Wang-Landau sampling for Quantum Monte Carlo

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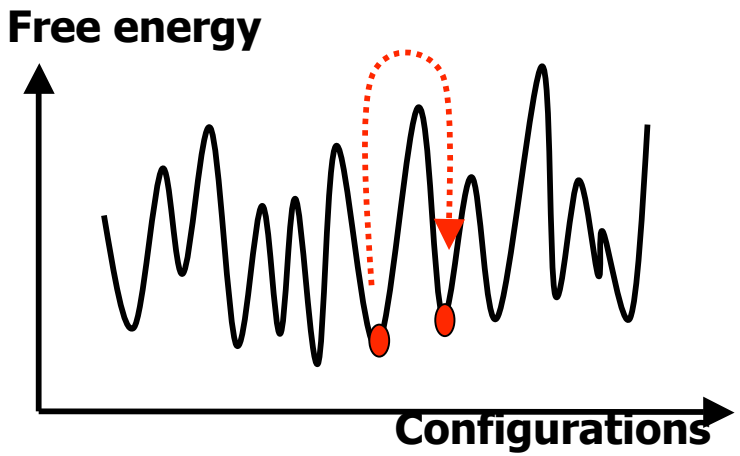
Overview

- Classical Monte Carlo
- First order phase transitions
- Classical Wang-Landau algorithm
- Extension to quantum systems
- Applications



Classical Monte Carlo simulations

- We 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 $\Delta A = \sqrt{\frac{\mathrm{Var}\, A}{M}}$

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

Markov chains and Metropolis algorithm

- 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:

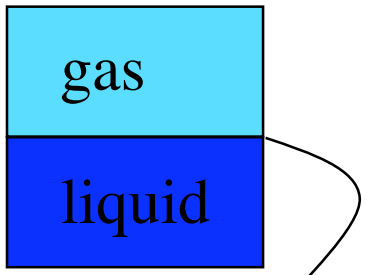
$$\frac{W_{x,y}}{W_{y,x}} = \frac{p_y}{p_x}$$

- Simplest algorithm due to Metropolis (1953): $W_{x,y} = \min[1, p_y / p_x]$

- Needs only relative probabilities (energy differences) $p_y / p_x = e^{-\beta(E_y - E_x)}$

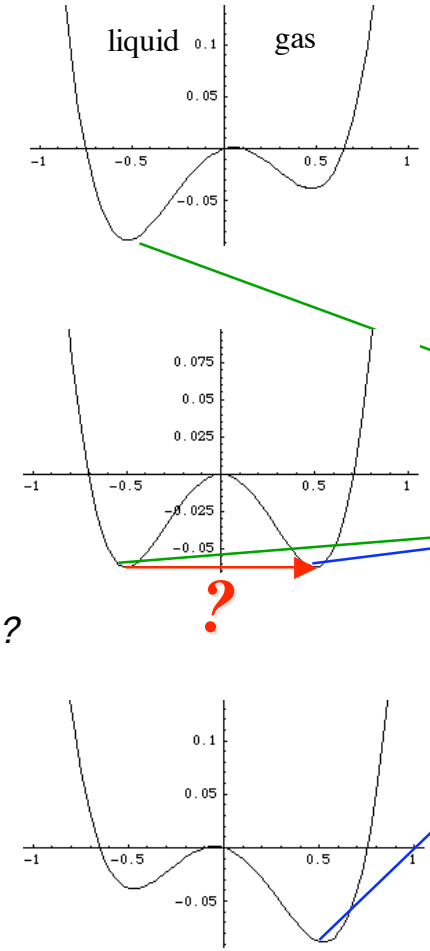
First order phase transitions

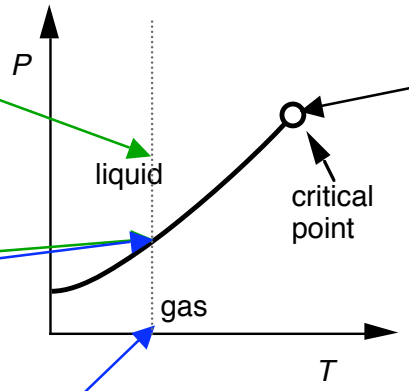
- Tunneling out of meta-stable state is suppressed exponentially

