Representations of Partition Functions and the Loop Algorithm

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- Representations of $\mathrm{tr}\, e^{-\beta H}$, and mapping between them
- Loop algorithm (with extension to infinite lattice size)
- QMC method for coupled spins and bosons

HGE, Advances in Physics 52, 1 (2003)

F.F. Assaad, HGE, Springer Lecture Notes (2008)

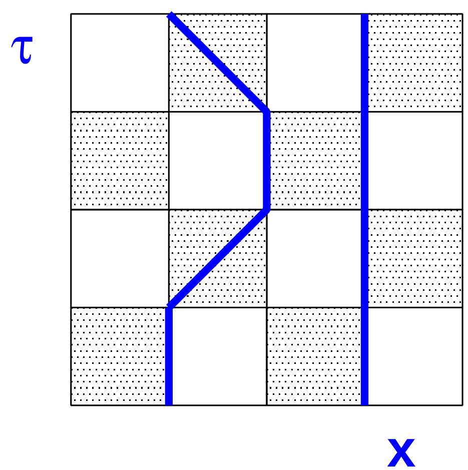
Representations of $\exp(-\beta \hat{H})$: Discrete time

1D Heisenberg: $$H = \sum_{\langle ij \rangle} \frac{J_x}{2} (S_i^+ S_j^- + S_j^+ S_i^-) + J_z S_i^z S_j^z$$

similar to tV-model: $$H = \sum_{\langle ij \rangle} t\,(c_i^\dagger c_j + c_j^\dagger c_i) + V\, n_i n_j$$

Trotter decomposition: $$Z = \mathrm{tr}\; e^{-\beta H} = \lim_{M\to\infty} \mathrm{tr}(e^{-\Delta\tau H_{\text{even}}}\; e^{-\Delta\tau H_{\text{odd}}})^M \qquad \Delta\tau = \frac{\beta}{M}$$

Insert $\{S^z\}$ eigenstates: $$Z = \lim_{M\to\infty} \sum_{\{S^z\}} \langle S^z_{(1)} | e^{-\Delta\tau H_1} | S^z_{(2)} \rangle \; \langle S^z_{(2)} | e^{-\Delta\tau H_2} | S^z_{(3)} \rangle \;\ldots$$



$$= \sum_{S^z} \prod_p W(S_p)$$

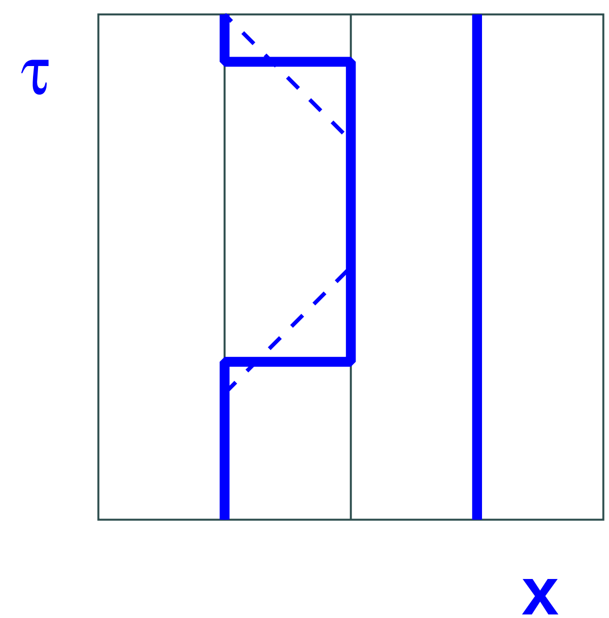
- Continuous worldlines of up-spins $S^z(x,\tau) = \uparrow$
- Similar representations for: fermions, bosons, higher spins

Representations of $\exp(-\beta\hat{H})$: Continuous time (1)

1D Heisenberg: $$H = \sum_{\langle ij\rangle} \frac{J_x}{2}(S_i^+ S_j^- + S_i^- S_j^+) + J_z S_i^z S_j^z = H_0 - V,$$ (V: spin flips)

Interaction repres.: $$Z = \text{tr}\; e^{-\beta H} = \boxed{\text{tr}\sum_{n=0}^{\infty} e^{-\beta H_0}\int_0^{\beta} d\tau_n \ldots \int_0^{\tau_2} d\tau_1\; V(\tau_1)\ldots V(\tau_n)}$$

- Leads to Worldline representation
- Worldlines are weighted with $e^{-\beta H_0} \to e^{\pm\frac{\tau}{4}J_z}$
- Get same repres. from $\lim_{\Delta\tau\to 0}\; \sinh\frac{\Delta\tau}{2}J_x = \frac{\Delta\tau}{2}J_x$
- Constant probability in time for spin-flip event: Poisson process   Beard,Wiese '96



- Store configurations by *events*

Continuous time (2)

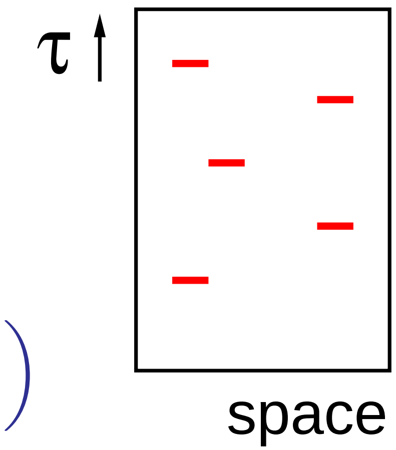
Aizenman et al. ('90,'94), Farhi and Gutmann ('92)

