7. Overview of modern QMC algorithms

Modern Monte Carlo algorithms

- Which system sizes can be studied?

temperature	local updates	modern algorithms
3D Tc	16'000 spins	16'000'000 spins
0.1 J	200 spins	1'000'000 spins
0.005 J	—	50'000 spins
3D Tc	32 bosons	1'000'000 bosons
0.1 t	32 bosons	10'000 bosons

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

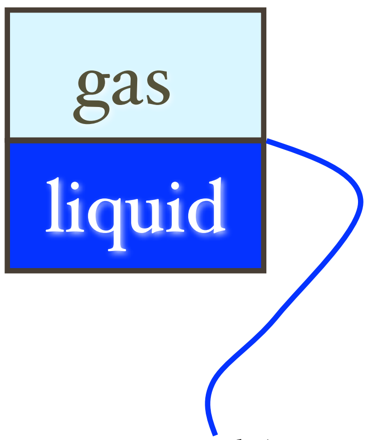
When to use path integrals?

- 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

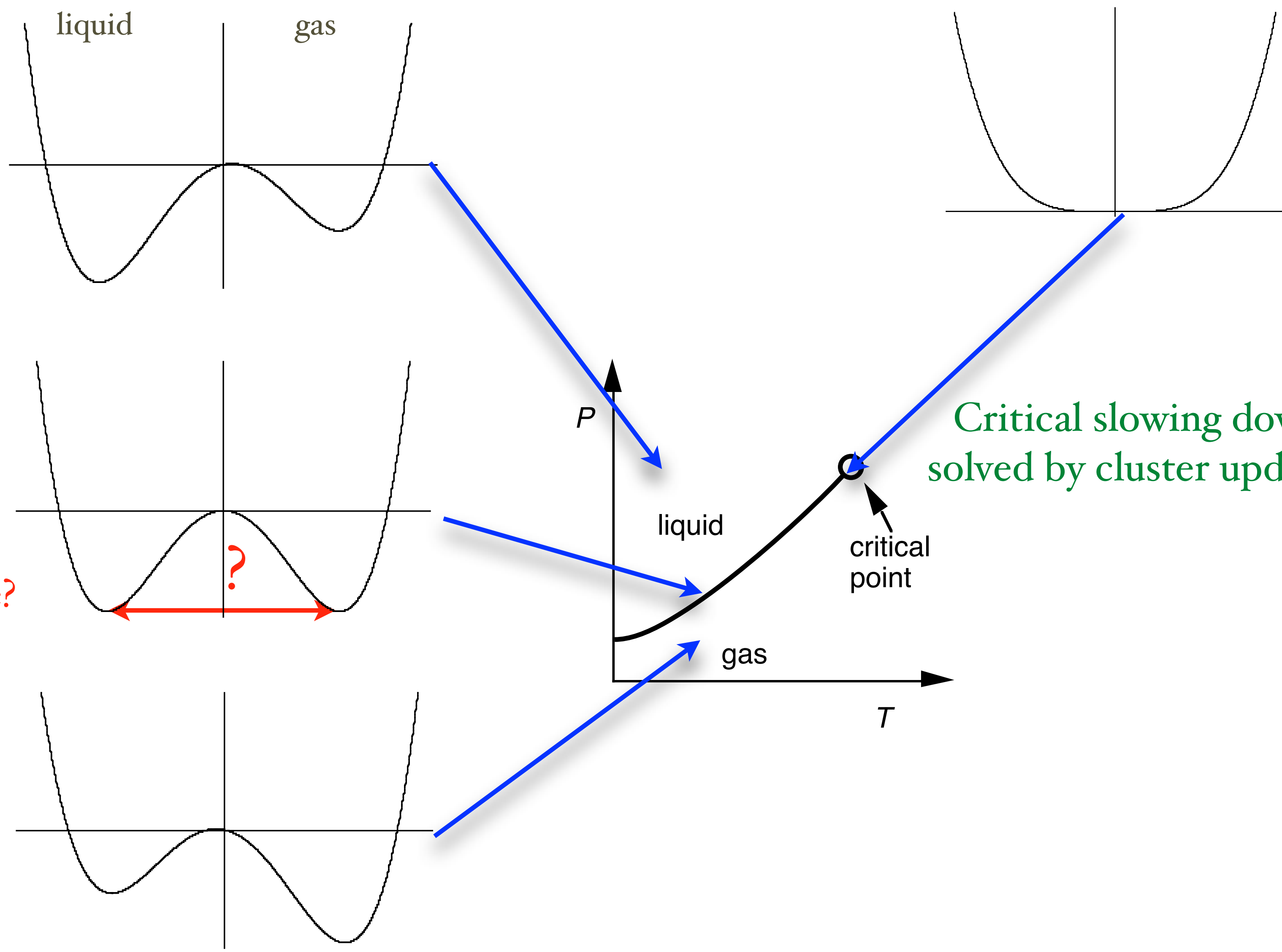
First order phase transitions

Tunneling out of meta-stable state is suppressed exponentially



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

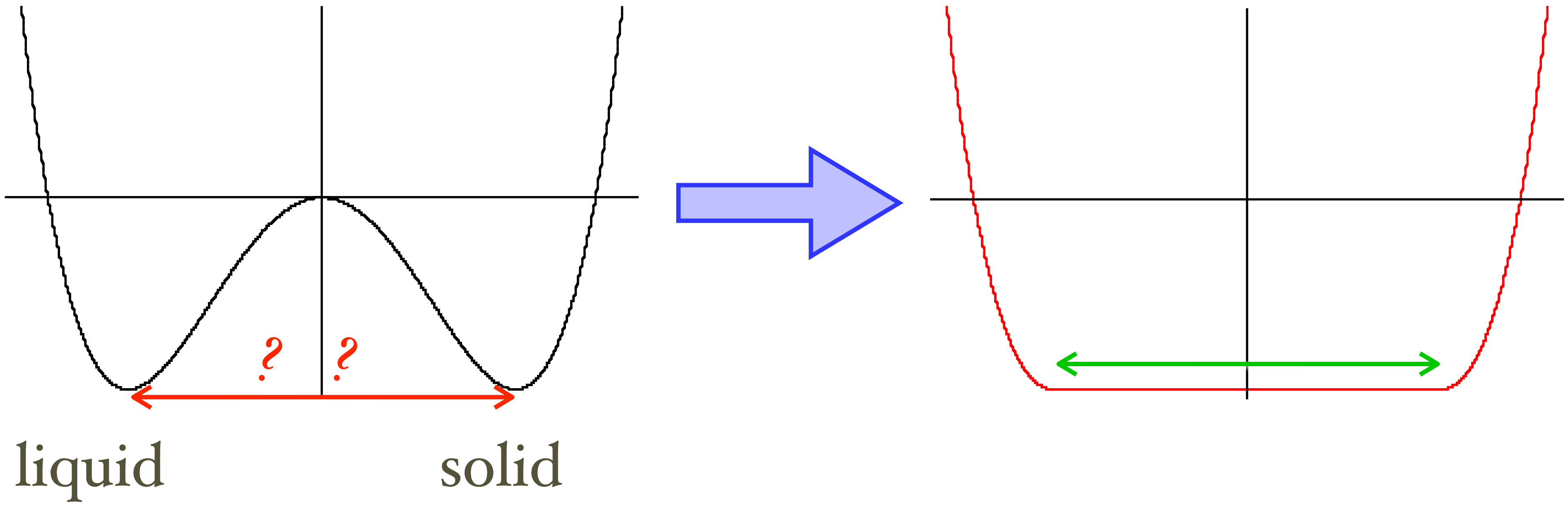
How can we tunnel out of metastable state?



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
  - Multicanonical sampling (Berg and Neuhaus, Phys. Rev. Lett. 1992)
  - Wang-Landau sampling (Wang and Landau, Phys. Rev. Lett. 2001)
  - Quantum version (MT, Wessel and Alet, Phys. Rev. Lett. 2003)
  - Optimized ensembles (Trebst, Huse and MT, Phys. Rev. E 2004)



Quantum systems

- Classical: $$Z = \sum_c e^{-E_c/k_B T} = \sum_E \rho(E) e^{-E/k_B T}$$