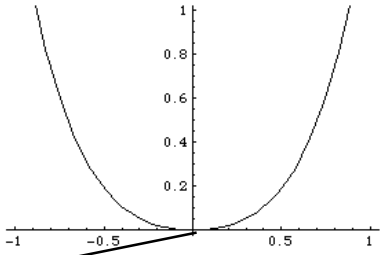


$$\tau \propto e^{-cL^{d-1}/T}$$

How can we tunnel out of metastable state?







Critical slowing down

At critical point was solved by cluster updates

The Wang-Landau method

- Directly calculates density of states $r(E)$ instead of canonical averages

- Acceptance rate proportional to inverse density of states

$$p_i = \frac{1}{\rho(E_i)} \text{ instead of } p_i = e^{-E_i/k_B T}$$

- All energy levels visited equally well

$$P(E) = \sum_c \delta_{E_c,E} \, P(c) \propto \rho(E) \frac{1}{\rho(E)} = 1$$

- Random walk in energy space
  - Flat histogram in energy space => *no tunneling problem*

- *Free energy accessible*

$$F = -k_B T \ln \sum_E \rho(E) e^{-E/k_B T}$$

- One simulation gives results for all T

F. Wang & D.P. Landau (2001)

The Wang-Landau algorithm

- Initially, $r(E)$ is unknown
  - Start with $r(E)$=1 and adjust iteratively

- Only a few modifications to usual sampling needed

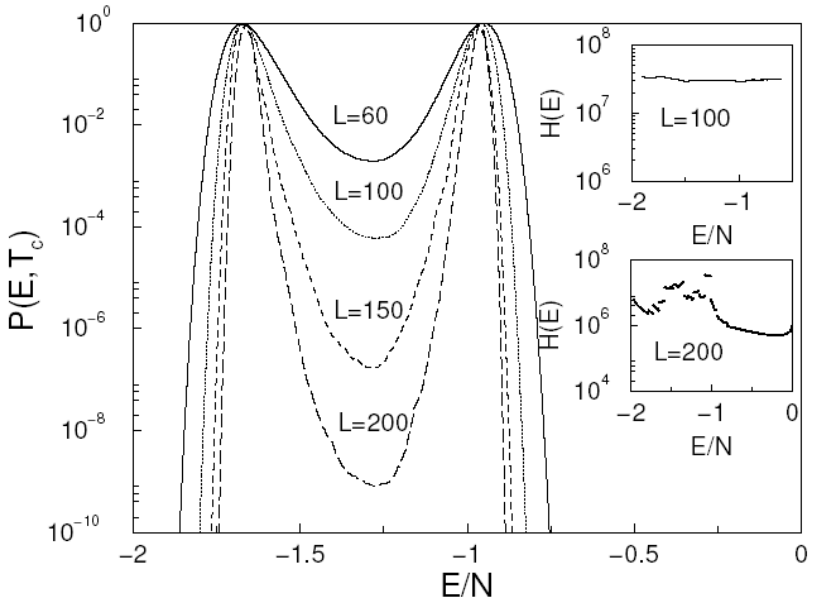
Start with modification factor $f=e$
do {
  do {
    Metropolis updates with transition probability $W[i \to j] = \min[1, r(E_i) / r(E_j)]$
    Adjust $r(E)$ at each step: $r(E) \leftarrow r(E) \times f$
    Increase histogram $H(E)$++
  } until histogram $H(E)$ is "flat" (e.g. 20%)
  decrease f (e.g. $f \leftarrow \sqrt{f}$)
  reset $H(E)$
} until $f - 1 \approx 10^{-8}$

