7. Overview of modern QMC algorithms
Modern Monte Carlo algorithms

• Which system sizes can be studied?

<table>
<thead>
<tr>
<th>temperature</th>
<th>local updates</th>
<th>modern algorithms</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D Tc</td>
<td>16’000 spins</td>
<td>16’000’000 spins</td>
</tr>
<tr>
<td>0.1 J</td>
<td>200 spins</td>
<td>1’000’000 spins</td>
</tr>
<tr>
<td>0.005 J</td>
<td>——</td>
<td>50’000 spins</td>
</tr>
<tr>
<td>3D Tc</td>
<td>32 bosons</td>
<td>1’000’000 bosons</td>
</tr>
<tr>
<td>0.1 t</td>
<td>32 bosons</td>
<td>10’000 bosons</td>
</tr>
</tbody>
</table>
When to use SSE?

• For quantum magnets
  • loop cluster algorithm if there is spin inversion symmetry
  • directed loops if there is no spin inversion symmetry

• For hardcore bosons:
  • loop cluster algorithm if there is particle-hole symmetry
  • directed loops if there is no particle-hole symmetry

• Which models?
  • 2-site interactions are rather straightforward
  • multi-site interactions require more thought
When to use path integrals?

- For Bose-Hubbard models
  - Use the worm algorithm in continuous time path integrals
  - This expands only in the hopping $t$ and not the much larger repulsion $U$

- For non-local in time actions
  - Appear in dissipative (Caldeira-Legget type) models, coupling to phonons, DMFT, ...
  - Cluster algorithms are again possible in case of spin-inversion symmetry
8. Wang-Landau sampling and optimized ensembles for quantum systems
First order phase transitions

Tunneling out of meta-stable state is suppressed exponentially

\[ \tau \propto \exp(-cL^{d-1}/T) \]

How can we tunnel out of metastable state?

Critical slowing down solved by cluster updates
First order phase transitions

- **Tunneling problem** at a first order phase transition is solved by *changing the ensemble* to create a flat energy landscape
Quantum systems

• Classical:
  \[ Z = \sum_c e^{-E_c / k_BT} = \sum_E \rho(E)e^{-E / k_BT} \]

• Quantum: \( \rho(E) \) is not accessible
  • formulation in terms of \textit{high-temperature series}
    \[ Z = \text{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \text{Tr}(-H)^n = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} g(n) \]
  • or \textit{perturbation series}
    \[ Z = \text{Tr} e^{-\beta H} = \text{Tr} e^{-\beta(H_0 + \lambda V)} = \sum_{n=0}^{\infty} \lambda^n g(n) \]

• Flat histogram, parallel tempering, histogram reweighting, etc done in order \( n \) of series expansion instead of energy
Stochastic Series Expansion (SSE)

• based on high temperature expansion, (A. Sandvik, 1991)

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

\[ = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{\alpha_1, \ldots, \alpha_n} \langle \alpha_1 | - H | \alpha_2 \rangle \langle \alpha_2 | - H | \alpha_3 \rangle \cdots \langle \alpha_n | - H | \alpha_1 \rangle \]

• also has a graphical representation in terms of world lines

• is very similar to path integrals
  • perturb in all terms of the Hamiltonian, not just off-diagonal terms
Wang–Landau sampling for quantum systems

- **SSE:**
  \[
  Z = \text{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \text{Tr} \left[ (-H)^n \right]
  \]
  \[
  = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{\alpha_1, \ldots, \alpha_n} \langle \alpha_1 \mid -H \mid \alpha_2 \rangle \langle \alpha_2 \mid -H \mid \alpha_3 \rangle \cdots \langle \alpha_n \mid -H \mid \alpha_1 \rangle
  \]
  \[
  \equiv \sum_{n=0}^{\infty} \frac{\beta^n}{n!} g(n)
  \]

- compare to classical Monte Carlo:
  \[
  Z = \sum_{c} e^{-E_c / k_B T} = \sum_{E} \rho(E) e^{-E / k_B T}
  \]

