Quantum Monte Carlo and the negative sign problem

or … how to earn one million dollar

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Complexity of many particle problems

- **Classical**
  - 1 particle: 6-dimensional ODE
    - 3 position and 3 velocity coordinates
  - N particles: 6N-dimensional ODE

$$m\frac{d^2\vec{x}}{dt^2} = \vec{F}$$

- **Quantum**
  - 1 particle: 3-dimensional PDE
  - N particles: 3N dimensional PDE

$$i\hbar\frac{\partial\Psi(\vec{x})}{\partial t} = -\frac{1}{2m}\Delta\Psi(\vec{x}) + V(\vec{x})\Psi(\vec{x})$$

- **Quantum or classical lattice model**
  - 1 site: q states
  - N sites: q^N states
- Effort grows exponentially with N
- *How can we solve this exponential problem?*

The Metropolis Algorithm (1953)

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

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(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed,

II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

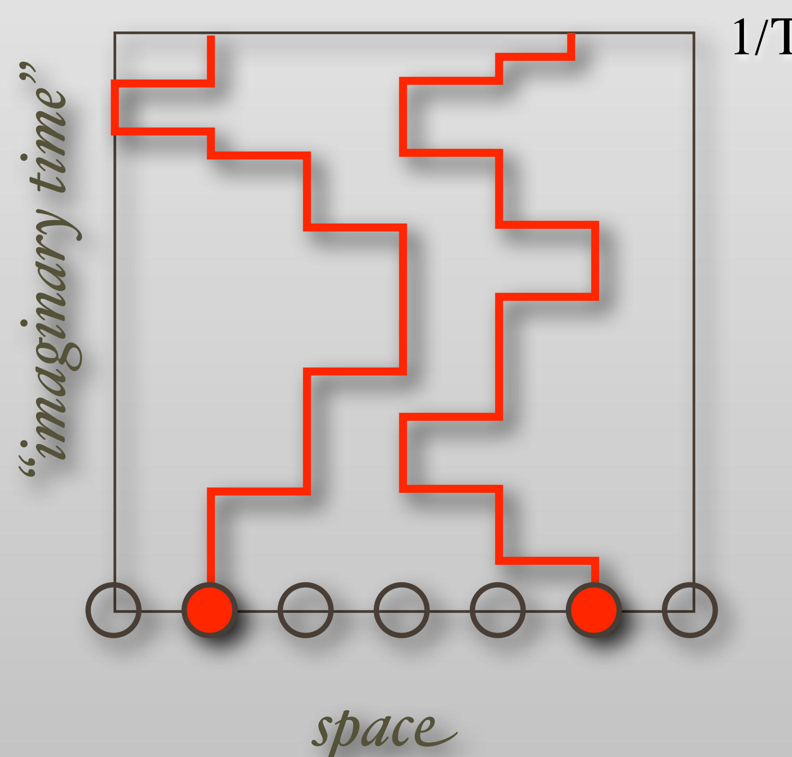
In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† con-

Mapping quantum to classical systems

- Classical: $$\langle A \rangle = \sum_c A_c e^{-E_c/T} \Big/ \sum_c e^{-E_c/T}$$
- Quantum: $$\langle A \rangle = \mathrm{Tr}\, A e^{-H/T} \Big/ \mathrm{Tr}\, e^{-H/T}$$
- Calculate exponential by integrating a diffusion equation

$$\frac{d\Psi}{d\tau} = -H\Psi \Rightarrow \Psi(1/T) = e^{-(1/T)H}\Psi(0)$$

- Map to „world lines“ of the trajectories of the particles
- use Monte Carlo samples these world lines

