Introduction to
Quantum Monte Carlo

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Outline

♦ Examples of QMC applications
♦ Representations and local updates
  ♦ World-line representations
    ♦ Discrete time
    ♦ Continuous time
  ♦ Path-integral representation
  ♦ Stochastic series expansion (SSE) representation
♦ Comparison
♦ The sign problem
What can modern QMC algorithms do?

♦ Local updates (before 1994)
  ♦ 200 spins
  ♦ T=0.1

♦ Cluster algorithms (after 1995)
  ♦ 2D quantum phase transition: 20'000 spins at T=0.005
  ♦ 2D square lattice: 1'000'000 spins at T=0.2

♦ Extended ensembles (Quantum Wang-Landau, Parallel Tempering)
  ♦ Allows efficient simulation of 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 quantum magnets and bosonic systems
Example 1: Quantum phase transitions

- Bilayer antiferromagnet

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

\( J \ll J_\perp \): spin gap, no long range order

\( J \gg J_\perp \): long range order

Quantum phase transition at \( J_\perp / J \approx 2.524(2) \)
- Spin gap vanishes
- Magnetic order vanishes
- Universal properties
Example 1: Critical exponents

- 2D quantum phase transition in a quantum Heisenberg antiferromagnet

- Simulations of 20,000 spins at low temperatures

<table>
<thead>
<tr>
<th>Model</th>
<th>$\beta$</th>
<th>$\nu$</th>
<th>$\eta$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>QMC results</td>
<td>$0.345 \pm 0.025$</td>
<td>$0.685 \pm 0.035$</td>
<td>$0.015 \pm 0.020$</td>
<td>$1.018 \pm 0.02$</td>
</tr>
<tr>
<td>no assumption</td>
<td>$0.3639 \pm 0.0035$</td>
<td>$0.7048 \pm 0.0030$</td>
<td>$0.034 \pm 0.005$</td>
<td>$0.02$</td>
</tr>
<tr>
<td>3D classical</td>
<td>$0.0035$</td>
<td>$0.0030$</td>
<td>$0.005$</td>
<td></td>
</tr>
<tr>
<td>Mean field</td>
<td>$1/2$</td>
<td>$1$</td>
<td>$0$</td>
<td></td>
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</tbody>
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- Consistent with classical 3D Heisenberg model exponents
- Can do quantum simulations with the same accuracy as classical
Example 2: Trapped atoms on optical lattices

- Bose-Hubbard model
  - Both soft- and hardcore
  - Harmonic trapping potential
- Realistic modeling of 1D, 2D, 3D traps
- Density profiles, Momentum distribution

\[ U / t = 6.7 \]

\[ U / t = 25.0 \]

Lattice depth

Review: 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
  \implies \text{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

\[ \langle A \rangle \approx A = \frac{1}{M} \sum_{i=1}^M A_{c_i} \]

  - Within a statistical error

\[ \Delta A = \sqrt{(1 + 2 \tau_A) \frac{\text{Var} A}{M}} \]

- Problem: we cannot calculate \( p_{c_i} = e^{-\beta E_{c_i}} / Z \) since we do not know \( Z \)
Metropolis algorithm builds a Markov chain

\[ c_1 \to c_2 \to \ldots \to c_i \to c_{i+1} \to \ldots \]

Transition probabilities \( W_{x,y} \) for transition \( x \to y \) need to fulfill

- Ergodicity: any configuration reachable from any other

\[ \forall x, y \exists n : (W^n)_{x,y} \neq 0 \]

- Detailed balance:

\[ \frac{W_{x,y}}{W_{y,x}} = \frac{p_y}{p_x} \]

Simplest algorithm due to Metropolis (1953):

\[ W_{x,y} = \min[1, \frac{p_y}{p_x}] \]

Needs only relative probabilities (energy differences)

\[ \frac{p_y}{p_x} = e^{-\beta(E_y - E_x)} \]
Quantum Monte Carlo simulations

♦ Not as “easy” as classical Monte Carlo

\[ Z = \text{Tr} \ e^{-\beta H} = \sum_c e^{-\beta E_c} \]

♦ Calculating the energy eigenvalue \( E_c \) is equivalent to solving the problem

♦ Need to find a mapping of the quantum partition function to a classical problem

\[ Z = \text{Tr} e^{-\beta H} \equiv \sum_c p_c \]

♦ Different approaches
  ♦ 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 $h$

$$H_{XXZ} = J_{xz}(S_1^x S_2^x + S_1^y S_2^y) + J_z S_1^z S_2^z - h(S_1^z + S_2^z)$$