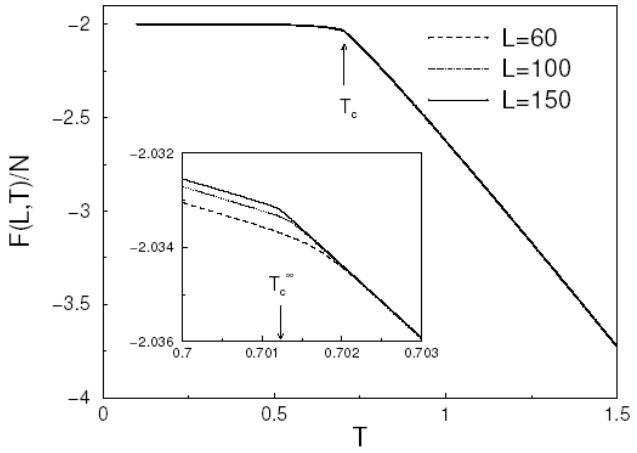
- Comments
  - Initially: multiplicative changes with large f allow rapid crude convergence
  - Finally: small f means fine structure of $r(E)$ can be mapped out

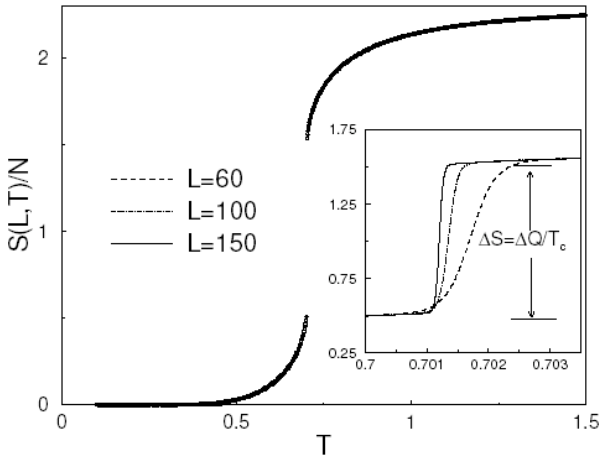
Example application of Wang-Landau sampling

- 10 states Potts model in 2D
  - First order phase transition
  - T_c=0.701

$$P(E,T_c) = \rho(E)e^{-E/k_BT_c}$$







Applications and Extensions

- First and second order phase transitions and disorder
  - F. Wang and D.P. Landau, (2001)
- Scaling analysis for Ising spin glasses
  - P. Dayal, et al., (2003).
- Improved sampling and optimized ensembles
  - S. Trebst, D. Huse, and M. Troyer, (2003)
  - C. Zhou and R.N. Bhatt, (2003)
  - B.J. Schulz et al., (2002).
  - C. Yamaguchi and N. Kawashima, (2002).
- Continuum simulations
  - Q. Yan et al., (2002).
  - M.S. Shell et al., (2002).
- Polymer films
  - T.S. Jan et al., (2002).
- Protein folding
  - N. Rathore et al., (2002).

Try out the Ψ-Mag Wang-Landau tutorial!

Quantum version of the Wang-Landau algorithm

- Density of states not accessible directly in quantum case
  - Classical $$Z = \sum_c e^{-E_c / k_B T} = \sum_E \rho(E) e^{-E / k_B T}$$
  - Quantum $$Z = \mathrm{Tr}\, e^{-\beta H}$$
- Quantum version based on SSE

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

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

$$= \sum_{n=0}^{\Lambda} \beta^n g(n)$$

- We have a similar expression as a sum over orders n instead of energies

Quantum version of the Wang-Landau algorithm

- We want flat histogram in order n
  - Use the Wang-Landau algorithm to get

$$Z = \sum_{n=0}^{\Lambda} \beta^n g(n) \qquad \text{from} \qquad Z = \sum_{n=0}^{\Lambda} \sum_{|\alpha\rangle} \sum_{(b_1,\ldots,b_\Lambda)} \frac{(\Lambda - n)!\beta^n}{\Lambda!} \langle \alpha | \prod_{i=1}^{\Lambda} (-H_{b_i}) | \alpha \rangle$$