- When $\hat{H}$ is a sum of operators with **discrete representation**

$$\hat{H} = -\sum J_b \, \hat{h}_b$$

then

$$\begin{aligned} e^{-\beta \hat{H}} &= e^{\beta \sum_b J_b} \lim_{\Delta t \to 0} \left(\prod_b e^{(-J_b + J_b \hat{h}_b)\Delta t} \right)^{\beta/\Delta t} \\ &= e^{\beta \sum_b J_b} \lim_{\Delta t \to 0} \left(\prod_b \{(1 - J_b \Delta t) + J_b \hat{h}_b \Delta t\} \right)^{\beta/\Delta t} \\ &= \text{Integral of } \left(\begin{array}{l} \textbf{Poisson distribution of operators } \hat{h}_b, \\ \text{in \textit{continuous imaginary time}, with rates } J_b. \end{array} \right) \end{aligned}$$



- Valid also for standard hopping representation

Representations of $\exp(-\beta\hat{H})$: SSE

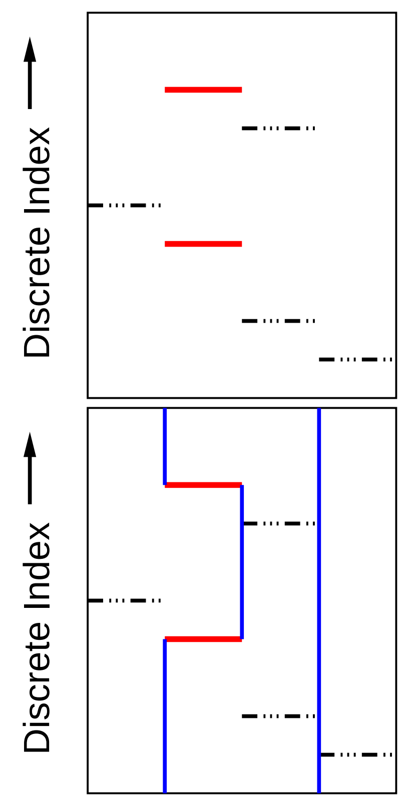
Stochastic Series Expansion (A. Sandvik)

Let $V = \hat{H} = \sum_{i=1}^{N} \hat{H}_i$, i.e. $\boxed{H_0 = 0}$. Then the interaction representation

$$Z = \mathrm{tr} \sum_{n=0}^{\infty} \int_0^{\beta} d\tau_n \ldots \int_0^{\tau_2} d\tau_1 \; V(\tau_1) \ldots V(\tau_n)$$

results in the SSE expansion of $e^{-\beta H}$:

$$\begin{aligned} Z &= \mathrm{tr}\, e^{-\beta\hat{H}} \\ &= \mathrm{tr} \textstyle\sum_{n=1}^{\infty} \frac{\beta^n}{n!} (-\hat{H})^n \\ &= \mathrm{tr} \textstyle\sum_{n=1}^{\infty} \frac{\beta^n}{n!} (-\hat{H}_1 - \hat{H}_2 - \ldots)(-\hat{H}_1 - \hat{H}_2 - \ldots)\ldots \\ &= \textit{Sum over } \underline{\textit{sequences of operators}} \end{aligned}$$



- ,,Trace" produces worldlines
- Similar to continuous time, but with discrete index space.
- Diagonal operators $S_i^z S_j^z$ occur explicitely
- Dynamical correlations are very expensive to measure, since a temporal distance τ corresponds to a convolution over index distances.

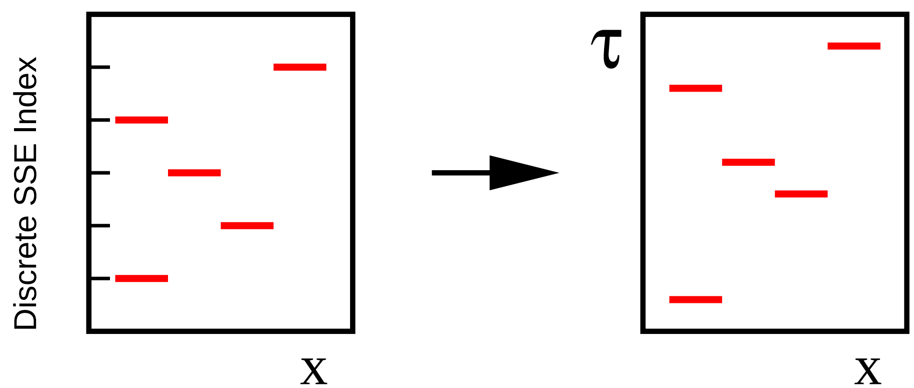
Efficient measurement of dynamical correlations in SSE

Michel, HGE '07

- Go back to interaction representation: **reintroduce time !**

$$Z = \mathrm{tr} \sum_{n=0}^{\infty} \int_0^{\beta} d\tau_n \ldots \int_0^{\tau_2} d\tau_1 \, V(\tau_1) \ldots V(\tau_n)$$

