sqrt{N} \langle Sign \rangle_{|p|}} = \frac{e^{\beta V \Delta f}}{\sqrt{N}}$$

  - Need of the order $N = \exp(2\beta V \Delta f)$ measurements for sufficient accuracy
  - Similar problem occurs for the observables
  - Exponential growth! Impossible to treat large systems or low temperatures

How bad is the sign problem?

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- The sign problem is basis-dependent
  - Diagonalize the Hamiltonian matrix $H|i\rangle = \varepsilon_i |i\rangle$

$$\langle A \rangle = \mathrm{Tr}\left[A \exp(-\beta H)\right] / \mathrm{Tr}\left[\exp(-\beta H)\right] = \sum_i \langle i|A_i|i\rangle \exp(-\beta\varepsilon_i) \Big/ \sum_i \exp(-\beta\varepsilon_i)$$

  - All weights are positive
  - But this is an *exponentially hard problem* since $\dim(H)=2^N$!
  - Good news: the sign problem is basis-dependent!

- But: the sign problem is still not solved
  - Despite decades of attempts

- Reminiscent of the NP-hard problems like traveling salesman etc.
  - No proof that they are exponentially hard
  - No polynomial solution either

The sign problem is NP-hard

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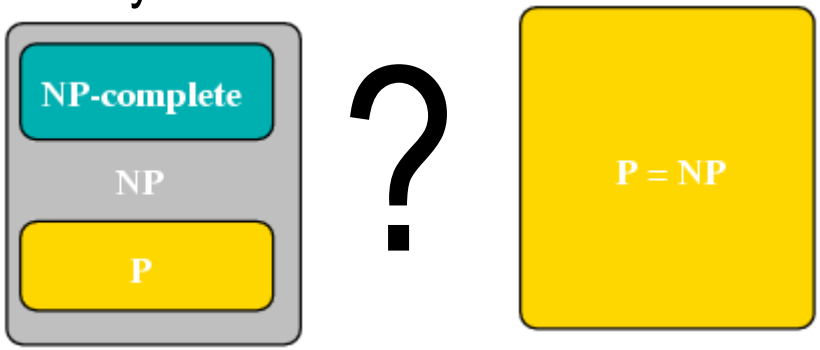
- See: M. Troyer and U. Wiese, Phys. Rev. Lett. (2005)
- Could use solution to the sign problem to obtain polynomial algorithm for all NP-complete problems (e.g. traveling salesman)
- This is bad news!
- Or not - if you solve it, you will get both
  - The Nobel price (??)
  - Plus additional 1.000.000 $$ from the Clay Foundation http://www.claymath.org



How to deal with the sign problem ?

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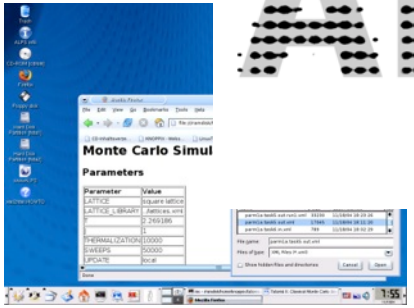
- The sign problem is NP-hard (worst-case complexity)
  - A general solution is almost certainly impossible

- What can we do?
  - Simulate models without a sign problem
    - Non-frustrated quantum magnets
    - Bosonic models (atomic BEC condensates)
    - Hubbard model in 1D
  - Brute force-approach
    - Live with the exponential scaling of the sign problem and stay on small lattices
  - Other exact algorithms
    - DMRG, exact diagonalization, or series expansion might be better
  - Special solutions for certain models still possible by a clever choice of the computational basis

The End

- Thank You for your attention!

Software project



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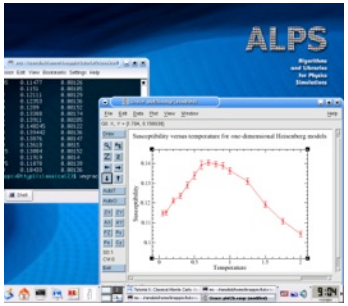

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