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

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

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

- Hamiltonian matrix in 2-site basis

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

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

- Traditionally employing local updates using Metropolis sampling
- Continuous time version can be constructed (Prokof'ev et al. 1996)
- Cluster updates using the loop algorithm (Evertz et al. 1993)
The Trotter-Suzuki decomposition

- Generic mapping of a quantum spin system onto a classical Ising model
  - basis of most QMC algorithms
  - not limited to special cases
- 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
  \[ Z = \text{Tr} e^{-\beta H} = \text{Tr} e^{-\beta (H_1 + H_2)} = \lim_{M \to \infty} \text{Tr} \left( (e^{-\Delta \tau (H_1 + H_2)} )^M \right) = \text{Tr} \left( (e^{-\Delta \tau H_1} e^{-\Delta \tau H_2} )^M \right) + O(\Delta \tau^2) \]
- Insert 2M sets of complete basis states
  \[ = \sum_{i_1, \ldots, i_{2M}} \langle i_1 | e^{-\Delta \tau H_1} | i_{2M} \rangle \langle i_{2M} | e^{-\Delta \tau H_2} | i_{2M-1} \rangle \cdots \langle i_3 | e^{-\Delta \tau H_1} | i_2 \rangle \langle i_2 | e^{-\Delta \tau H_2} | i_1 \rangle \]
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

$$Z = \sum_{i_1,\ldots,i_{2M}} \langle i_1 | e^{-\Delta\hat{H}_1} | i_{2M} \rangle \langle i_{2M} | e^{-\Delta\hat{H}_2} | i_{2M-1} \rangle \cdots \langle i_3 | e^{-\Delta\hat{H}_1} | i_2 \rangle \langle i_2 | e^{-\Delta\hat{H}_2} | i_1 \rangle$$

♦ Each of the
  ♦ matrix elements
  $\langle i_{j+1} | e^{-\Delta\hat{H}_{1,2}} | i_j \rangle$
  ♦ corresponds to a
  ♦ row of shaded plaquettes and equals
  ♦ the product over those plaquettes
The weights for the spin-1/2 Heisenberg model

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

\[ Z = \sum_{C} W(C) = \sum_{C} \prod_{\text{plaquettes } p} w(C_p) \]

- Conservation of magnetization on each bond

- The only allowed plaquette-configurations are

<table>
<thead>
<tr>
<th>( C_p )</th>
<th>[ e^{-\Delta J/4} ]</th>
<th>[ e^{\Delta J/4} \text{ch}(\Delta \tau J/2) ]</th>
<th>[ e^{\Delta J/4} \text{sh}(\Delta \tau J/2) ]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \omega(C_p) )</td>
<td></td>
<td></td>
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</table>

- Ferromagnet (J<0)
  - All weights are positive

- Antiferromagnet on a bipartite lattice
  - perform a gauge transformation on one sublattice

\[ \frac{J}{2}(S_i^+S_j^- + S_i^-S_j^+) \quad S_i^\pm \rightarrow (-1)^{l_i}S_i^\pm \quad -\frac{J}{2}(S_i^+S_j^- + S_i^-S_j^+) \]

- Frustrated antiferromagnet:
  - we have a sign problem
Worldlines

♦ Each valid configuration is represented by continuous worldlines

Sampling over all (important) worldline configurations

♦ According to the above weight
♦ Try to generate a new configurations from a given one
Local updates

♦ Move the world lines locally using Metropolis
  ♦ probabilities given by the resulting plaquette weights

♦ Consider the limit of small $\Delta\tau$
  ♦ Insert or remove two kinks

\[
P_{\rightarrow} = \min[1, (\Delta\tau J / 2)^2] \\
P_{\leftarrow} = \min[1, 1/(\Delta\tau J / 2)^2]
\]

♦ Shift a kink

\[
P_{\rightarrow} = P_{\leftarrow} = 1 \\
P = \Delta\tau J / 2
\]
Local updates

♦ Problems:
  ♦ Restricted to canonical ensemble
  ♦ No change of magnetization, particle number, winding number
  ♦ Critical slowing down

♦ Solution for classical Monte Carlo: cluster algorithms

♦ Try the same for the quantum case
  ♦ Loop algorithm (talk by H.G. Evertz)
  ♦ Worm update (talk by S. Trebst)
  ♦ Directed loops (talk by F. Alet)
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 \( M \))

\[ \Delta \tau = \frac{\beta}{M} \]