  - Small change in acceptance rates for diagonal updates

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

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

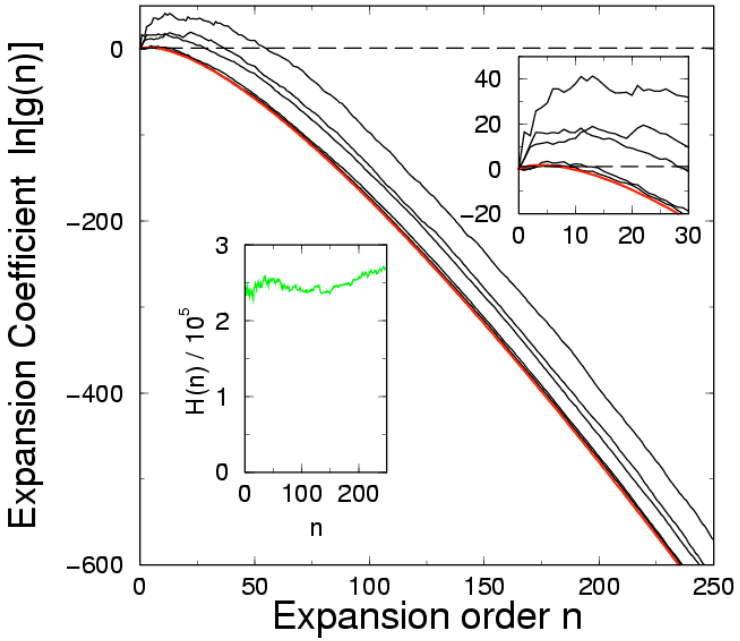
- Nonlocal updates (directed loops, …) do not change n and thus remain unchanged!
- Cutoff L limits temperatures to b < L / E_0

