Quantum Monte Carlo

Seminar

Quantum problems of mesoscopic physics

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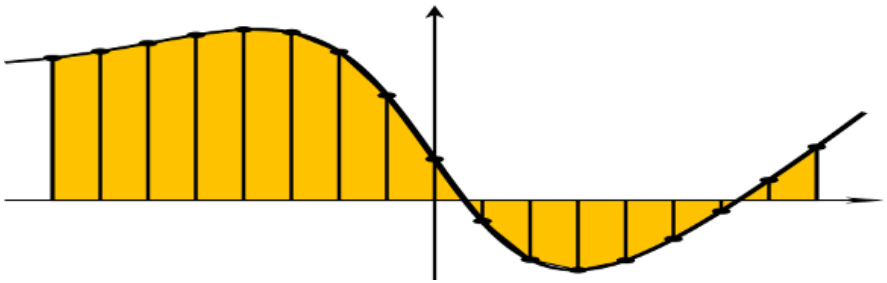
Contents

What are Monte Carlo methods?

- Monte Carlo methods are a statistical approach to solving integrals.
- The usual methods evaluate integrals on a regular grid.
- Monte Carlo methods choose points at random.

$$I = \int_a^b dx\ f(x) \approx \frac{b-a}{N} \sum_{i=1}^{N} f(x_i)$$

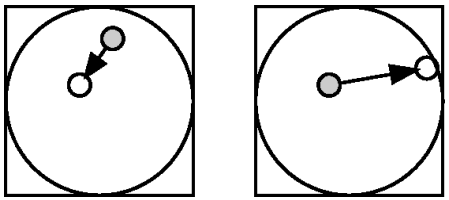


Importance Sampling

- The largest weights of a function are often in a small subinterval, e.g. the partition function $Z = \int dx_1 \cdots dx_N dp_1 \cdots dp_N e^{-\beta E(x_1,p_1,\ldots,x_N,p_N)}$.
- Importance Sampling samples many points in the region where the integrand is large and few elsewhere.
- Crucial reduction of computing time.

Markov chains

- To generate configurations according to a probability distribution $w(x)$ construct a Markov chain.
  New points are generated according to a probability distribution that depends on the current position.



- Solutions have to be ergodic.
- One special solution is detailed balance:

$$w(x)T(x \to x') = w(x')T(x' \to x)$$

The Metropolis algorithm

- The Metropolis algorithm is an ergodic solution to the detailed balance condition.
- Split the transition probability into an selection and an acceptance probability.

$$T(x \to x') = \omega_{xx'} A_{xx'}$$

- Accept the new configuration with the probability

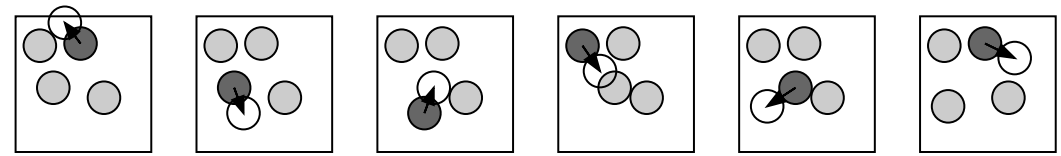
$$A_{xx'} = min\left(1, \frac{\omega_{x'x} w(x')}{\omega_{xx'} w(x)}\right)$$

Example: Simulation of a monatomic gas

- In the canonical or (NVT) ensemble the configurations should be weighed according to the Boltzman factor $\rho(X) \propto \exp(-\beta E(X))$.

Algorithm for a monatomic gas

1. Choose a random particle i.
2. Calculate a random trial displacement Δx and $x_i' = x_i + \Delta x$.
3. Accept the new configuration with probability $min\left(1, exp(-\beta(U(x'^N) - U(r^N)))\right)$.