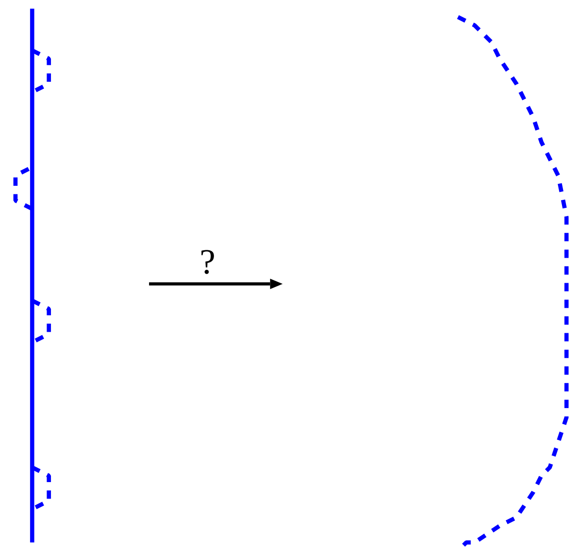
- **Stochastic mapping from SSE to continuous imaginary time τ:**
  Given an SSE operator sequence, choose ordered times τ_i uniformly between 0 and β for all operators



- Then measure correlations in time via FFT
- Saves factor O(volume) vs. measurement in SSE representation

Local Updates of continuous worldlines are very slow

Local Updates are like random walks:



Problems:

- Very long autocorrelation times (e.g. $\tau \sim \max(\xi, \frac{1}{\Delta})^2$)
- Not ergodic (Magnetization, Particle number, Winding number)

Loop Algorithm

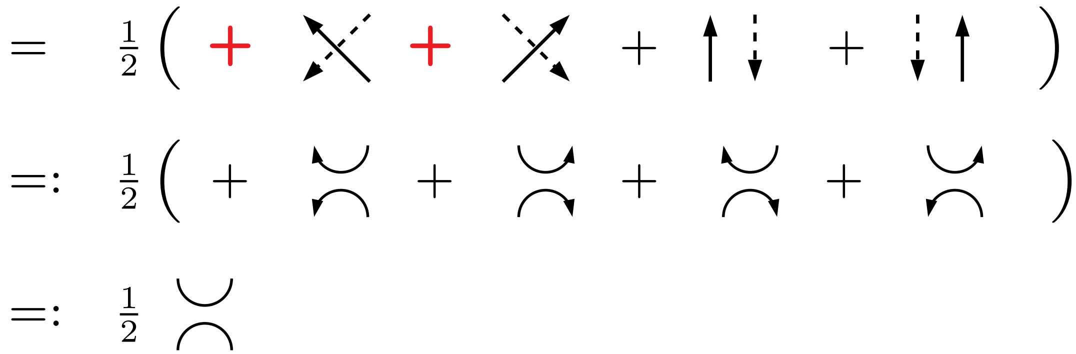
- Ergodic, any dimension, almost no autocorrelations
- Can measure off-diagonal operators
- But restricted range of models

- Cluster algorithm
- Based on *exact mapping* to *Worldlines + Loops*
- Provides loop representation: "improved estimators" as observables
- Sign problem can be removed in loop representation in some cases: meron algorithm

- Many generalizations

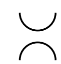
Loop representation of Heisenberg AF

$$-\hat{\vec{S}}_i\hat{\vec{S}}_j + \frac{1}{4} = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)\ \frac{1}{\sqrt{2}}\left(\langle\uparrow\downarrow| - \langle\downarrow\uparrow|\right)$$ **= Singlet projection operator**

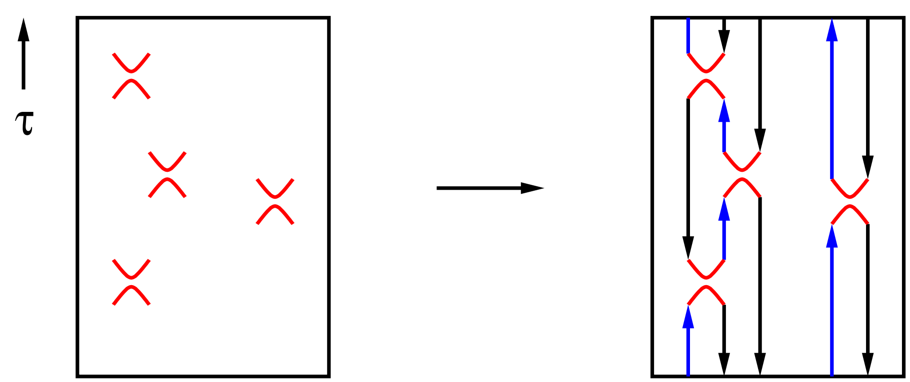


on bipartite lattice

: allowed spin configurations

$\Rightarrow$ Partition function $Z = \mathrm{tr}\, e^{-\beta\hat{H}} \sim \mathrm{tr}\ e^{\beta\frac{J}{2}\sum_{\langle ij\rangle}}$  (in any dimension)

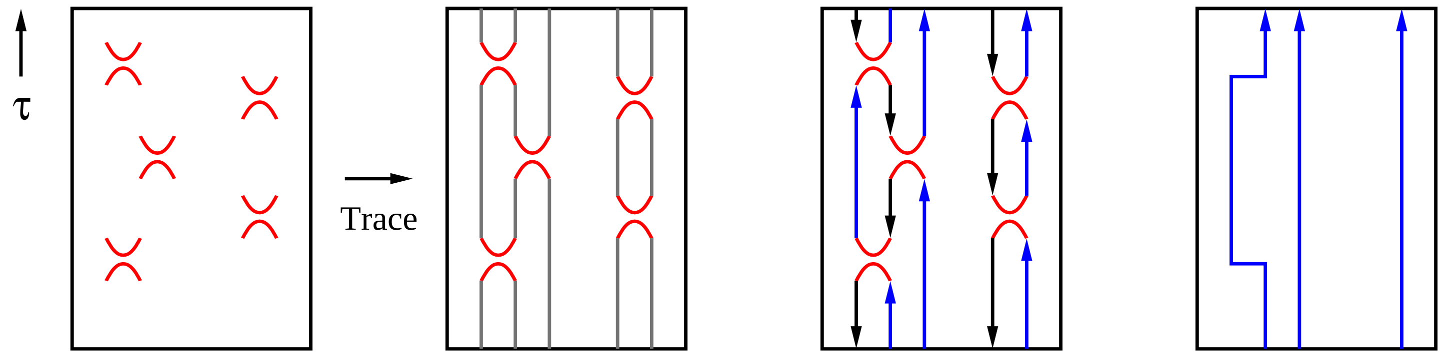
- $\Rightarrow$ Poisson distribution of operators
- Trace produces Loop representation:



