

PERIMETER SCHOLARS INTERNATIONAL

April 5-23, 2010, Course on “Quantum Spin Simulations”

Anders W. Sandvik, Boston University

PART3: Quantum Monte Carlo Methods

Introduction; path integrals and series representation

SSE algorithm for the $S=1/2$ Heisenberg model

- some details needed to make a simple but very efficient program
- essentially lattice-independent (bipartite) formulation

Examples: properties of chains, ladders, planes

- critical state of the Heisenberg chain and odd number of coupled chains
- gapped (quantum disordered) state of even number of coupled chains
- long-range order in 2D

The valence-bond basis and resonating valence-bond states

- alternative to single-spin \uparrow, \downarrow basis; properties of the basis
- exact solution of the frustrated chain at the “Majumdar-Ghosh” point
- amplitude-product states
- projector QMC method

Néel to VBS quantum phase transition

- J-Q models; evidence for “deconfined” quantum criticality

Path integrals in quantum statistical mechanics

We want to compute a thermal expectation value

$$\langle A \rangle = \frac{1}{Z} \text{Tr}\{Ae^{-\beta H}\}$$

where $\beta=1/T$ (and possibly $T \rightarrow 0$). How to deal with the exponential operator?

“Time slicing” of the partition function

$$Z = \text{Tr}\{e^{-\beta H}\} = \text{Tr}\left\{\prod_{l=1}^L e^{-\Delta_\tau H}\right\} \quad \Delta_\tau = \beta/L$$

Choose a basis and insert complete sets of states;

$$Z = \sum_{\alpha_0} \sum_{\alpha_1} \cdots \sum_{\alpha_{L-1}} \langle \alpha_0 | e^{-\Delta_\tau H} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | e^{-\Delta_\tau H} | \alpha_1 \rangle \langle \alpha_1 | e^{-\Delta_\tau H} | \alpha_0 \rangle$$

Use approximation for imaginary time evolution operator. Simplest way

$$Z \approx \sum_{\{\alpha\}} \langle \alpha_0 | 1 - \Delta_\tau H | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | 1 - \Delta_\tau H | \alpha_1 \rangle \langle \alpha_1 | 1 - \Delta_\tau H | \alpha_0 \rangle$$

Leads to error $\propto \Delta_\tau$. Limit $\Delta_\tau \rightarrow 0$ can be taken

Example: hard-core bosons

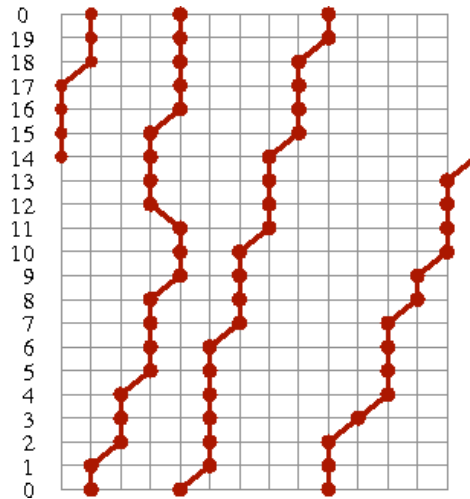
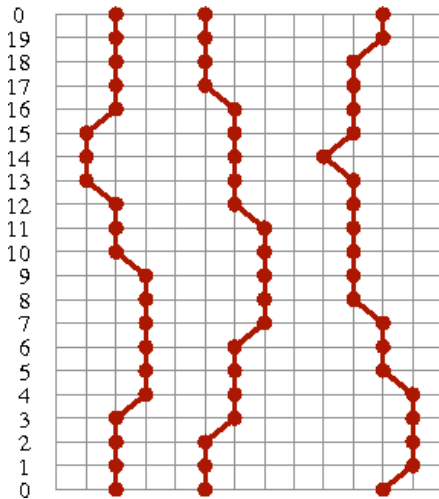
$$H = K = - \sum_{\langle i,j \rangle} K_{ij} = - \sum_{\langle i,j \rangle} (a_j^\dagger a_i + a_i^\dagger a_j) \quad n_i = a_i^\dagger a_i \in \{0, 1\}$$

Equivalent to S=1/2 XY model

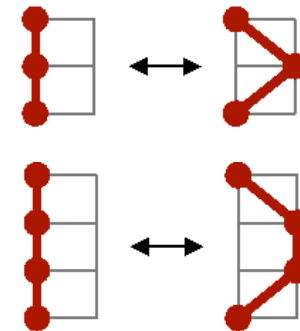
$$H = -2 \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) = - \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+), \quad S^z = \pm \frac{1}{2} \sim n_i = 0, 1$$

“World line” representation of

$$Z \approx \sum_{\{\alpha\}} \langle \alpha_0 | 1 - \Delta_\tau H | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | 1 - \Delta_\tau H | \alpha_1 \rangle \langle \alpha_1 | 1 - \Delta_\tau H | \alpha_0 \rangle$$



world line moves for
Monte Carlo sampling



$$Z = \sum_{\{\alpha\}} W(\{\alpha\}), \quad W(\{\alpha\}) = \Delta_\tau^{n_K} \quad n_K = \text{number of “jumps”}$$

Expectation values

$$\langle A \rangle = \frac{1}{Z} \sum_{\{\alpha\}} \langle \alpha_0 | e^{-\Delta\tau} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | e^{-\Delta\tau H} | \alpha_1 \rangle \langle \alpha_1 | e^{-\Delta\tau H} A | \alpha_0 \rangle$$

We want to write this in a form suitable for MC importance sampling

$$\langle A \rangle = \frac{\sum_{\{\alpha\}} A(\{\alpha\}) W(\{\alpha\})}{\sum_{\{\alpha\}} W(\{\alpha\})} \longrightarrow \langle A \rangle = \langle A(\{\alpha\}) \rangle_W$$

$W(\{\alpha\}) =$ weight

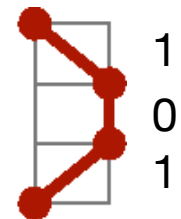
$A(\{\alpha\}) =$ estimator

For any quantity diagonal in the occupation numbers (spin z):

$$A(\{\alpha\}) = A(\alpha_n) \quad \text{or} \quad A(\{\alpha\}) = \frac{1}{L} \sum_{l=0}^{L-1} A(\alpha_l)$$

Kinetic energy (here full energy). Use

$$K e^{-\Delta\tau K} \approx K \quad K_{ij}(\{\alpha\}) = \frac{\langle \alpha_1 | K_{ij} | \alpha_0 \rangle}{\langle \alpha_1 | 1 - \Delta\tau K | \alpha_0 \rangle} \in \left\{ 0, \frac{1}{\Delta\tau} \right\}$$



Average over all slices \rightarrow count number of kinetic jumps

$$\langle K_{ij} \rangle = \frac{\langle n_{ij} \rangle}{\beta}, \quad \langle K \rangle = -\frac{\langle n_K \rangle}{\beta} \quad \langle K \rangle \propto N \rightarrow \langle n_K \rangle \propto \beta N$$

There should be of the order βN “jumps” (regardless of approximation used)