- flat histogram obtained by changing the ensemble:
  - classically:
    \[
    e^{-\beta E_c} \rightarrow \frac{1}{\rho(E)}
    \]
  - quantum:
    \[
    \frac{\beta^n}{n!} \rightarrow \frac{1}{g(n)}
    \]
Wang-Landau updates in SSE

- We want flat histogram in order $n$
  - Use the Wang-Landau algorithm to get
    \[
    Z = \sum_{n=0}^{\Lambda} \beta^n g(n) \quad \text{from} \quad Z = \sum_{n=0}^{\Lambda} \sum_{\left\{ b_1, \ldots, b_{\Lambda} \right\}} \frac{(\Lambda - n)! \beta^n}{\Lambda!} \langle \alpha \prod_{i=1}^{\Lambda} (-H_{b_i}) | \alpha \rangle
    \]
  - Small change in acceptance rates for diagonal updates
    \[
    P[1 \rightarrow H_{(i,j)}^d] = \min \left( 1, \frac{\beta N_{\text{bonds}} \langle \alpha | H_{(i,j)}^d | \alpha \rangle}{\Lambda - n} \right) \xrightarrow{\text{Wang-Landau}} \min \left( 1, \frac{N_{\text{bonds}} \langle \alpha | H_{(i,j)}^d | \alpha \rangle g(n)}{\Lambda - n} g(n+1) \right)
    \]
    \[
    P[H_{(i,j)}^d \rightarrow 1] = \min \left( 1, \frac{\Lambda - n + 1}{\beta N_{\text{bonds}} \langle \alpha | H_{(i,j)}^d | \alpha \rangle} \right) \xrightarrow{\text{Wang-Landau}} \min \left( 1, \frac{\Lambda - n + 1}{N_{\text{bonds}} \langle \alpha | H_{(i,j)}^d | \alpha \rangle} g(n) g(n-1) \right)
    \]
- Loop update does not change $n$ and is thus unchanged!
- Cutoff $\Lambda$ limits temperatures to $\beta < \Lambda / E_0$
The first test

- L=10 site Heisenberg chain with $\Lambda = 250$

The graph shows the behavior of various quantities as a function of temperature, indicated by the temperature cutoff due to finite L.
Wang–Landau sampling for quantum systems

- Example: 3D quantum Heisenberg antiferromagnet
Speedup at first order phase transition

- Greatly reduced tunneling times at free energy barriers
  - Example: stripe rotation in 2D hard-core bosons

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

Friday, 9 July 2010
Perturbation expansion

- Instead of temperature a coupling constant can be changed
- Based on finite temperature perturbation expansion

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

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

\[= \sum_{n_\lambda=0}^{\Lambda} \lambda^{n_\lambda} g(n_\lambda) \quad \text{count of } \lambda \text{ terms} \]

- Flat histogram in order \( n_\lambda \) of perturbation expansion
Perturbation series by Wang-Landau

- We want flat histogram in order $n_\lambda$
- Use the Wang-Landau algorithm to get $Z = \sum_{n=0}^{\Lambda} \lambda^n g(n_\lambda)$ from $Z = \sum_{n=0}^{\Lambda} \sum_{\alpha \{b_1, \ldots, b_{\Lambda}\}} (\Lambda - n)! \beta^n \frac{\prod_{i=1}^{\Lambda} (-H_{b_i}) |\alpha\rangle \lambda^{n_\lambda(b_1, \ldots, b_{\Lambda})}}{\Lambda!}$$

- Small change in acceptance rates for diagonal updates

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

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

- Loop update does not change $n$ and is thus unchanged!
- Cutoff $\Lambda$ limits value of $\lambda$ for which the series converges
The antiferromagnetic bilayer