- Can work purely in loop representation, e.g. Merons to solve sign problem Chandrasekharan, Wiese '99,....
- At each time τ, pairs of sites belonging to the same loop are in a *singlet state*: ,,Valence bond basis"

Loop *algorithm*

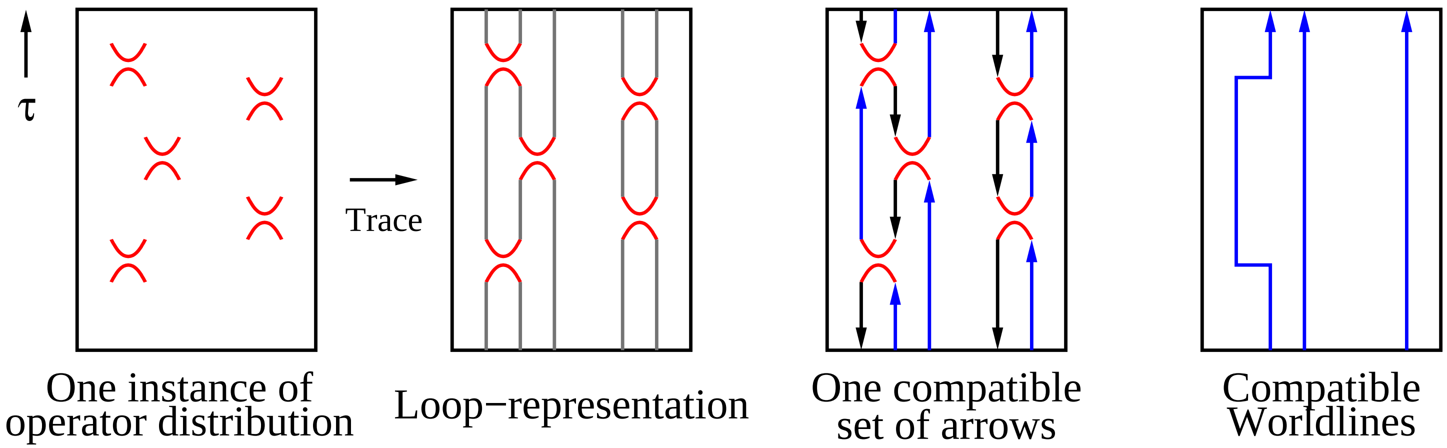
- **Switch between operator and worldline representation**

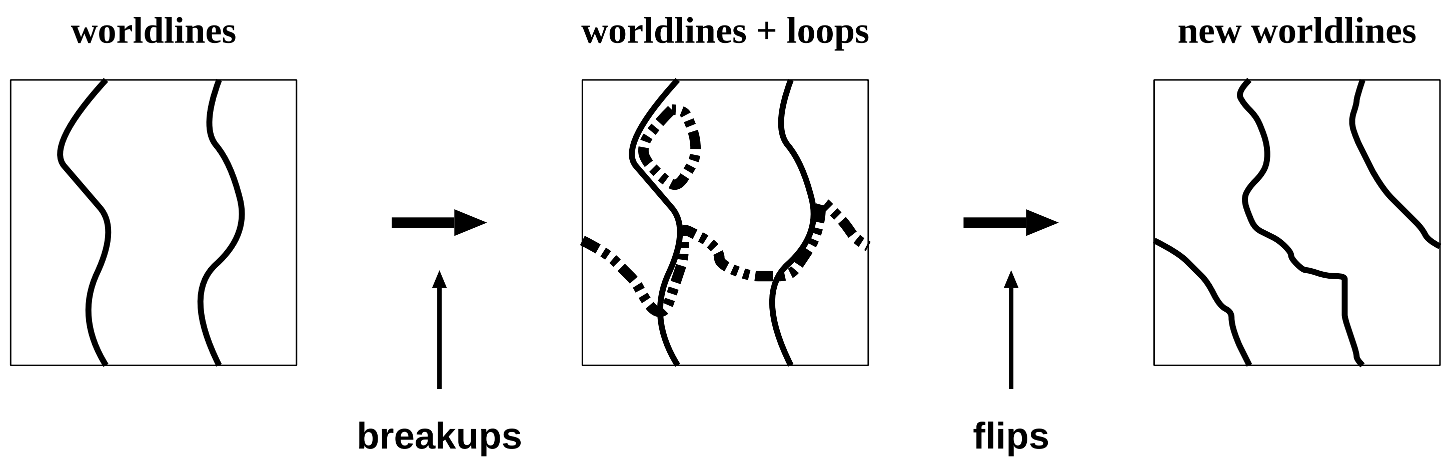


One instance of operator distribution | Loop−representation | One compatible set of arrows | Compatible Worldlines