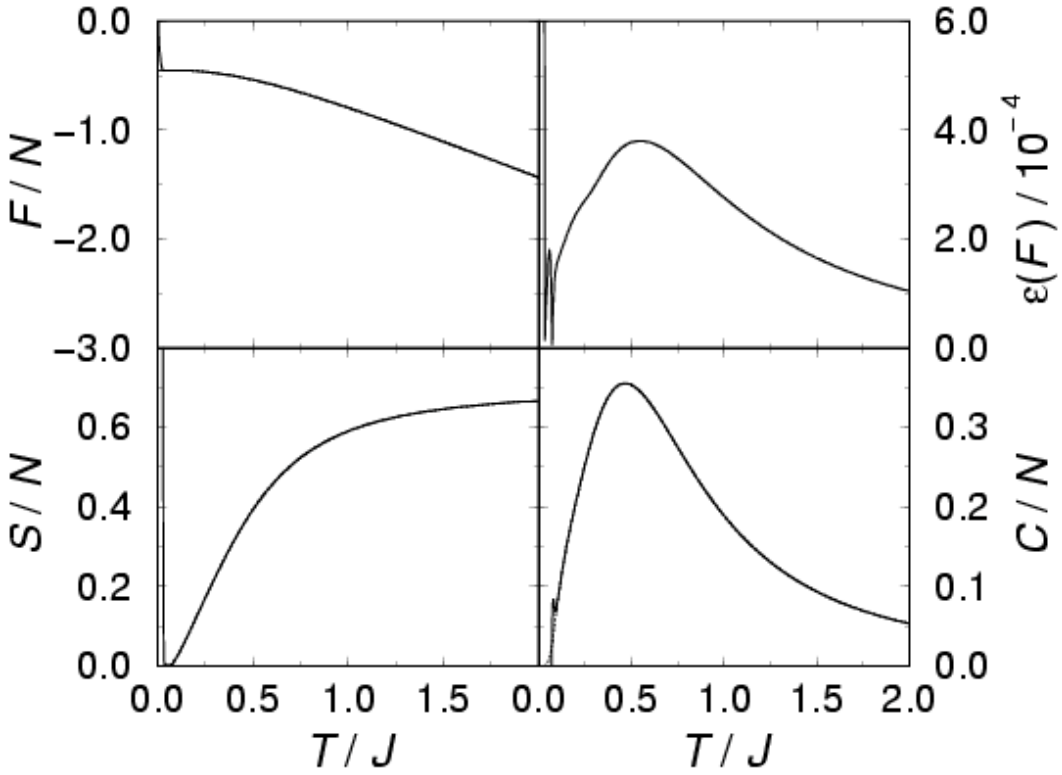
A first test

- L=10 site Heisenberg chain with L = 250
  - Free energy and entropy available
  - One simulation for all temperatures
  - Clear limit of reliability

    $T>0.05J$ due to cutoff

$$H = J\sum_{i=1}^{10} \vec{S}_i \cdot \vec{S}_{i+1}$$

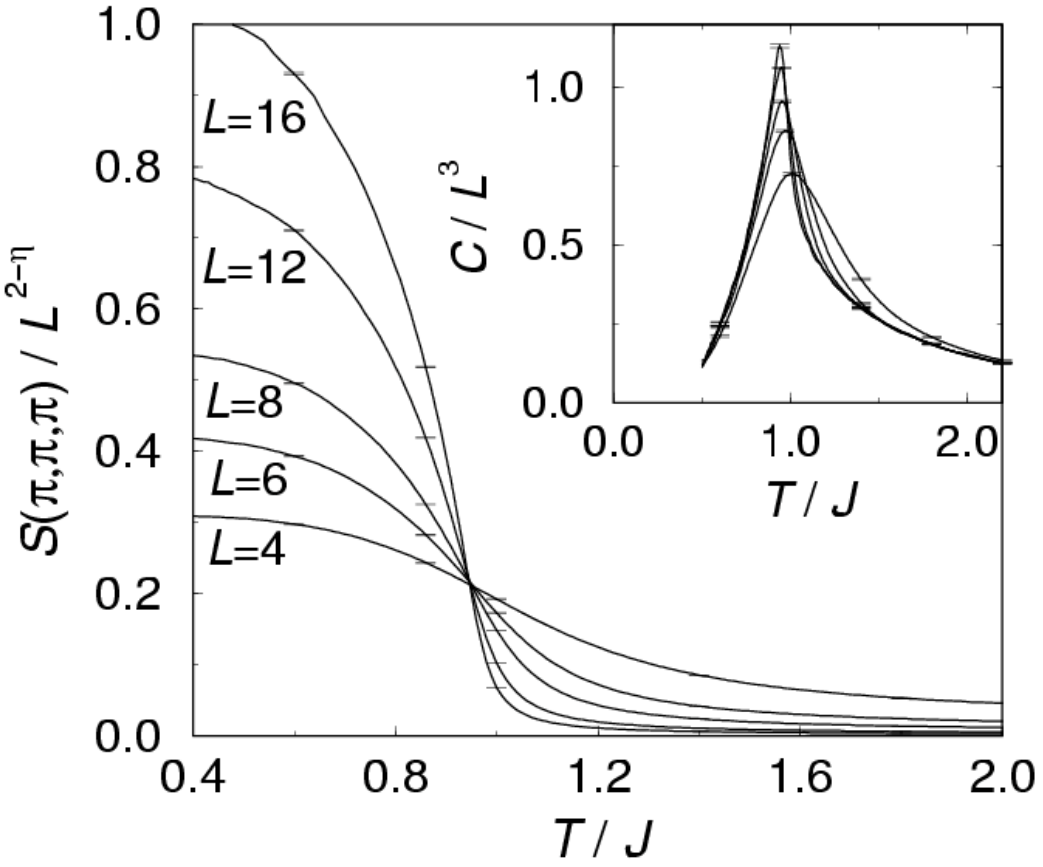




Thermal phase transitions

- 3D Heisenberg antiferromagnet
  - Second order phase transition at T_c=0.947J
  - Parallelization via splitting of the n-range among several CPUs