Quantum phase transition at $J_\perp / J \approx 2.524(2)$

- Spin gap vanishes
- Magnetic order vanishes
- Universal properties

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

$J >> J_\perp$: long range order
Quantum phase transition

• Quantum phase transition in bilayer quantum Heisenberg antiferromagnet
Summary

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

• High-temperature series
  \[ Z = \sum_{n=0}^{\infty} \beta^n g(n) \]

• 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

• Optimized ensembles are also possible
9. The negative sign problem in quantum Monte Carlo
Quantum Monte Carlo

• Not as easy as classical Monte Carlo

\[ Z = \sum_c e^{-E_c / k_B T} \]

• Calculating the eigenvalues \( E_c \) is equivalent to solving the problem

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

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

• “Negative sign” problem if some \( p_c < 0 \)
In mapping of quantum to classical system

\[ Z = \text{Tr} e^{-\beta H} = \sum_{i} p_i \]

there is a “sign problem” if some of the \( p_i < 0 \)

Appears e.g. in simulation of electrons when two electrons exchange places (Pauli principle)
The negative sign problem

- Sample with respect to absolute values of the weights

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

- Exponentially growing cancellation in the sign

\[
\langle \text{sign} \rangle = \frac{\sum_i p_i}{\sum_i |p_i|} = Z/Z_{|p|} = e^{-\beta V (f - f_{|p|})}
\]

- Exponential growth of errors

\[
\frac{\Delta \text{sign}}{\langle \text{sign} \rangle} = \frac{\sqrt{\langle \text{sign}^2 \rangle} - \langle \text{sign} \rangle}{\sqrt{M} \langle \text{sign} \rangle} \approx \frac{e^\beta V (f - f_{|p|})}{\sqrt{M}}
\]

- NP-hard problem (no general solution) [Troyer and Wiese, PRL 2005]
Is the sign problem exponentially hard?

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

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

- All weights are positive
- But this is an \textit{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
  - No proof that they are exponentially hard
  - No polynomial solution either
What is a solution of the sign problem?

- Consider a fermionic quantum system with a sign problem (some $p_i < 0$)

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

- Where the sampling of the bosonic system with respect to $|p_i|$ scales polynomially

$$T \propto \epsilon^{-2} N^n \beta^m$$

- A solution of the sign problem is defined as an algorithm that can calculate the average with respect to $p_i$ also in polynomial time

- Note that changing basis to make all $p_i \geq 0$ might not be enough: the algorithm might still exhibit exponential scaling
Complexity of decision problems

- Partial hierarchy of decision problems
  - **Undecidable** (“This sentence is false”)
  - **Partially decidable** (halting problem of Turing machines)
  - **EXPSPACE**
    - Exponential space and time complexity: diagonalization of Hamiltonian
  - **PSPACE**
    - Exponential time, polynomial space complexity: Monte C
  - **NP**
    - Polynomial complexity on non-deterministic machine
    - Traveling salesman problem
    - 3D Ising spin glass
  - **P**
    - Polynomial complexity on Turing machine
Complexity of decision problems

• Some problems are harder than others:
  • Complexity class $\mathsf{P}$
    • Can be solved in polynomial time on a Turing machine
    • Eulerian circuit problem
    • Minimum spanning Tree (decision version)
    • Detecting primality
  • Complexity class $\mathsf{NP}$
    • Polynomial complexity using non-deterministic algorithms
    • Hamiltonian cycle problem
    • Traveling salesman problem (decision version)
    • Factorization of integers
    • 3D spin glasses
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 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.
The complexity class NP

• Polynomial time complexity on a *nondeterministic* machine
  • Can execute both branches of an if-statement, but branches cannot merge again
  • Has exponential number of CPUs but no communication

• *It can* in polynomial time
  • Test all possible paths on the graph to see whether there is a Hamiltonian cycle
  • Test all possible configurations of a spin glass for a configuration smaller than a given energy $\exists c: E_c < E$

• *It cannot*
  • Calculate a partition function since the sum over all states cannot be performed
    
    $Z = \sum_c \exp(-\beta \varepsilon_c)$
**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 \( \forall Q \in NP : Q \leq P \)
  - This means that solving it in polynomial time solves all problems in NP too

- **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 was found
  - Exponential complexity has not been proven either

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

- The situation is similar to the sign problem
The Ising spin glass: **NP-complete**

- **3D Ising spin glass**
  \[ H = -\sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j \quad \text{with} \quad J_{ij} = 0, \pm 1 \]

- **The NP-complete question is:** “Is there a configuration with energy \( \leq E_0 \)?”