Loop algorithm

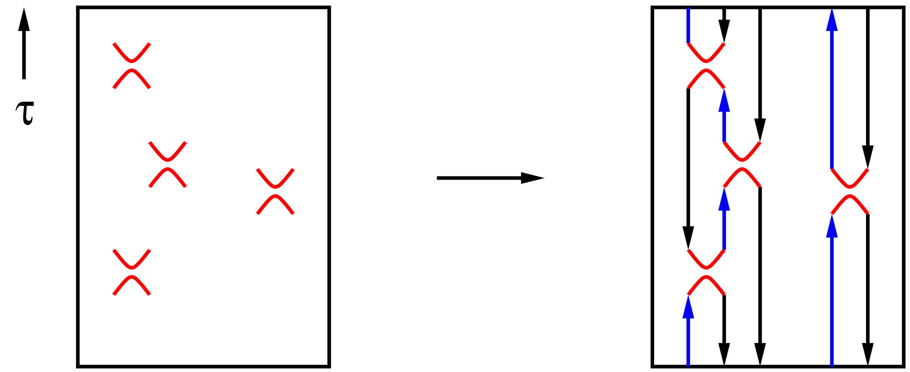
- **Switch between operator and worldline representation**



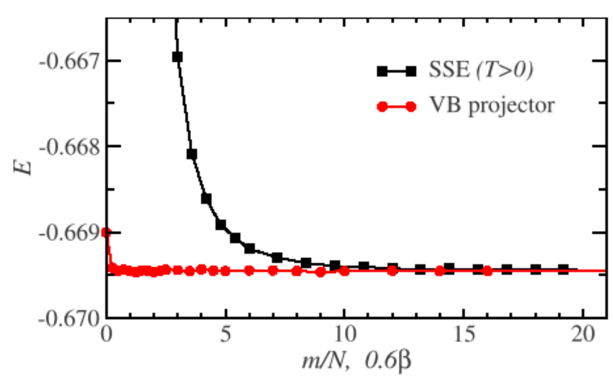


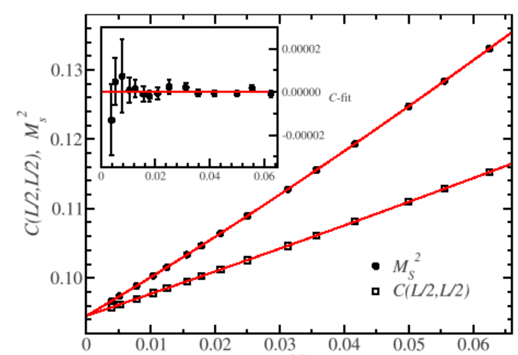
- Change of configuration on large scale (ξ, ξ_t)
- Note: with SSE representation: almost same, discrete index.
- Ferromagnet: similar.

Projector MC in valence bond basis



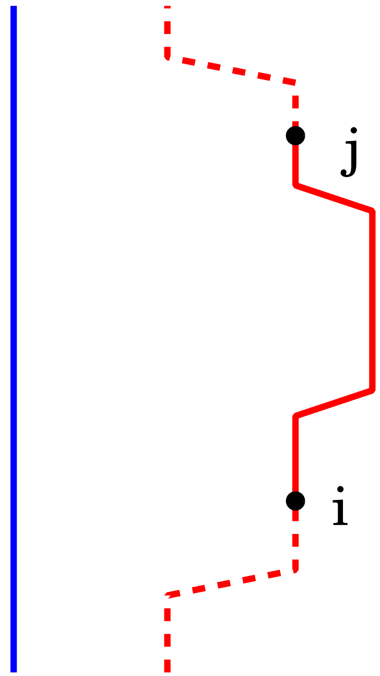
- At each time τ, pairs of sites belonging to the same loop are in a singlet
- $\Rightarrow$ after many applications of $\hat{H}$, only singlets remain = Valence bond state = RVB state
- Ground state $|\psi_0\rangle = \lim_{\theta\to\infty} \mathrm{e}^{-\theta\hat{H}}|\psi_{trial}\rangle$
- Projector Monte Carlo ($\rightarrow$ ground state magnetization 0.30749(1)) Sandvik 2005; Sandvik,HGE 2010





Single Particle Greens function:

Brower, Chandrasekharan, Wiese '98



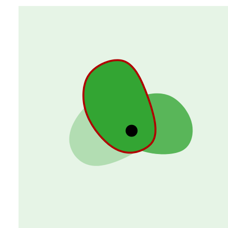
contributes to $\langle S_i^+ S_j^- \rangle, \ \langle c_i^\dagger c_j \rangle$

Simulations on infinite lattices: $L \equiv \infty$ and $\beta \equiv \infty$

- Two-point Greens functions get contributions only from sites on the *same* loop
- $\Rightarrow$ Probability of large loops decays like correlation length
- Infinite system: Simulate single loop with fixed starting point, in an "infinite" spin system

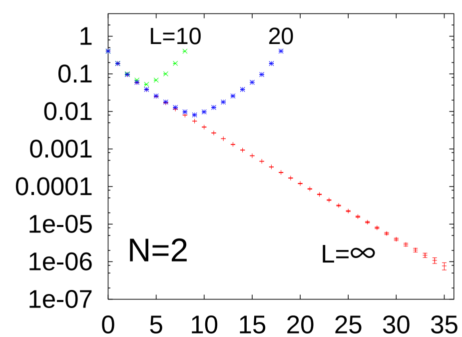
- $\Longrightarrow$ equilibrates region around origin. Reaches distance r with prob. $e^{-r/\xi}$.