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



Quantum version – perturbation expansion

- Instead of temperature a coupling constant can be varied

$$H = H_0 + \lambda V$$

- Based on finite temperature perturbation expansion

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

$$\approx \sum_{n=0}^{\Lambda} \sum_{|\alpha\rangle} \sum_{(b_1,\ldots,b_\Lambda)} \frac{(\Lambda - n)!\beta^n}{\Lambda!} \langle \alpha | \prod_{i=1}^{\Lambda} (-H_{b_i}) | \alpha \rangle \lambda^{n_\lambda(b_1,\ldots,b_\Lambda)}$$

$$= \sum_{n_\lambda=0}^{\Lambda} \lambda^{n_\lambda} g(n_\lambda)$$

$n_\lambda(b_1,\ldots,b_n)$ counts # of λ terms

- Flat histogram in order n_l of perturbation expansion

Perturbation series by Wang-Landau

- We want flat histogram in order n_l
  - Use the Wang-Landau algorithm to get

$$Z = \sum_{n_\lambda=0}^{\Lambda} \lambda^{n_\lambda} g(n_\lambda) \quad \text{from} \quad Z = \sum_{n=0}^{\Lambda} \sum_{|\alpha\rangle} \sum_{(b_1,\ldots,b_\Lambda)} \frac{(\Lambda-n)!\beta^n}{\Lambda!} \langle\alpha| \prod_{i=1}^{\Lambda} (-H_{b_i}) |\alpha\rangle \lambda^{n_\lambda(b_1,\ldots,b_\Lambda)}$$

  - Small change in acceptance rates for diagonal updates

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

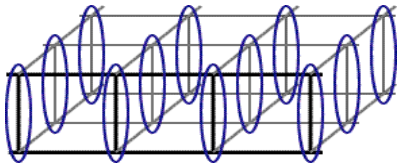
$$P[H^d_{(i,j)} \to 1] = \min\left(1, \frac{\Lambda - n + 1}{\beta N_{bonds} \langle\alpha|H^d_{(i,j)}|\alpha\rangle}\right) \xrightarrow{\text{Wang-Landau}} \min\left(1, \frac{\Lambda - n + 1}{\beta N_{bonds} \langle\alpha|H^d_{(i,j)}|\alpha\rangle} \frac{g(n_\lambda)}{g(n_\lambda - \Delta n_\lambda)}\right)$$