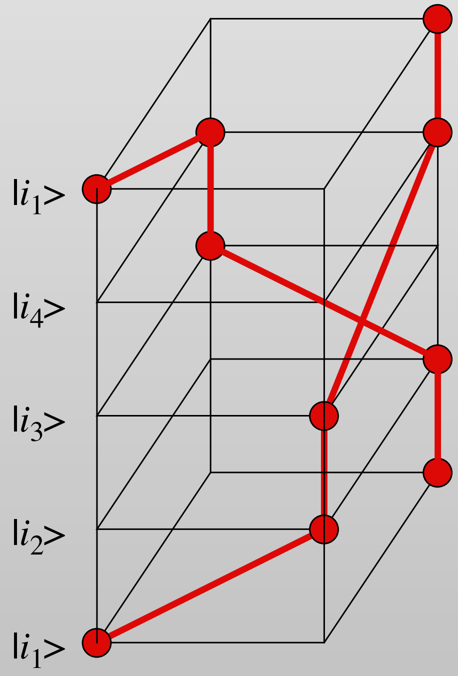


The negative sign problem

- 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

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

- 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?

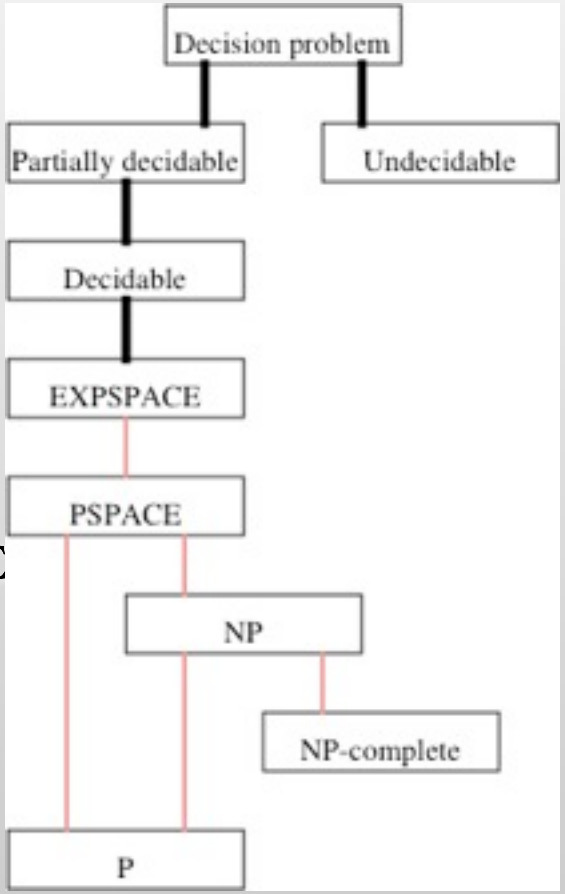
- The sign problem is basis-dependent
  - Diagonalize the Hamiltonian matrix $H|i\rangle = \varepsilon_i|i\rangle$