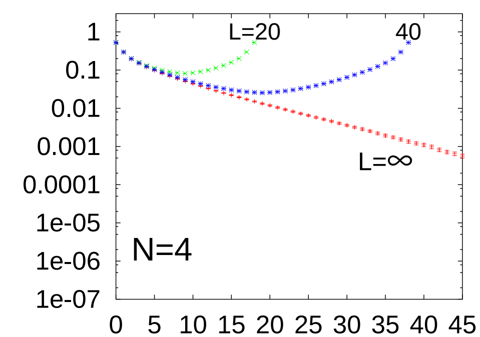
  Can grow without bounds $\Longrightarrow$ Simulates directly at $L = \infty$ and/or $\beta = \infty$



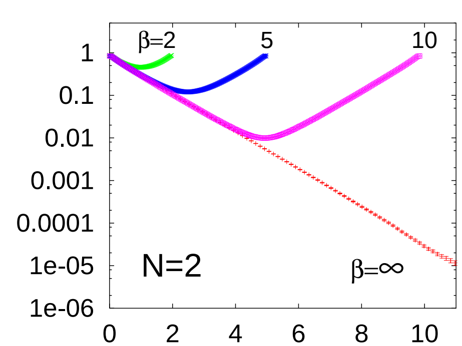
- **Example: Heisenberg spin ladder with N chains**

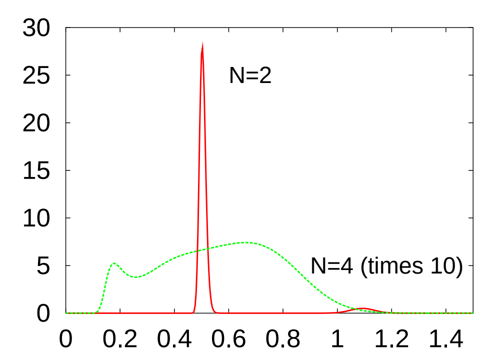
- Spatial correl. at $L = \infty$:





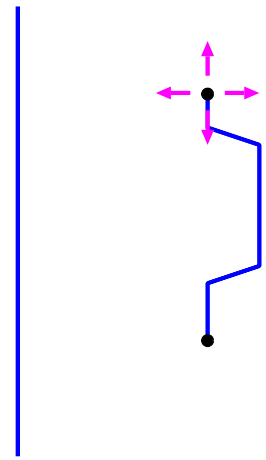
- Temporal correlations: choose infinite size: $\Rightarrow$ get $\beta \equiv \infty$ (and $L \equiv \infty$)
- Can take limits $q \to 0$ and $\omega \to 0$ directly
- Get full dynamics $S(q, i\omega)$.





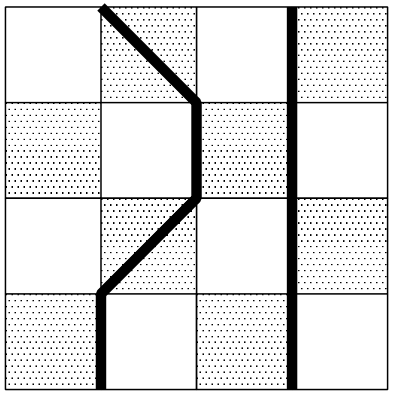
Efficient general methods: Worms and Directed Loops

Prokof'ev, Svistunov, Tupitsyn, 1998; Sandvik, Syljuasen, 2003

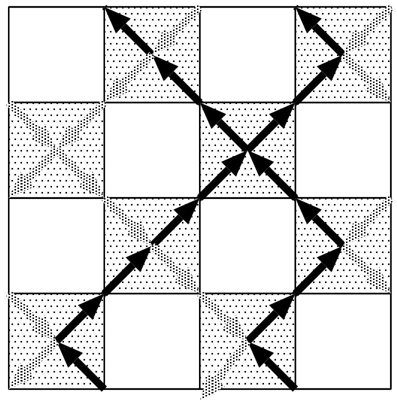


- **Introduce 2 sources. Allow them to move**
- Local updates
- When sources meet and annihilate, a valid sourceless configuration is reached again
- Applicable to any model.
- Ergodic
- Intermediate states contribute to Greens functions
- Directed loops: efficient update designed such that for isotropic couplings the loop-algorithm is recovered

Loop algorithm in vertex language

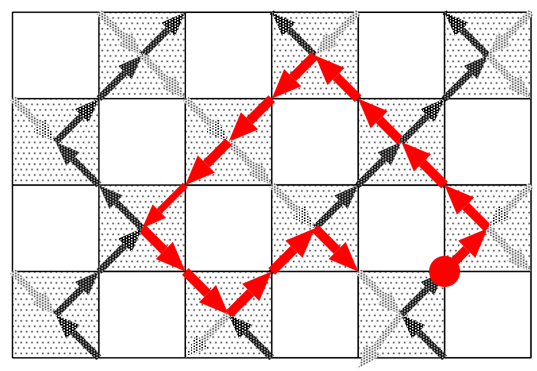


worldline language

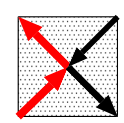


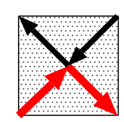
vertex language

- At each vertex, 2 arrows enter and 2 leave: arrow configuration has *"zero divergence"*
- $\Rightarrow$ Difference between configurations also has zero divergence, i.e. it lies on loops
- Solution: Each such loop follows arrows, which are then flipped