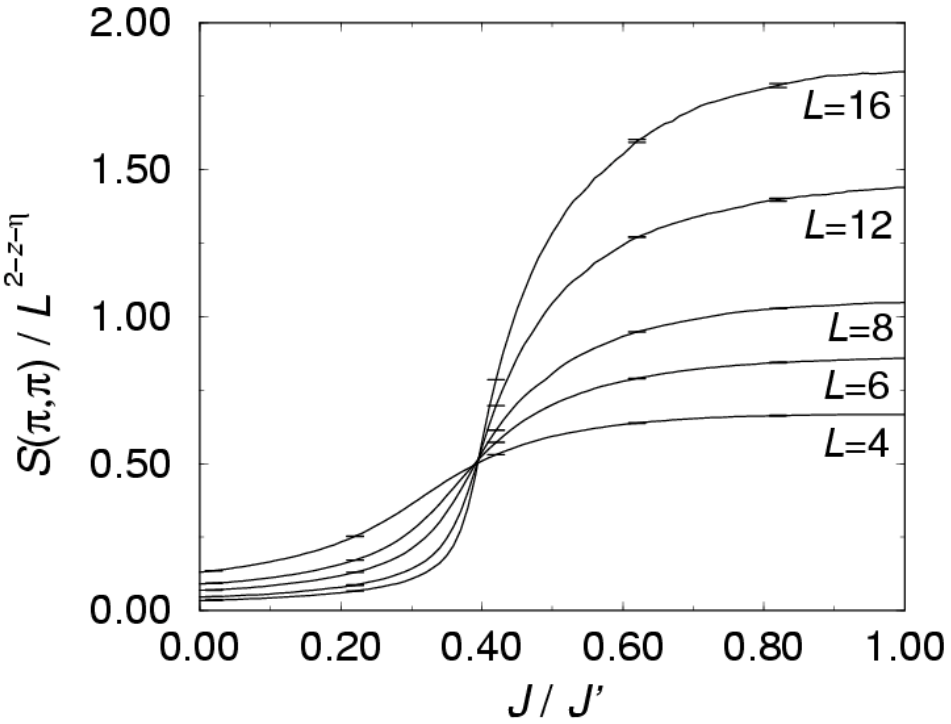
- Nonlocal updates (directed loops, …) do not change n_λ and thus remain unchanged!
- Cutoff L limits value of l for which the series converges

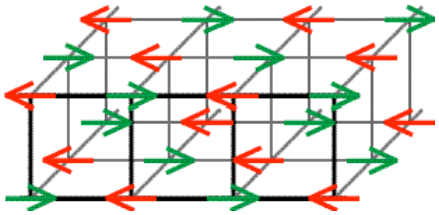
Quantum phase transition

- Bilayer Heisenberg Antiferromagnet
  - Single simulation gives results for all values of $\lambda = J/J'$
  - Quantum phase transition at $\lambda = 0.396$
  - Parallelization as in thermal case