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

  - 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

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

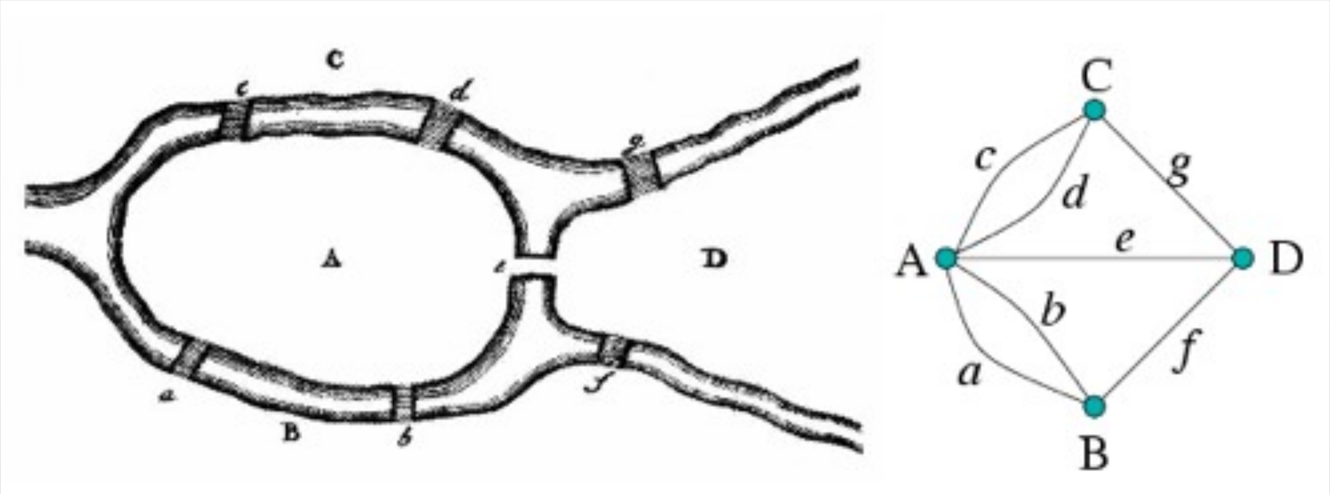


Complexity of decision problems

- 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

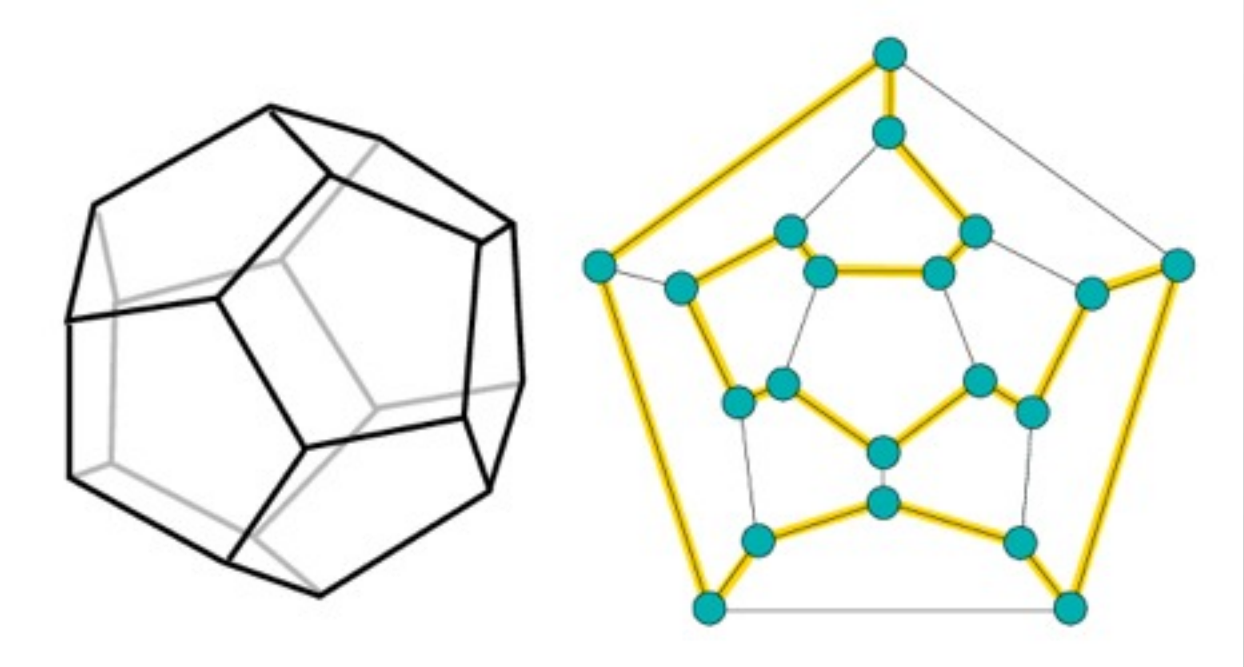
- The Eulerian circuit problem
  - Seven bridges in Königsberg (now Kaliningrad) crossed the river Pregel
  - Can we do a roundtrip by crossing each bridge exactly once?
  - Is there a closed walk on the graph going through each edge exactly once?