- The limit \( \Delta \tau \to 0 \) can be taken in the construction of the algorithm! (Prokof'ev et al. 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
Path integral representation

- 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

- Continuous time representation
- Discrete local objects (kinks, changes in wordline-configuration)
- Local updates of kinks using Metropolis
- Improved update scheme using Worm update (Prokofev et al., 1997)

**Talk by S. Trebst**
Path integral representation

- **Perturbation expansion:**

\[
H = H_0 + V, \quad H_0 = \sum_{<i,j>} J^{z}_{ij} S^z_i S^z_j - \sum_i h S^z_i, \quad V = \sum_{<i,j>} J^{xy}_{ij} (S^x_i S^x_j + S^y_i S^y_j)
\]

\[
Z = \text{Tr}(e^{-\beta H}) = \text{Tr}(e^{-\beta H_0} \text{Te}^{-\int_0^\beta d\tau V(\tau)})
\]

\[
Z = \text{Tr}(e^{-\beta H_0} (1 - \int_0^\beta d\tau V(\tau)) + \int_0^\beta d\tau_2 \int_0^\tau_2 d\tau_1 V(\tau_2) V(\tau_1) + ...))
\]

- Each term represented by a world line configuration
Local updates in continuous time

♦ Shift a kink

![Diagram showing kink shift]

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

![Diagram showing kink insertion/removal]

\[ P = 1 \quad P = (\Delta \tau J / 2)^2 \to 0 \]

♦ Vanishing acceptance rate: \[ P_\rightarrow = \min[1, (\Delta \tau J / 2)^2] \to 0 \]

♦ Solution: Integrate over all possible insertion in a finite time window

\[ P_\rightarrow = \int_0^\Lambda \int_\tau_1^\Lambda (J / 2)^2 d\tau_2 d\tau_1 \to \frac{\Lambda^2 J^2}{8} \neq 0 \]
Stochastic series expansion (SSE) approach

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

Talk by F. Alet
Decomposing the Hamiltonian for SSE

- Break up the Hamiltonian into offdiagonal and diagonal bond terms

\[ H = \sum_{\langle i, j \rangle} H_{(i,j)}^o + H_{(i,j)}^d \]

- Example: Heisenberg antiferromagnet

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

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

\[
= \sum_{\langle i, j \rangle} H_{(i,j)}^o + \sum_{\langle i, j \rangle} H_{(i,j)}^d
\]

with

\[
H_{(i,j)}^o = \frac{J_{xy}}{2} (S_i^+ S_j^- + S_i^- S_j^+)
\]

\[
H_{(i,j)}^d = J_z S_i^z S_j^z - \frac{h}{z} (S_i^z + S_j^z)
\]

convert site terms into bond terms

split into diagonal and offdiagonal bond terms
High temperature series expansion

- Expansion in inverse temperature

\[ Z = \text{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \text{Tr}(-H^n) \]

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

- Using the bond Hamiltonians

\[ H_{b_i} \in \bigcup_{i,j} \{ H_{(i,j)}^d, H_{(i,j)}^o \} \]
Ensuring positive diagonal bond weights

- **SSE expansion:**

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

\[
= \sum_{n=0}^{\infty} \sum_{\{\alpha\}} \sum_{(b_1,\ldots,b_n)} W(|\alpha\rangle, (b_1,\ldots,b_n)) 
\]

- Negative matrix elements are the bond weights

  - Need to make all matrix elements non-positive

  - Diagonal matrix elements: subtract an energy shift \( C \geq \frac{|J_z|}{4} + |h| \)

    - Does not change the physics

\[
H_{(i,j)}^d = J_z S_i^z S_j^z - \frac{h}{z} (S_i^z + S_j^z) - C 
\]
Positivity of off-diagonal bond weights

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

\[ H_{(i,j)}^o = \frac{J_{xy}}{2} (S_i^+ S_j^- + S_i^- S_j^+) \]

- Ferromagnet \((J_{xy} < 0)\)
  - no problem

- Antiferromagnet on a bipartite lattice
  - perform a gauge transformation on one sublattice

\[ \frac{J_{xy}}{2} (S_i^+ S_j^- + S_i^- S_j^+) \rightarrow S_i^\pm \rightarrow (-1)^{|l|} S_i^\pm \rightarrow -\frac{J_{xy}}{2} (S_i^+ S_j^- + S_i^- S_j^+) \]