- Quantum: ρ(E) is not accessible
  - formulation in terms of *high-temperature series*

$$Z = \mathrm{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \mathrm{Tr}(-H)^n = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} g(n)$$

  - or *perturbation series*

$$Z = \mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr}\, e^{-\beta(H_0 + \lambda V)} = \sum_{n=0}^{\infty} \lambda^n g(n)$$

- Flat histogram, parallel tempering, histogram reweighting, etc done in order *n* of series expansion instead of energy

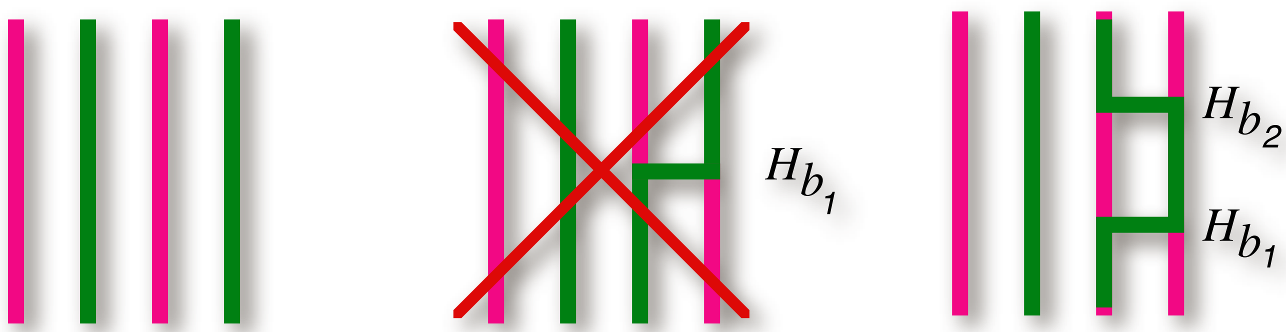
Stochastic Series Expansion (SSE)

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

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

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

- 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:

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

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

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

- 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: $e^{-\beta E_c} \to \dfrac{1}{\rho(E)}$
  - quantum: $\dfrac{\beta^n}{n!} \to \dfrac{1}{g(n)}$