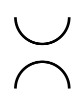


- There are 2 possible paths *out* of each vertex:





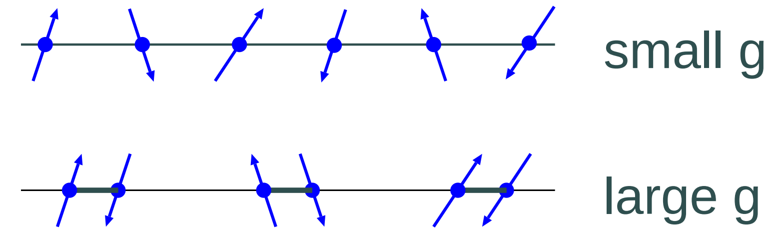
- Horizontal path corresponds to loop-operator



Spins and Bosons: divide and conquer

Spin - Peierls Transition

- Structural phase transition due to interaction of phonons with spins or electrons

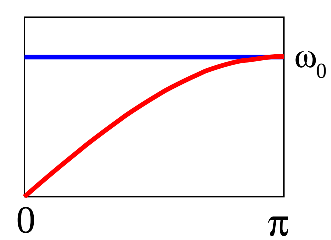


- **Example:** 1D Heisenberg chain coupled to phonons

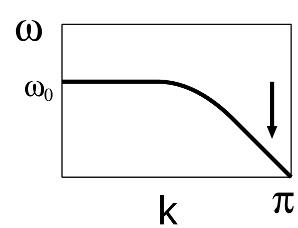
$$\hat{H} = \sum_{i=1}^{N} \hat{\mathbf{S}}_i \hat{\mathbf{S}}_{i+1} \underbrace{\left\{ \begin{array}{lll} 1 + \mathbf{g} & \hat{x}_i & \text{bond phonons} \\ 1 + \mathbf{g} & (\hat{x}_i - \hat{x}_{i+1}) & \text{site phonons} \end{array} \right\}}_{f(\{\hat{x}_i\})} + \underbrace{\frac{1}{2} \sum_q \hat{p}_q^2 + \omega^2(q)\, \hat{x}_q^2}_{\hat{H}_{ph}}$$

- $T = 0$: Quantum Phase Transition at g_c to dimerized phase

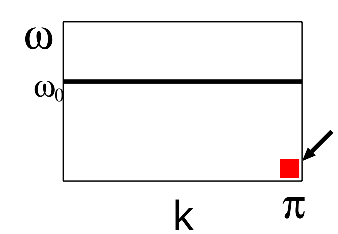
- Issue: **Does g_c depend on bare dispersion ?**



- Spectra: **Phonon softening ?**



or **central peak ?**



Phonons: some difficulties

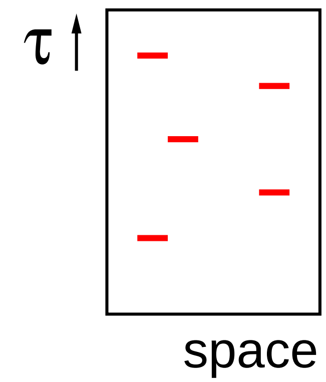
- First quantization: $(1 + g(x_i - x_{i+1})\, S_i S_{i+1}$:

  Very slow phonon convergence with updates local in imaginary time; especially for acoustical phonons $(\omega(q=0)=0)$

- Second quantization: $...(b_i^\dagger + b_i - b_{i+1}^\dagger - b_{i+1})\, S_i S_{i+1}$:

  Sign problem !

QMC method for dynamical phonons



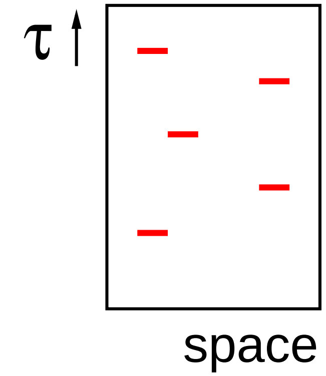
- **Interaction representation** with $\hat{H}_{ph}$ as diagonal part:

$$Z = \mathrm{Tr}_s \sum_{n=0}^{\infty} \sum_{S_n^\tau} \int_0^\beta d\tau_n \ldots \int_0^{\tau_2} d\tau_1 \int \mathcal{D}x \underbrace{\prod_{l=0}^{n} f(\{x(\tau)\}) S_n^\tau[l]}_{\text{spin operator sequence}} \underbrace{\int \exp\left(-\int_0^\beta d\tau \, H_{ph}(\{x(\tau)\})\right)}_{\text{phonon path integral}}$$

Spin-phonon coupling $f(\{x(\tau)\})$ acts at space-time locations of spin-operators

- Effective action for phonon coordinates contains $\log f(\{x_l\})$: not bilinear

QMC method for dynamical phonons



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Spin-phonon coupling $f(\{x(\tau)\})$ acts at space-time locations of spin-operators

- Effective action for phonon coordinates contains $\log f(\{x_l\})$: not bilinear

- Phonon update proposal: Replace $f(x) = 1 + gx$ by $f^{\text{prop}} = \exp(gx)$ $\Rightarrow$ bilinear

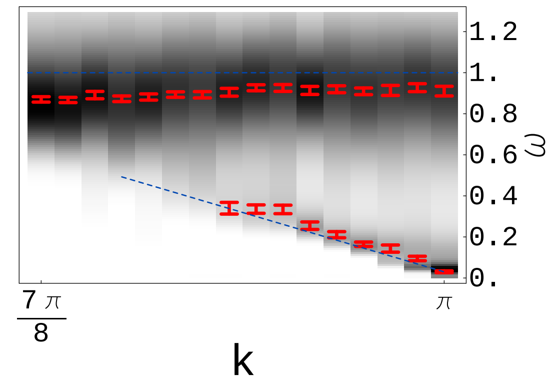
$\Rightarrow$ generate new phonon configuration in (ω_n, k) space ; *accept* with physical S_{eff}

- Spin update : *Directed loops* in spin operators (fast).