- 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

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

- Extend operator string to fixed length $\Lambda$ by adding extra unit operators:

$$H_{id} = -1 \quad n: \text{number of non-unit operators}$$

$$Z = \sum_{n=0}^{\Lambda} \sum_{\alpha} \sum_{(b_1, \ldots, b_{\Lambda})} \frac{(\Lambda - n)! \beta^n}{\Lambda!} \langle \alpha \prod_{i=1}^{\Lambda} (-H_{b_i}) \alpha \rangle \quad H_{b_i} \in \{H_{id}\} \cup \bigcup_{\langle i, j \rangle} \{H_{d}^{d}, H_{o}^{o}\}$$

- Ensure $\Lambda$ large enough during thermalization

  - Such that e.g. $n_{\max} < \frac{3}{4} \Lambda$  

  - $n_{\max} > \langle n \rangle \propto \beta V$
The SSE configuration space

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

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

♦ Example for a four site system:

\[
\Lambda = 5
\]
\[
n = 4
\]
\[
|\alpha\rangle = | \downarrow \uparrow \uparrow \downarrow \rangle
\]
\[
S_{\Lambda} = (H_{(1,2)}^d, H_{(3,4)}^o, 1, H_{(3,4)}^o, H_{(1,2)}^d)
\]

♦ Sample over all possible configurations
  ♦ According to the above weights
  ♦ Need a way to generate new configurations from a given one
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:
    \[ \chi = \beta \left( \langle \alpha | \sum_i S_i^z | \alpha \rangle \right)^2 \]

- Some look a bit more involved:
  - Equal time diagonal correlations:
    \[ \langle D_1 D_2 \rangle = \left( \frac{1}{n+1} \sum_{p=0}^{n} d_2[p] d_1[p] \right) \text{, where} \ d_i[p] = \langle \alpha(p) | D_i | \alpha(p) \rangle \]
  - Imaginary time depended diagonal correlations:
    \[ \langle D_1(\tau) D_2(0) \rangle = \sum_{\Delta p=0}^{n} \left( \frac{\tau}{\Delta p} \right)^{\Delta p} \left( 1 - \frac{\tau}{\beta} \right)^{n-\Delta p} C_{12}(\Delta p) \]
    \[ C_{12}(\Delta p) = \frac{1}{n+1} \sum_{p=0}^{n} d_1[p+\Delta p] d_2[p] \]
Comparing path integrals and SSE

- **Perturbation Expansion:** \( H = H_0 + V \)
  \[
  Z = \text{Tr}(e^{-\beta H_0}(1 - \int_0^\beta d\tau V(\tau) + \int_0^\beta d\tau_2 \int_0^{\tau_2} d\tau_1 V(\tau_2)V(\tau_1) + \ldots)) \]

- **Decomposition into bond terms:** \( V = \sum_b H^o_b \)
  \[
  Z = \sum_{n=0}^{\infty} \sum |\alpha\rangle \sum_{b^o_1,\ldots,b^o_n} \beta \int_0^{\tau_n} d\tau_n \int_0^{\tau_{n-1}} d\tau_{n-1} \ldots \int_0^{\tau_1} d\tau_1 W(\alpha,\{b^o\},\{\tau\}) \]
  \[
  W(\alpha,\{b^o\},\{\tau\}) = (-1)^n \left( e^{-\beta E_0} \prod_{p=1}^n e^{-\tau_p (E_p - E_{p-1})} \right) \langle \alpha | \prod_{p=1}^n H^o_{b_p} | \alpha \rangle
  \]

- **Compare to SSE**
  \[
  Z = \sum_{n=0}^{\infty} \sum |\alpha\rangle \sum (b_1,\ldots,b_n) W(|\alpha\rangle, (b_1,\ldots,b_n))
  \]
Comparing path integrals and SSE

♦ Relation between the weights:

♦ Given: \( \{b^0\} = (b^0_1, ..., b^0_n) \)

\[
\sum_m \sum_{\{b\}=(b_1, ..., b_m)} W(\alpha, \{b\}) = \int_0^{\beta} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 \ W(\alpha, \{b^0\}, \{\tau\})
\]

♦ Operator string longer in SSE, including diagonal terms
♦ In perturbation expansion need to also sample over the continuum times (Sandvik et al. 1997)
Comparing path integrals and SSE

- **World lines in path integrals**
  - Advantage
    - Diagonal terms treated exactly
  - Disadvantage
    - Continuous imaginary time