Wang-Landau updates in SSE

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

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

  - Small change in acceptance rates for diagonal updates

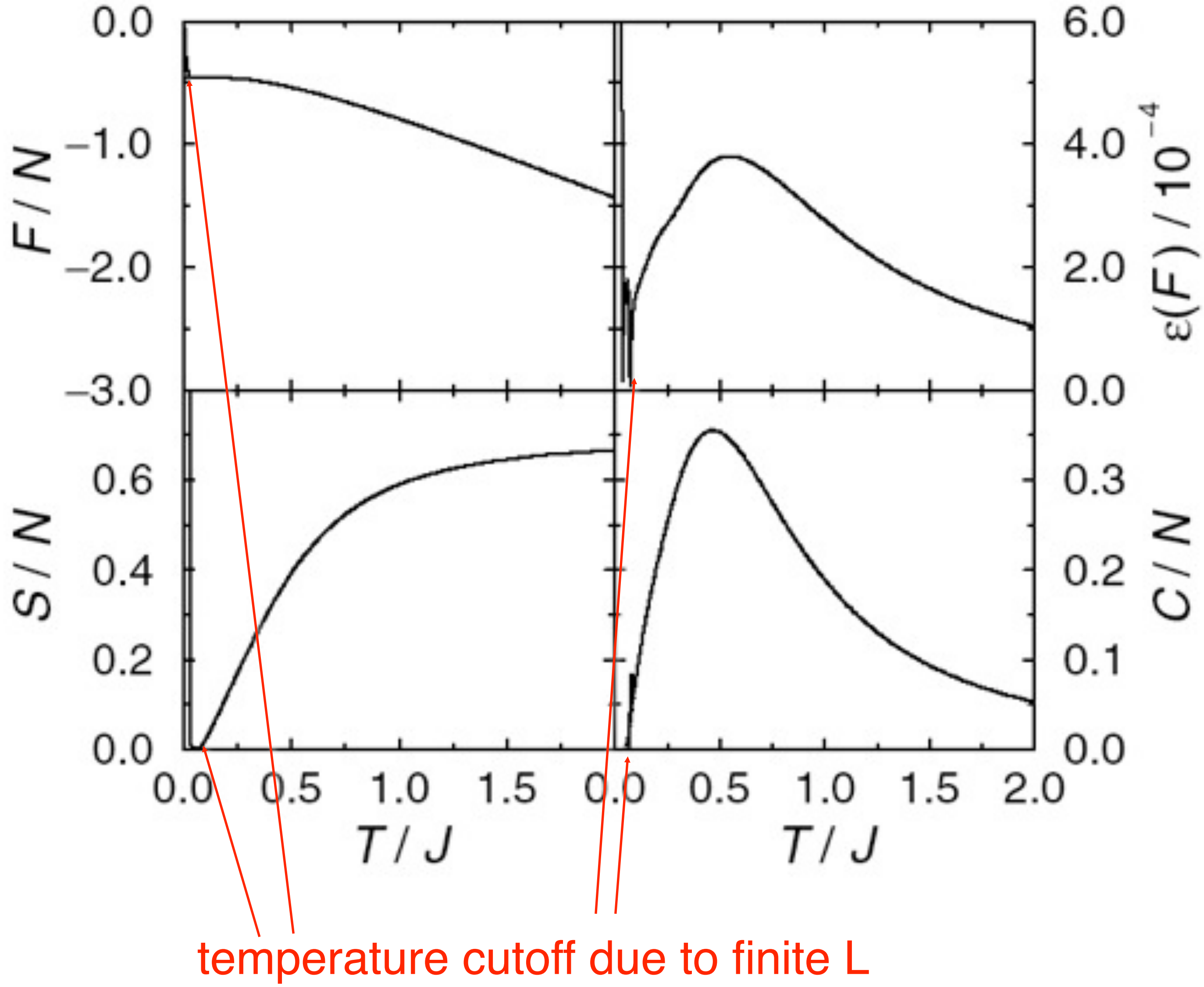
$$P[1 \to H^d_{(i,j)}] = \min\left(1, \frac{\beta N_{bonds} \langle\alpha|H^d_{(i,j)}|\alpha\rangle}{\Lambda - n}\right) \xrightarrow{\text{Wang–Landau}} \min\left(1, \frac{N_{bonds} \langle\alpha|H^d_{(i,j)}|\alpha\rangle}{\Lambda - n} \frac{g(n)}{g(n+1)}\right)$$

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

- Loop update does not change n and is thus unchanged!
- Cutoff Λ limits temperatures to $\beta < \Lambda / E_0$