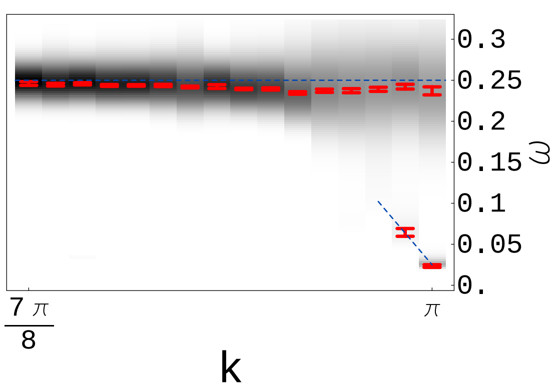
- Can use any bare dispersion $\omega(q)$

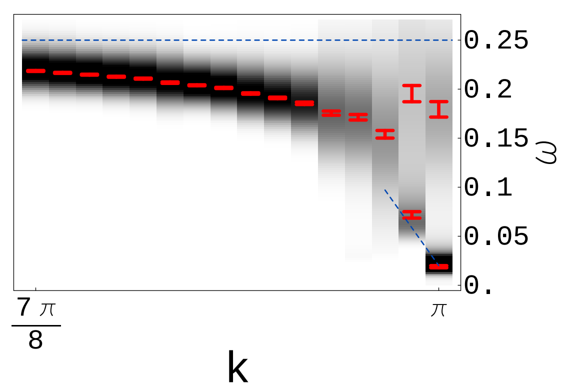
Optical bond phonons $(1 + g\hat{x}_i)S_iS_{i+1}$

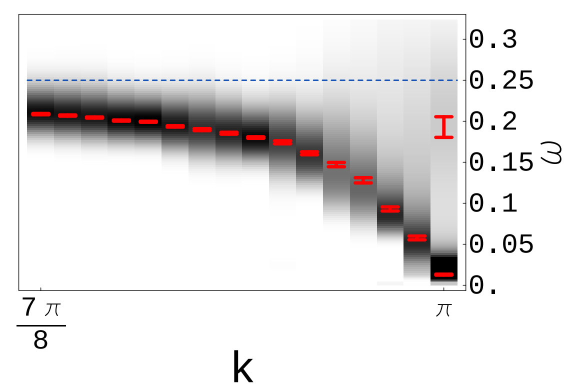
- Dispersion at large $\omega_0 \gtrsim J$:
  Second phonon branch
  develops at g_c from **central peak**



- Dispersion at small $\omega_0 = 0.25J$: Bare phonons **soften** and join central peak







Site phonons $1 + g(x_i - x_{i+1})S_iS_{i+1}$: QMC results

- Gapless acoustic phonons:

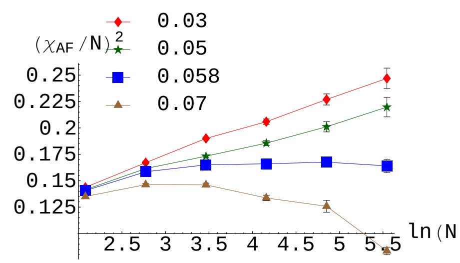
DMRG paper (PRL) concluded that $g_c = 0$!?

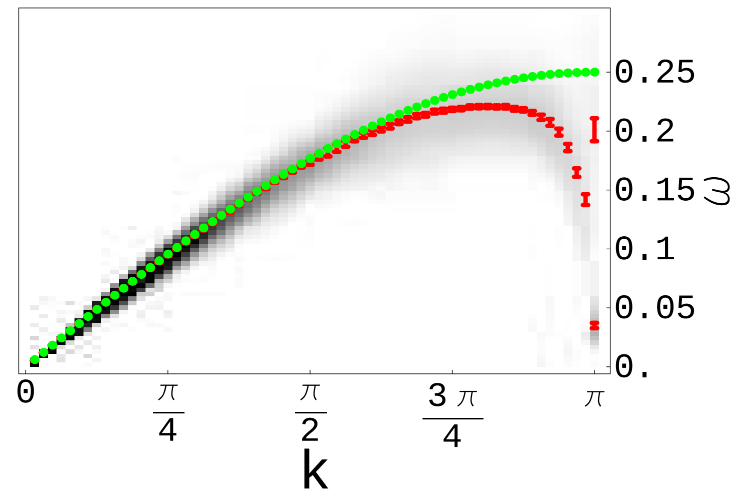
(measured magnetization M, incorrectly assumed $M(N) \propto \Delta_S(N)$)

QMC:

KT transition at $g_c = 0.058(2)$

Not affected by gapless mode !





Conclusions

- Representations of partition function (discrete, continuous, SSE)
- Common framework: Interaction representation
- Representation is different issue than update algorithm
- Loop algorithm: cluster method switching between loop and spin representations
- Infinite size lattices
- Generalization: worms and directed loops
- Efficient algorithm for coupled spins and phonons, with arbitrary phonon dispersions