  - 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

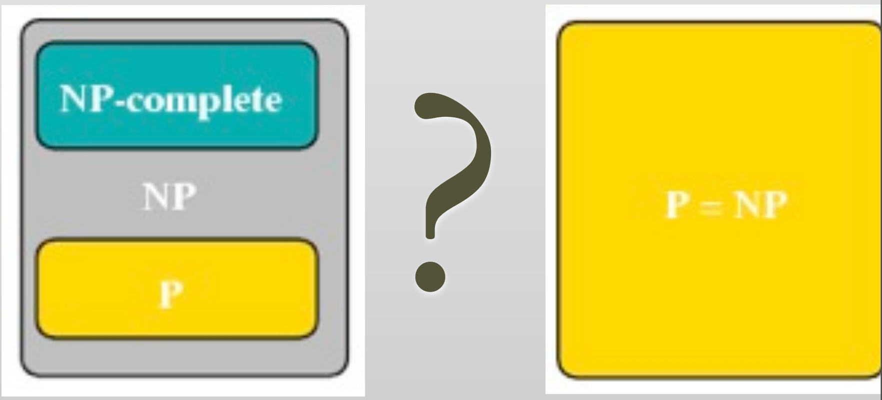
The P versus NP problem

- 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

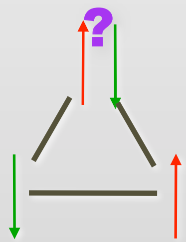
- 3D Ising spin glass $H = -\sum_{\langle i,j \rangle} J_{ij} \sigma_j \sigma_j$ with $J_{ij} = 0, \pm 1$
- The NP-complete question is: "Is there a configuration with energy $\leq E_0$?"

- 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 $J_{ij} = 0, \pm 1$

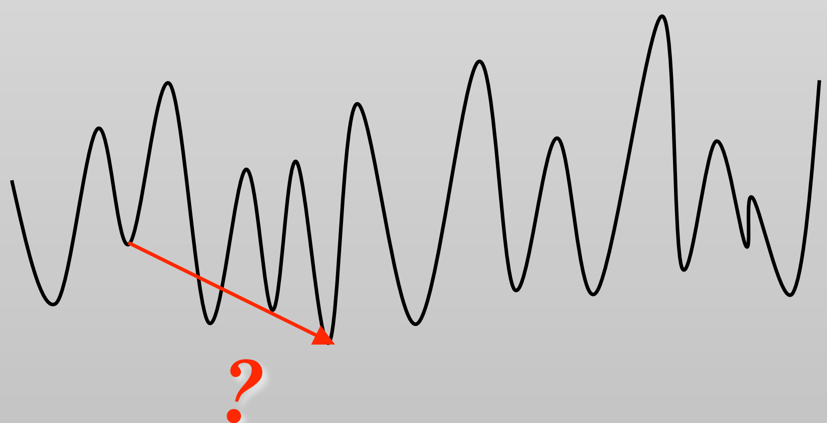
- Frustration leads to NP-hardness of Monte Carlo



- Exponentially long tunneling and autocorrelation times

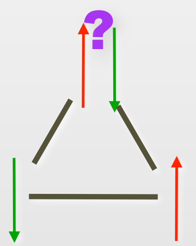
$$c_1 \to c_2 \to \ldots \to c_i \to c_{i+1} \to \ldots$$

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



Frustration

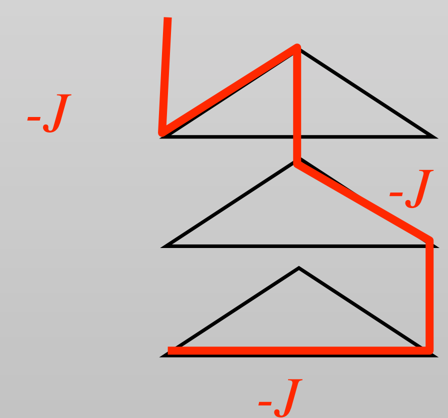
- Antiferronmagnetic couplings on a triangle:



  - 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 $(-J)^3$



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

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)