- **Solution by Monte Carlo:**
  - Perform a Monte Carlo simulation at \( \beta = N \ln 2 + \ln N + \ln \frac{3}{2} + \frac{1}{2} \)
  - Measure the energy:
    \[ \langle E \rangle < E_0 + \frac{1}{2} \quad \text{if there exists a state with energy } \leq E_0 \]
    \[ \langle E \rangle > E_0 + 1 \quad \text{otherwise} \]
  - A Monte Carlo simulation can decide the question
The Ising spin glass: \textbf{NP-complete}

- 3D Ising spin glass is NP-complete
  \[ H = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j \] with \( J_{ij} = 0, \pm 1 \)

- Frustration leads to NP-hardness of Monte Carlo

- Exponentially long tunneling and autocorrelation times

\[ \Delta A = \sqrt{\left( \overline{A} - \langle A \rangle \right)^2} = \sqrt{\frac{\text{Var} A}{M} \left(1 + 2 \tau_A \right)} \]
Frustration

- Antiferromagnetic couplings on a triangle:
  - Leads to “frustration”, cannot have each bond in lowest energy state
  - With random couplings finding the ground state is NP-hard

- Quantum mechanical:
  - negative probabilities for a world line configuration
  - Due to exchange of fermions

Negative weight $(-J)^3$
Solving an NP-hard problem by QMC

- Take 3D Ising spin glass \( H = \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j \) with \( J_{ij} = 0, \pm 1 \)

- View it as a quantum problem in basis where \( H \) it is not diagonal

\[
H^{(SG)} = \sum_{\langle i,j \rangle} J_{ij} \sigma^x_i \sigma^x_j \text{ with } J_{ij} = 0, \pm 1
\]

- The randomness ends up in the sign of offdiagonal matrix elements
- Ignoring the sign gives the ferromagnet and loop algorithm is in \( \mathbb{P} \)

\[
H^{(FM)} = -\sum_{\langle i,j \rangle} \sigma^x_i \sigma^x_j
\]

- The sign problem causes NP-hardness

- solving the sign problem solves all the NP-complete problems and prove \( \text{NP}=\mathbb{P} \)
Summary

• A “solution to the sign problem” solves all problems in NP
• Hence a general solution to the sign problem does not exist unless P=NP
  • If you still find one and thus prove that NP=P you will get
    • 1 million US $!
    • A Nobel prize?
    • A Fields medal?

• What does this imply?
  • A general method cannot exist
  • Look for specific solutions to the sign problem or model-specific methods
The origin of the sign problem

- We sample with the wrong distribution by ignoring the sign!

- We simulate bosons and expect to learn about fermions?
  - will only work in insulators and superfluids

- We simulate a ferromagnet and expect to learn something useful about a frustrated antiferromagnet?

- We simulate a ferromagnet and expect to learn something about a spin glass?
  - This is the idea behind the proof of NP-hardness
Working around the sign problem

1. Simulate “bosonic” systems
   • Bosonic atoms in optical lattices
   • Helium-4 supersolids
   • Nonfrustrated magnets

2. Simulate sign-problem free fermionic systems
   • Attractive on-site interactions
   • Half-filled Mott insulators

3. Restriction to quasi-1D systems
   • Use the density matrix renormalization group method (DMRG)

4. Use approximate methods
   • Dynamical mean field theory (DMFT)
The secret of Monte Carlo

- Small ideas are enough to make big progress
- However one needs the right idea - most unfortunately fail