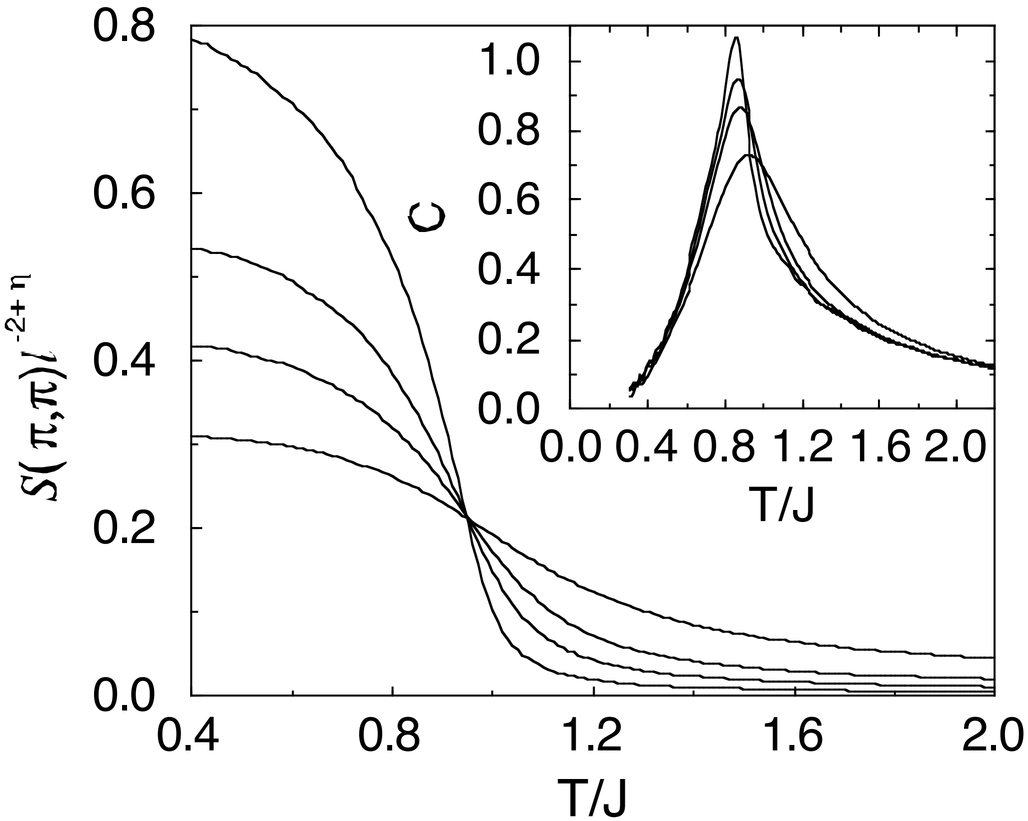
The first test

- L=10 site Heisenberg chain with Λ = 250



Wang-Landau sampling for quantum systems

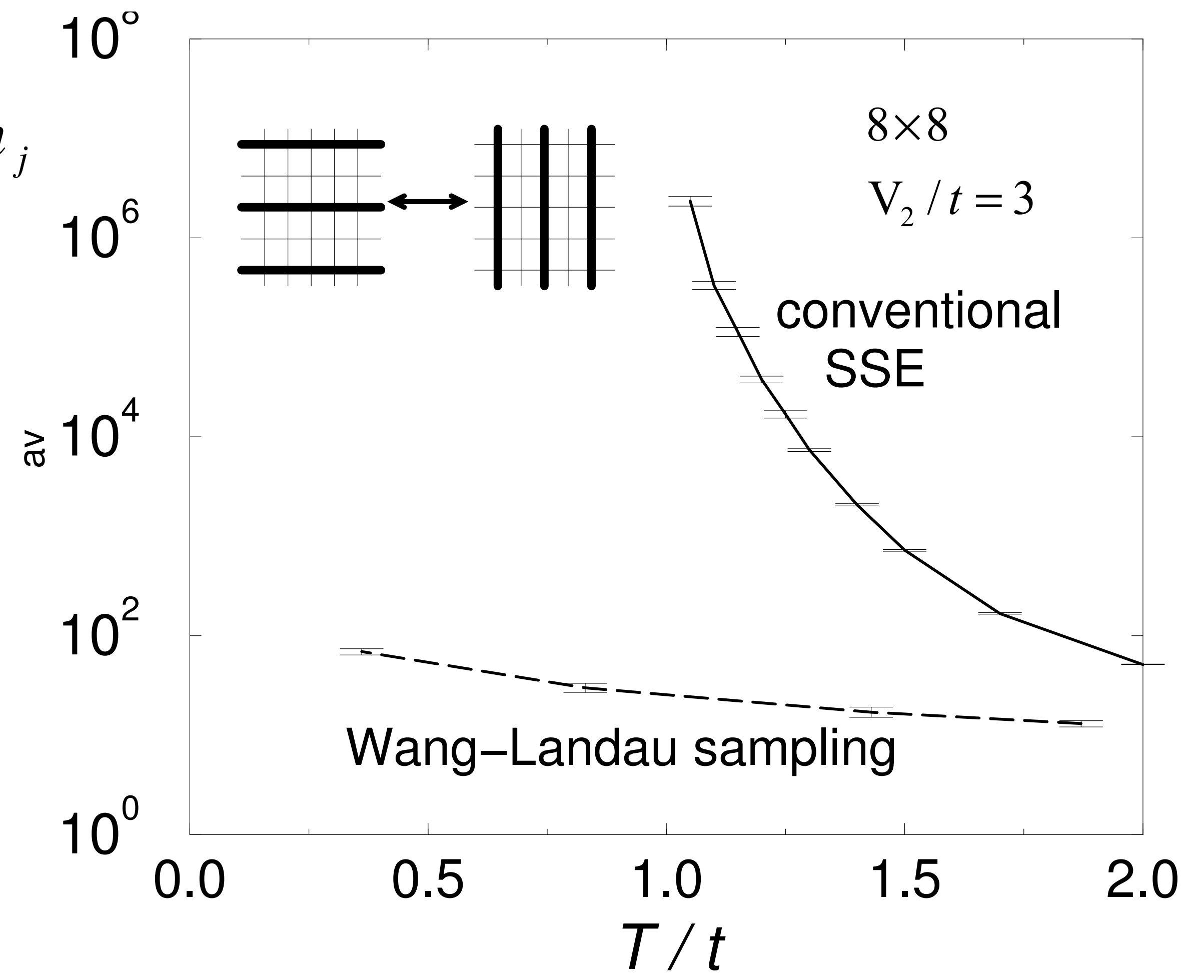
- Example: 3D quantum Heisenberg antiferromagnet