- Average of physical quantity $A = \frac{1}{n}\sum_{\nu=0}^{n} A_\nu$

Partition functions and density matrices

- In quantum mechanics the density matrix generalizes the classical Boltzmann distribution. The probability $\pi(x)$ of being at position x is given as

$$\pi(x) = \frac{1}{Z}\,\rho(x, x, \beta)$$
$$\rho(x, x', \beta) = \left\langle x' \left| \exp(-\beta \hat{H}) \right| x \right\rangle$$
$$Z = Tr(exp(-\beta \hat{H}))$$

- An exact solution for the density matrix can only be computed for simple examples (e.g. free particles).

High temperature limit

- A simple general expression for the density matrix does not exist.

$$e^{-\beta(\hat{T}+\hat{V})} = e^{-\beta\hat{T}} e^{-\beta\hat{V}} e^{-\frac{\beta^2}{2}[\hat{T},\hat{V}]},$$

  if $[\hat{T}+\hat{V},[\hat{T},\hat{V}]] = 0$.
- Neglecting the operator $[\hat{T},\hat{V}]$ yields an error of order β^2.
- For high temperatures (small β) the density matrix can be approximated as:

$$\rho(x,x',\beta) \approx \left\langle x' \left| e^{-\beta\hat{T}} \right| x \right\rangle \; e^{-\beta V(x)}$$

The path integral

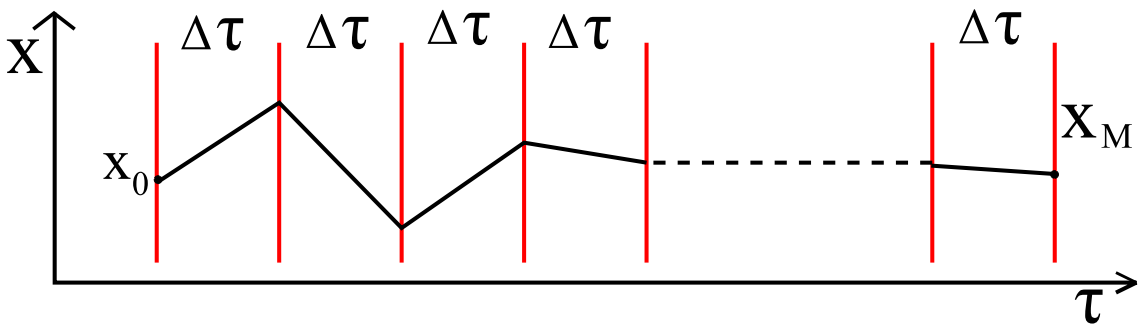
- To use the high temperature approximation, devide β in M small fragments $\Delta\tau = \frac{\beta}{M}$.

$$e^{-\beta(\hat{T}+\hat{V})} = \left[e^{-\Delta\tau(\hat{T}+\hat{V})}\right]^M$$

- The partition function can be written as

$$\int dx_0 \left\langle x_0 \left| e^{-\beta\hat{H}} \right| x_0 \right\rangle = \int dx_0 dx_1 \dots dx_{M-1}$$
$$\times \langle x_0|e^{-\Delta\tau\hat{H}}|x_1\rangle\langle x_1|e^{-\Delta\tau\hat{H}}|x_2\rangle \cdots \langle x_{M-1}|e^{-\Delta\tau\hat{H}}|x_M\rangle,$$

with $x_M = x_0$.



Path integral representation of the partition function

$$Z = \underbrace{\int \int dx_0 \dots dx_{M-1}}_{\text{sum of paths}} \underbrace{\langle x_0 | e^{-\Delta\tau \hat{H}} | x_1 \rangle \cdots \langle x_{M-1} | e^{-\Delta\tau \hat{H}} | x_M \rangle}_{\text{weight } \pi \text{ of path}}$$

- Quantum system of N particles is equivalent to a classical system of NM particles.
- The path integral maps the d-dimensional quantum system to a d+1-dimensional system. The extra dimension corresponds to the index k in x_k, going from 0 to β in steps $\Delta\tau = \frac{\beta}{M}$.