- **World lines in SSE**
  - Advantage
    - Integer index instead of time
  - Disadvantage
    - Perturbation also in diagonal terms
The negative sign problem

♦ In mapping of quantum to classical system

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

♦ “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:

\[
\langle A \rangle = \frac{\sum_i A_i p_i}{\sum_i p_i} = \frac{\sum_i A_i \text{sgn} p_i |p_i|}{\sum_i |p_i|} = \frac{\langle A \text{Sign} \rangle_{|p|}}{\langle \text{Sign} \rangle_{|p|}}
\]

♦ Sampling \( Z_{|p|} = \sum_i |p_i| \)
The negative sign problem

- The average sign becomes very small:

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

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

- The error of the sign:

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

- 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
Is the sign problem exponentially hard?

♦ The sign problem is basis-dependent
  ♦ Diagonalize the Hamiltonian matrix \( H|i\rangle = \mathcal{E}_i|i\rangle \)

\[ \langle A \rangle = \frac{\text{Tr}[A \exp(-\beta H)]}{\text{Tr}[\exp(-\beta H)]} = \sum_i \langle i | A | i \rangle \exp(-\beta \mathcal{E}_i) \Big/ \sum_i \exp(-\beta \mathcal{E}_i) \]

♦ All weights are positive
♦ But this is an \textit{exponentially hard problem} since \( \text{dim}(H) = 2^N \)!
♦ 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
  ♦ No proof that they are exponentially hard
  ♦ No polynomial solution either
Complexity of decision problems

♦ Some problems are harder than others:

♦ Complexity class $P$
  ♦ Can be solved in polynomial time on a Turing machine
  ♦ Eulerian circuit problem
  ♦ Minimum spanning Tree (decision version)

♦ Complexity class $NP$
  ♦ Polynomial complexity using non-deterministic algorithms
  ♦ Hamiltonian circle problem
  ♦ Traveling salesman problem (decision version)
The complexity class P

♦ The Eulerian circuit problem
  ♦ Seven bridges in Königsberg (now Kaliningrad) crossed the river Pregel
  ♦ Can we do a roundtrip by crossing each bridge exactly once?
  ♦ Is there a closed walk on the graph going through each edge exactly once?

Looks like an expensive task by testing all possible paths.
♦ Euler: Desired path exits only if the coordination of each edge is even.
♦ This is of order $O(N^2)$
♦ Concerning Königsberg: NO!
The complexity class NP

- The Hamiltonian cycle problem
  - Sir Hamilton's Icosian game:
  - Is there a closed walk on the graph going through each vertex exactly once?

- Looks like an expensive task by testing all possible paths.
- No polynomial algorithm is known
- Nor a proof that it cannot be constructed
- Concerning the Icosian game: YES!
NP-hardness and NP-completeness

♦ Polynomial reduction
  ♦ Two decision problems Q and P:
    ♦ $Q \leq P$: there is an polynomial algorithm for Q, provided there is one for P
    ♦ Typical proof: Use the algorithm for P as a subroutine in an algorithm for P
    ♦ Many problems have been reduced to other problems

♦ NP-hardness
  ♦ A problem P is **NP-hard**, if $\forall Q \in NP: Q \leq P$

♦ NP-completeness
  ♦ A problem P is **NP-complete**, if P is NP-hard and $P \in NP$
  ♦ Most Problems in NP were shown to be NP-complete
The P versus NP problem

♦ Hundreds of important NP-complete problems in computer science
  ♦ Despite decades of research no polynomial time algorithm has been found
  ♦ Exponential complexity has not been proven either

♦ The P versus NP problem
  ♦ Is P=NP or is P≠NP?
  ♦ One of the millennium challenges of the Clay Math Foundation
    http://www.claymath.org
  ♦ 1 million US$ for proving either P=NP or P≠NP

♦ The situation is similar to the sign problem
  ♦ Despite decades of research no general polynomial time algorithm has been found
  ♦ Exponential complexity has not been proven either
The sign problem is NP-hard

- See: M. Troyer and U. Wiese, Report cond-mat/0408370
- Use the following theorem:
  - A problem is NP-hard, if \( \exists Q : Q \text{ NP-complete} \land Q \leq P \)
  - \( Q \) is the 3D classical spin glass problem
- This is bad news!
- Or not - if you solve it, you will get both
  - The Nobel price (??)
  - And the 1 Million US$...
How can we deal with the sign problem?

♦ 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
  ♦ Meron-Cluster approach
  ♦ Special choice of basis