Speedup at first order phase transition

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

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



Perturbation expansion

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

with $H = H_0 + \lambda V = \sum_i \lambda^{n_\lambda(i)} H_i$

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

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

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

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

- Flat histogram in order n_λ of perturbation expansion

Perturbation series by Wang-Landau

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

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

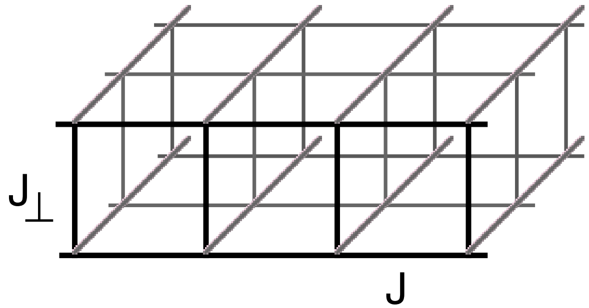
  - Small change in acceptance rates for diagonal updates

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

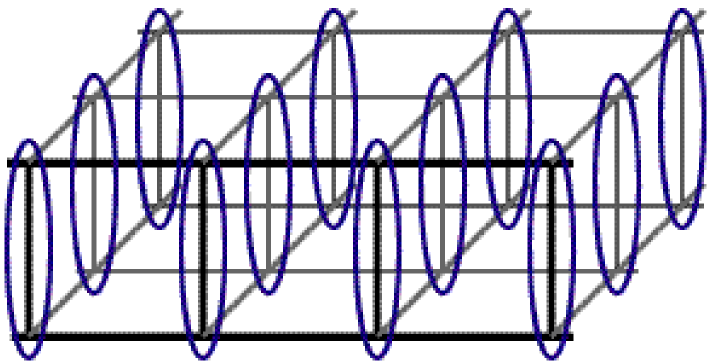
$$P[H^d_{(i,j)}\to 1]=\min\left(1,\frac{\Lambda-n+1}{\beta N_{bonds}\langle\alpha|H^d_{(i,j)}|\alpha\rangle}\right)\xrightarrow{\text{Wang-Landau}}\min\left(1,\frac{\Lambda-n+1}{\beta N_{bonds}\langle\alpha|H^d_{(i,j)}|\alpha\rangle}\frac{g(n_\lambda)}{g(n_\lambda-\Delta n_\lambda)}\right)$$

- Loop update does not change n and is thus unchanged!
- Cutoff Λ limits value of λ for which the series converges