Polymer picture

- Each particle is represented by a ring-polymer.
- Adjacent beads are connected are coupled by a harmonic spring.

$$\rho(x_i, x_j, \beta) = \langle x_j | e^{-\Delta\tau \hat{H}} | x_i \rangle = \frac{1}{(2\pi\Delta\tau)^{3N/2}} e^{-\Delta\tau V(x_j)} e^{-(x_j - x_i)^2/(2\Delta\tau)}$$

- Interatomic forces occur only if the imaginary time index s is the same.

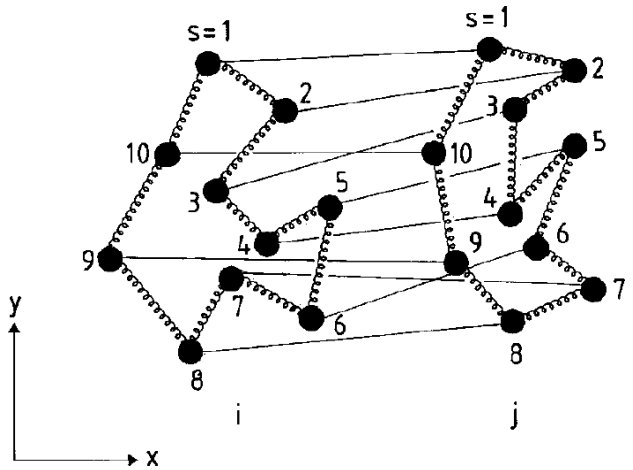
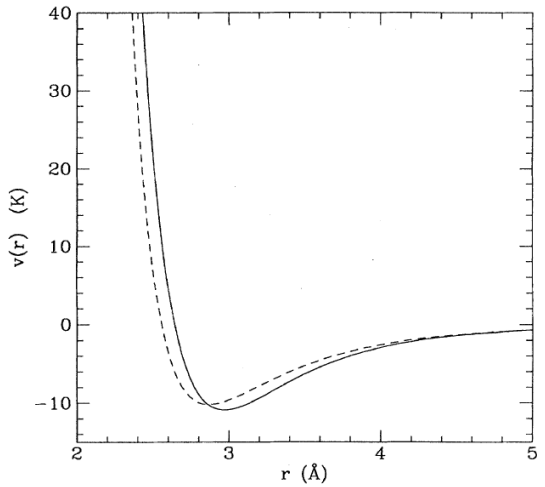


Figure: Representation of two quantum particles in two dimensions.

Simulation of superfluid ^{4}He

- The interactions between atoms can be described by a pair potential

$$H = -\frac{\hbar}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} V(|x_i - x_j|) \ .$$



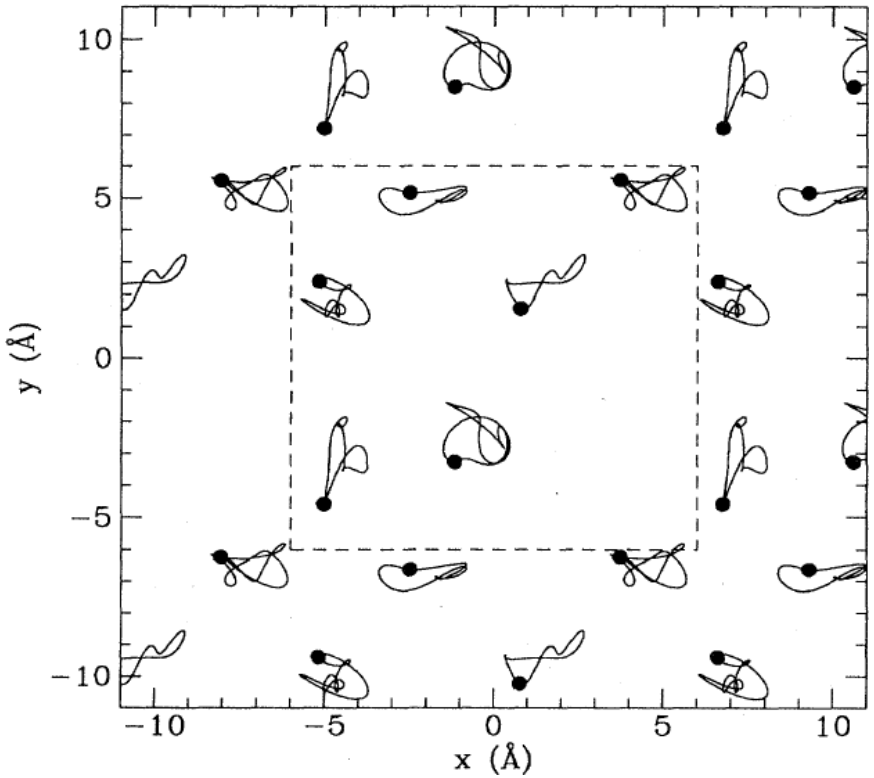
- ^{4}He atoms have the statistical properties of bosons. For a bosonic system the partition function has the form