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



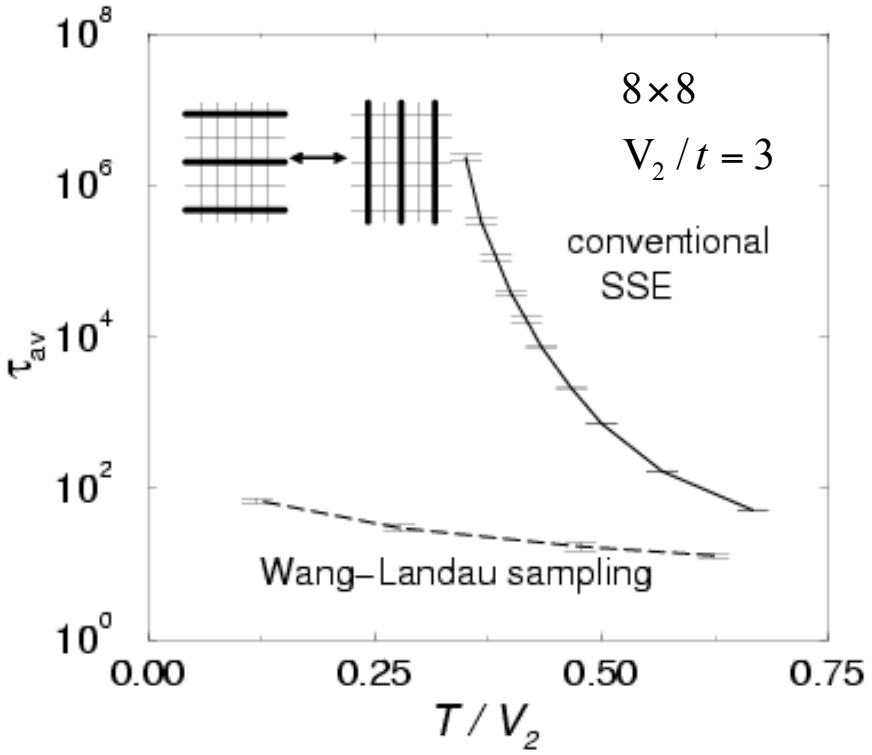




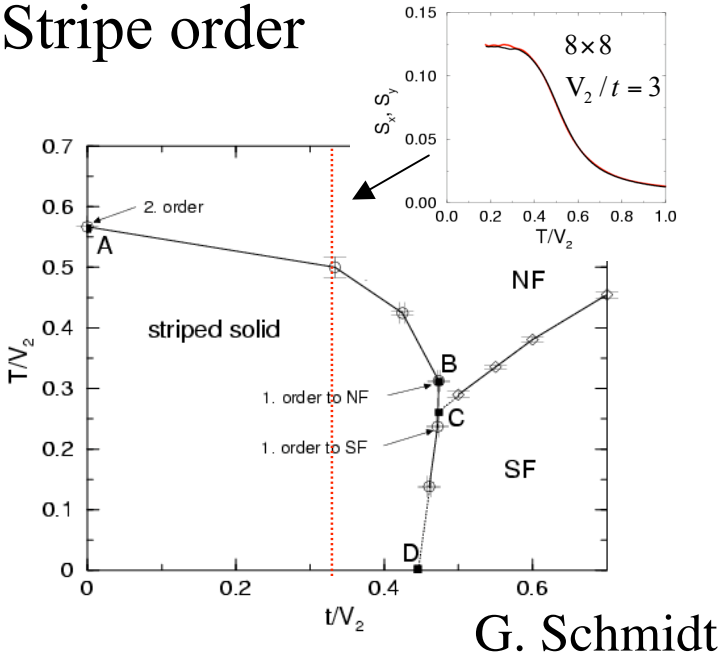
Speedup at first order phase transitions

- Greatly reduced tunneling times at free energy barriers
  - 2D hard-core bosons

$$H = -t \sum_{\langle i,j \rangle} \left(a_i^\dagger a_j + h.c. \right) + V_2 \sum_{\langle\langle i,j \rangle\rangle} n_i n_j$$



Stripe order



G. Schmidt

Summary

- Extension of Wang-Landau sampling to quantum systems
- Stochastically evaluate series expansion coefficients
  - High-temperature series

$$Z = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} g(n)$$

  - Perturbation series

$$Z = \sum_{n_\lambda=0}^{\infty} \lambda^{n_\lambda} g(n_\lambda)$$

- Features
  - Flat histogram in the expansion order
  - Allows calculation of free energy
  - Like classical systems, allows tunneling through free energy barriers

Qantum Wang-Landau in ALPS

- Application *qmc/qwl*
- Allows high temperature expansions for isotropic spin-1/2 systems
- You can reproduce the data presented here in the *qwl tutorial*.

Tutorial V: Quantum Wang-Landau Monte Carlo Simulations

- Tutorial I: Running and evaluating MC simulations using ALPS
- Tutorial II: Classical Monte Carlo Simulations
- Tutorial III: Quantum Monte Carlo Simulations (SSE)
- Tutorial IV: Quantum Monte Carlo Simulations (worm code)
- **Tutorial V: Quantum Wang-Landau Monte Carlo Simulations**
- Tutorial VI: Density Matrix Renormalization Group for a particle in a box (non-interacting DMRG)

Part I: Thermodynamics of Heisenberg quantum spin chains

The ferromagnetic Heisenberg chain

The parameter file **qwl/parm1** sets up a Monte Carlo simulation of the quantum mechanical Heisenberg **ferromagnet** on a **one-dimensional chain** with 40 sites, using the quantum Wang-Landau (QWL) method.

```
LATTICE="chain lattice"
MODEL="spin"
LATTICE_LIBRARY="../lattices.xml"
MODEL_LIBRARY="../models.xml"
S        = 1/2
L        = 40
T_MIN    = 0.1
T_MAX    = 10.0
DELTA_T  = 0.1
CUTOFF   = 500
{J = -1}
```