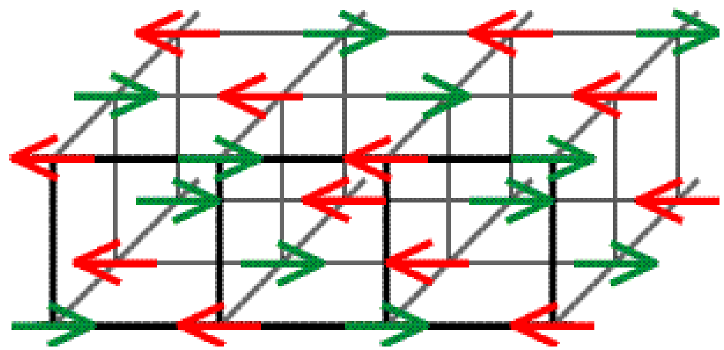
The antiferromagnetic bilayer



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



$J \gg J_\perp$: long range order

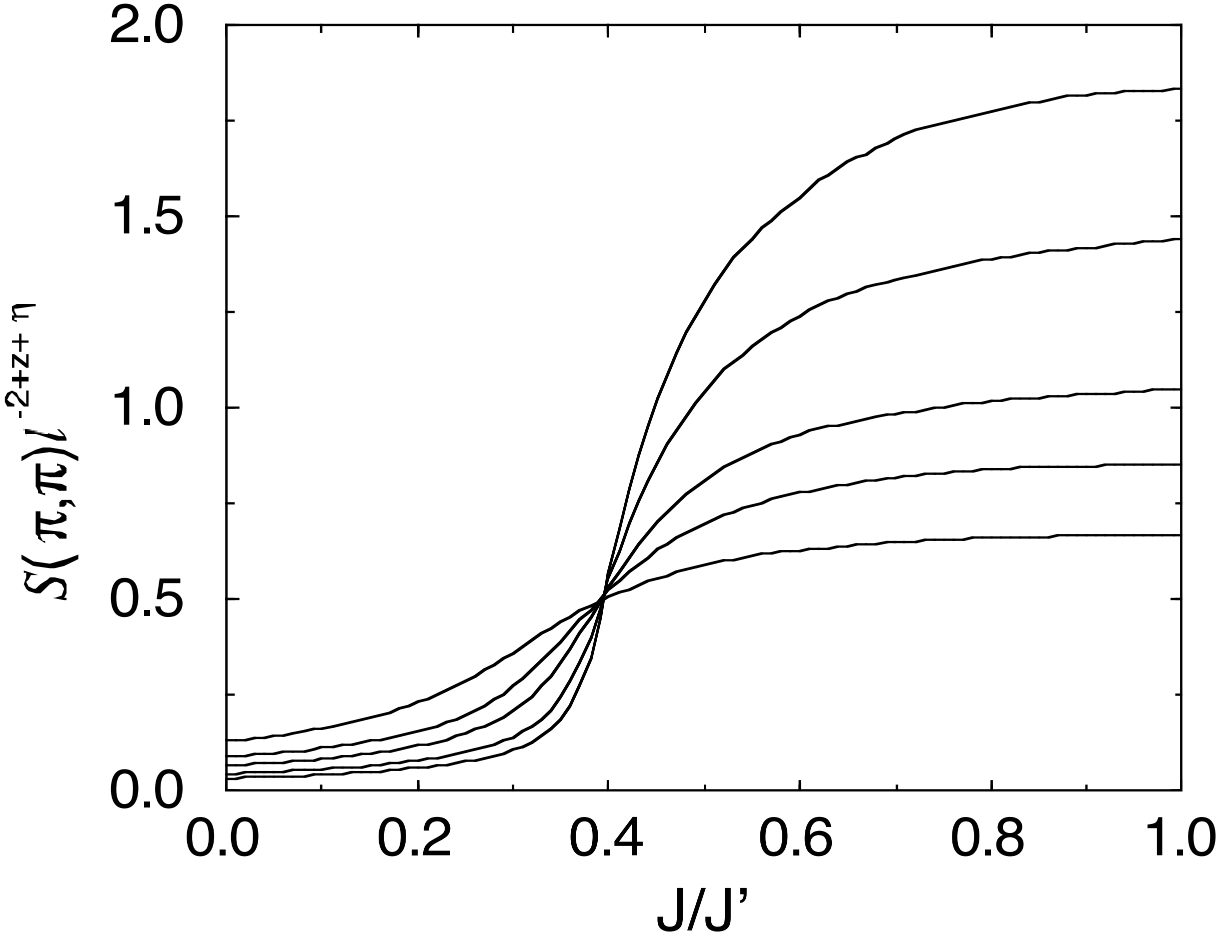


Quantum phase transition at $J_\perp / J \approx 2.524(2)$

Spin gap vanishes
Magnetic order vanishes
Universal properties

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

$$Z = \mathrm{Tr}\, e^{-\beta H} \equiv \sum_c p_c$$

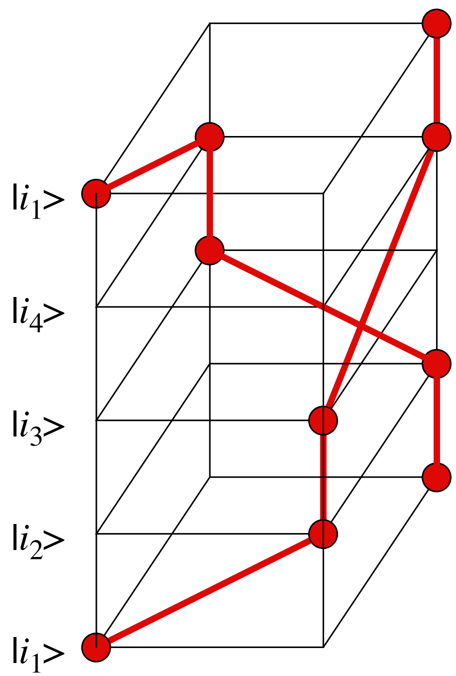
- "Negative sign" problem if some $p_c < 0$

The negative sign problem

- In mapping of quantum to classical system

$$Z = \mathrm{Tr} e^{-\beta H} = \sum_i p_i$$

- 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

$$\langle A \rangle = \sum_i A_i p_i \Big/ \sum_i p_i = \frac{\sum_i A_i \,\mathrm{sgn}\, p_i |p_i| \Big/ \sum_i |p_i|}{\sum_i \mathrm{sgn}\, p_i |p_i| \Big/ \sum_i |p_i|} \equiv \frac{\langle A \cdot sign \rangle_{|p|}}{\langle sign \rangle_{|p|}}$$

- Exponentially growing cancellation in the sign

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

- Exponential growth of errors

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

- 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 $H|i\rangle = \varepsilon_i |i\rangle$

$$\langle A\rangle = \mathrm{Tr}[A\exp(-\beta H)]/\mathrm{Tr}[\exp(-\beta H)] = \sum_{\mathrm{i}} \langle i|A_i|i\rangle \exp(-\beta\varepsilon_i) \Big/ \sum_{\mathrm{i}} \exp(-\beta\varepsilon_i)$$

  - All weights are positive
  - But this is an *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 $p_i < 0$

$$\langle A \rangle = \mathrm{Tr}[A\exp(-\beta H)]/\mathrm{Tr}[\exp(-\beta H)] = \sum_{\mathrm{i}} A_i p_i \Big/ \sum_{\mathrm{i}} p_i$$

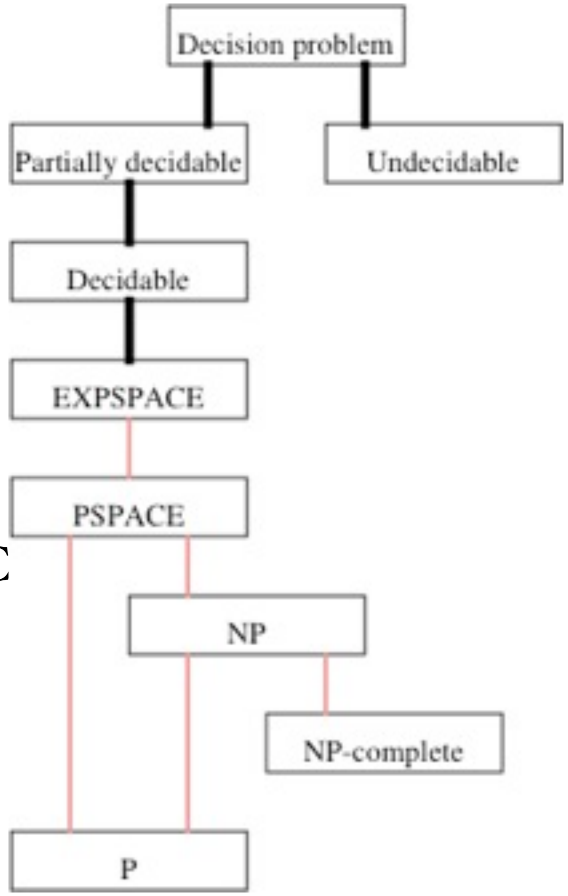
- Where the sampling of the bosonic system with respect to $|p_i|$ scales polynomially