$$Z_B = \frac{1}{N!}\sum_P \int dX_0 \cdots dX_{M-1} \langle X_0 | e^{-\Delta\tau \hat{H}} | X_1 \rangle \cdots \langle X_{M-1} | e^{-\Delta\tau \hat{H}} | X_M \rangle \ ,$$

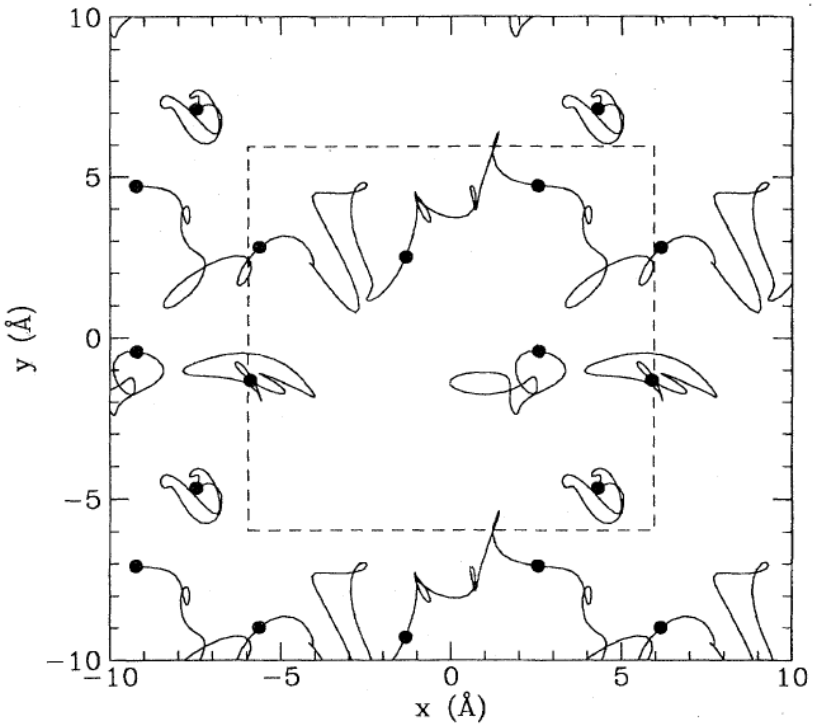
with the new boundary condition $PX_M = X_0$ where P is a permutation of particles.

Simulation of superfluid ^{4}He

- Paths can close on any permutation of their starting positions.



(a) The trace of six He-Atoms in a box with periodic boundary conditions at 4 K.



(b) At 0.75 K.