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

- 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

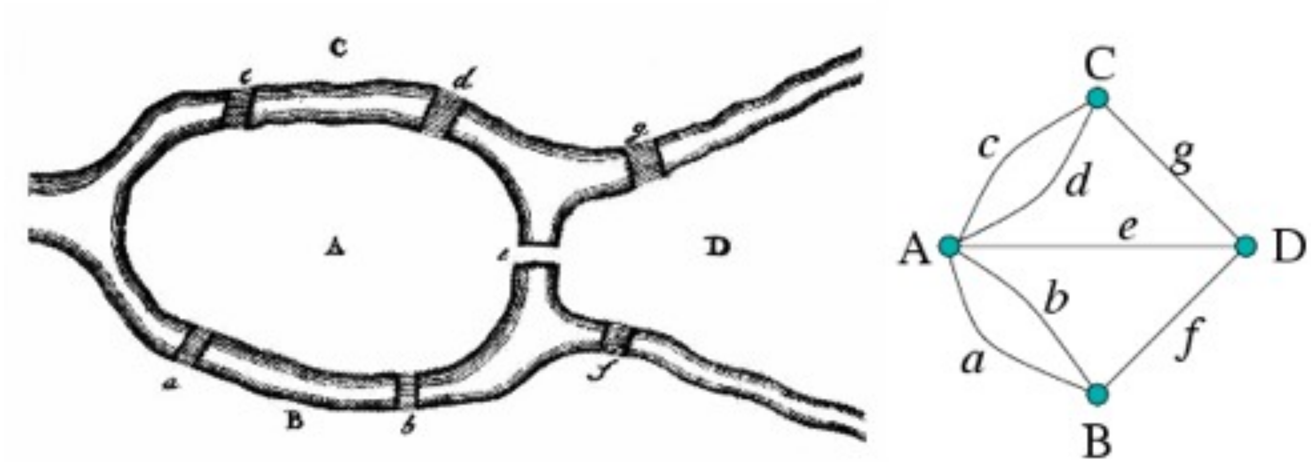


Complexity of decision problems

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

The complexity class P

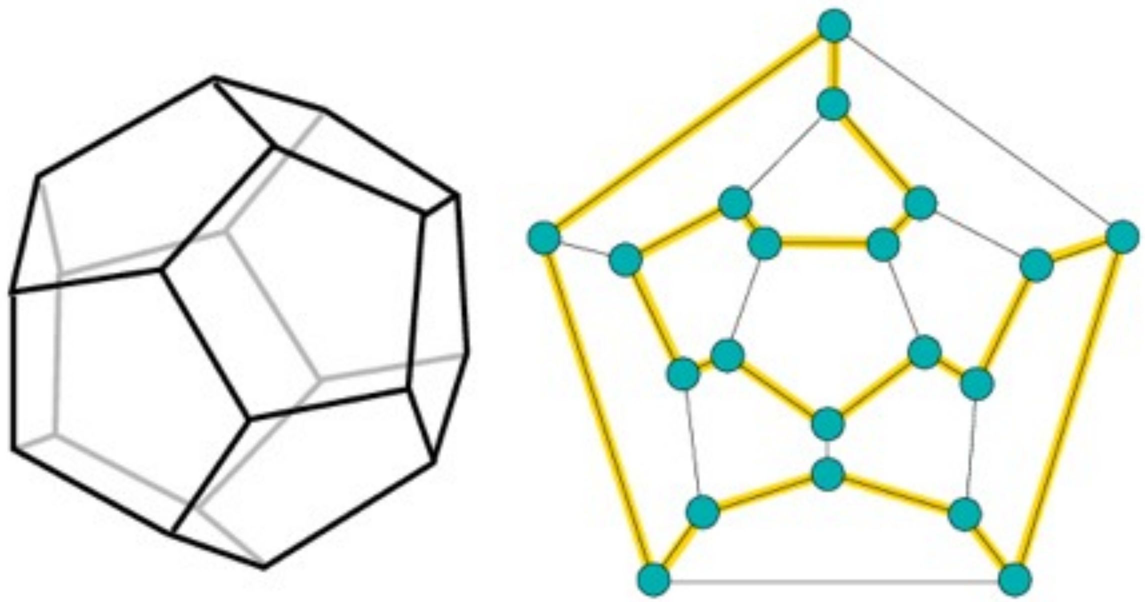
- The Eulerian circuit problem
  - Seven bridges in Königsberg (now Kaliningrad) crossed the river Pregel
  - Can we do a roundtrip by crossing each bridge exactly once?
  - Is there a closed walk on the graph going through each edge exactly once?



  - 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 $O(N^2)$
  - Concering Königsberg: NO!