Calculating properties

- Particle density: $\langle \rho(r) \rangle = \frac{1}{M} \left\langle \sum_{i,m} \delta(r - r_{im}) \right\rangle$
- Energy: $E = \langle \hat{H} \rangle$
- Specific heat: $C_v = -\beta^2 \frac{dE}{d\beta}$

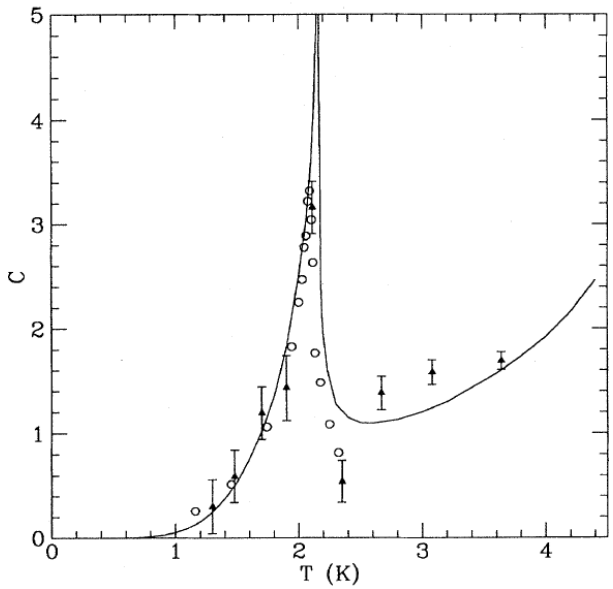


Figure: Specific heat of ^{4}He: solid line, experiment (Wilks, 1967), triangles, PIMC calculations (Ceperley and Pollock, 1986).

Quantum Ising Model

$$\hat{H} = \underbrace{-J\sum_{\langle ij\rangle}\hat{\sigma}_i^z\hat{\sigma}_j^z}_{\hat{H}_1} + \underbrace{-\Gamma\sum_i\hat{\sigma}_i^x}_{\hat{H}_2}$$

- The Mth approximant of the partition function is

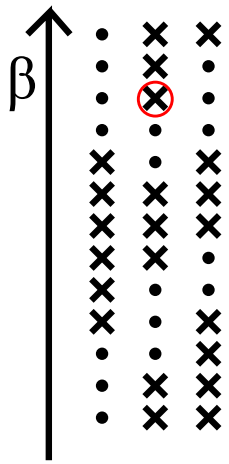
$$Z \approx Tr\left[e^{-\frac{\beta}{M}\hat{H}_1}e^{-\frac{\beta}{M}\hat{H}_2}\right]^M$$

$$= \sum_{\{S_i^k\}}\prod_{k=1}^{M}\prod_{i=1}^{N} e^{\frac{\beta J}{M}S_i^kS_{i+1}^k}\left\langle S_i^k\left|e^{\frac{\Gamma\beta}{M}\hat{\sigma}_i^x}\right|S_i^{k+1}\right\rangle$$

- System can be mapped to a 2-dimensional classical system.

$$Z = C_m\sum_{\{S_i^k\}}\exp\left[\sum_{k=1}^{M}\sum_{i=1}^{N}\left(\frac{\beta J}{M}S_i^kS_{i+1}^k + K_mS_i^kS_i^{k+1}\right)\right]$$

Sampling the Quantum Ising Model



- Attempt to flip the circled spin.
- Calculate the weights before and after the spin flip
- Accept the new configuration with

$$min\left(1, \frac{\pi_{after}}{\pi_{before}}\right) = min\left(1, \frac{e^{K_m - K_m}e^{\frac{\beta J}{M} + \frac{\beta J}{M}}}{e^{-K_m + K_m}e^{-\frac{\beta J}{M} - \frac{\beta J}{M}}}\right) = 1$$

Modifications

- The model can easily be extended to higher dimensions.

- The ferromagnetic interactions and the magnetic fields can be chosen randomly.

$$\hat{H} = -\sum_{\langle ij \rangle} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \sum_i \Gamma_i \hat{\sigma}_i^x$$

Summary

- Monte Carlo methods rely on repeated random sampling, and are useful for systems witch a large number of degrees of freedom.
- Importance Sampling increases the efficiency of Monte Carlo methods.
- The path integral method allows to sample quantum system configurations with the appropriate Boltzman factor.
- For bosonic systems we have to sample the path space and the permutation space.