The complexity class NP

- The Hamiltonian cycle problem
  - Sir Hamilton's Icosian game:
  - Is there a closed walk on 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

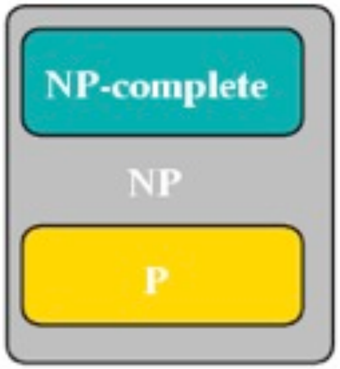
- It can in polynomial time
  - Test all possible paths on the graph to see whether there is a Hamiltonian cycle
  - Test all possible configurations of a spin glass for a configuration smaller than a given energy $\exists c : E_c < E$

- It cannot
  - Calculate a partition function since the sum over all states cannot be performed

$$\cancel{Z = \sum_c \exp(-\beta\varepsilon_c)}$$

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 $\forall Q \in NP: \quad Q \leq P$
  - 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



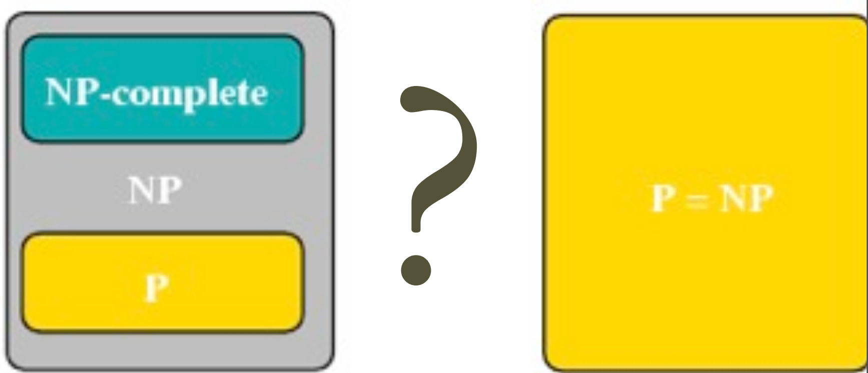
The P versus NP problem

- 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≠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≠NP



- The situation is similar to the sign problem

The Ising spin glass: NP-complete

- 3D Ising spin glass $H = -\sum_{\langle i,j \rangle} J_{ij}\sigma_j\sigma_j$ with $J_{ij} = 0, \pm 1$
- The NP-complete question is: "Is there a configuration with energy $\leq E_0$?"

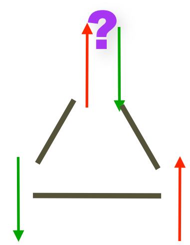
- Solution by Monte Carlo:
  - Perform a Monte Carlo simulation at $\beta = N\ln 2 + \ln N + \ln\frac{3}{2} + \frac{1}{2}$
  - Measure the energy: $\langle E \rangle < E_0 + \frac{1}{2}$ if there exists a state with energy $\leq E_0$

    $\langle E \rangle > E_0 + 1$ otherwise
  - A Monte Carlo simulation can decide the question

The Ising spin glass: NP-complete

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

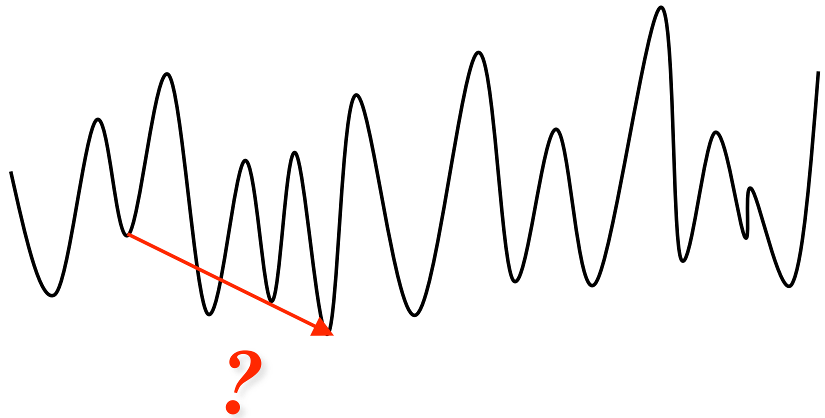
- Frustration leads to NP-hardness of Monte Carlo



- Exponentially long tunneling and autocorrelation times

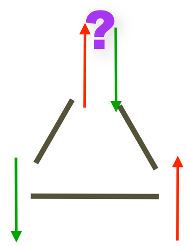
$$c_1 \to c_2 \to \ldots \to c_i \to c_{i+1} \to \ldots$$

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



Frustration

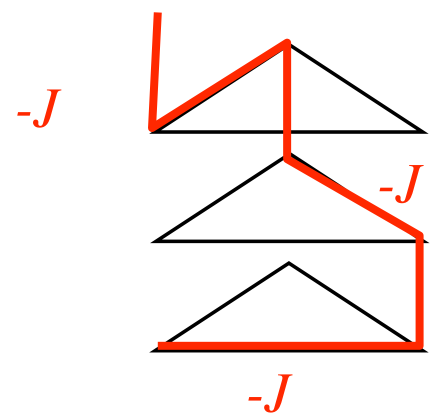
- Antiferronmagnetic couplings on a triangle:



  - 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 $H = \sum_{\langle i,j \rangle} J_{ij}\sigma_j\sigma_j$ with $J_{ij} = 0, \pm 1$
- View it as a quantum problem in basis where *H* it is not diagonal

$$H^{(SG)} = \sum_{\langle i,j \rangle} J_{ij}\sigma^x{}_j\sigma^x{}_j \text{ with } J_{ij} = 0, \pm 1$$

  - The randomness ends up in the sign of offdiagonal matrix elements
  - Ignoring the sign gives the ferromagnet and loop algorithm is in P

$$H^{(FM)} = -\sum_{\langle i,j \rangle} \sigma^x{}_j\sigma^x{}_j$$

  - The sign problem causes NP-hardness
- solving the sign problem solves all the NP-complete problems and prove NP=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