Quantum Monte Carlo

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The need for Quantum Monte Carlo

Many-Body Quantum Mechanics:

Schrödinger equation

\[ i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \]

Time Evolution operator

\[ \hat{U}(t) = e^{-\frac{it}{\hbar} \hat{H}} \]

Thermal Expectation value

\[ \langle \mathcal{O} \rangle = \frac{\text{Tr} \ e^{-\beta \hat{H}} \mathcal{O}}{\text{Tr} \ e^{-\beta \hat{H}}} \]

T=0 Expectation Value

\[ \langle \mathcal{O} \rangle = \langle \Psi | \mathcal{O} | \Psi \rangle \]

Would like to solve the dynamic, thermodynamic, and groundstate properties of a system
Consider the Time Independent Schrödinger Equation

$$\hat{H} |\Psi_n\rangle = E_n |\Psi_n\rangle$$

matrix $M \times M$ $M$ vector

Then for example the thermal expectation value:

$$\langle \mathcal{O} \rangle = \frac{\sum_{i=1}^{M} e^{-\beta E_i} \langle \Psi_i | \mathcal{O} | \Psi_i \rangle}{\sum_{i=1}^{M} e^{-\beta E_i}}$$

ie. we can solve the model thermodynamic properties if we can solve the eigenvalue problem (i.e. diagonalize the Hamiltonian)

Many efficient eigenvalue libraries exist (LAPACK, ARPACK...)
Difficulty: Hilbert space is exponential

Consider a spin 1/2 system (e.g. electron spin)

$$S^z = \pm \frac{1}{2}$$

two states

For an N-spin system, the Hilbert space is $$M = 2^N$$

If each vector element is an integer (4 bytes), the memory needed to store it can be calculated:

- $$N = 9$$, 2048 bytes
- $$N = 40$$, $$\sim 10^{12}$$ bytes
- $$N = 256$$, $$\sim 10^{77}$$ bytes
Can we diagonalize “parts” of the Hamiltonian?

For example, assume: \( \hat{H} = \hat{T} + \hat{V} \)

\[
e^{-\beta \hat{H}} \neq e^{-\beta \hat{T}} e^{-\beta \hat{V}} \quad \text{no}
\]

since \([\hat{T}, \hat{V}] \neq 0\)

to see this: compare Taylor expansions of

\[
e^{\lambda (\hat{A} + \hat{B})} \quad \text{and} \quad e^{\lambda \hat{A}} e^{\lambda \hat{B}}
\]

only agree up to order \(O(\lambda^2)\)
Numerical Methods for Quantum Systems

- Exact diagonalization
  
  obtain full spectrum

\[ \langle O \rangle = \frac{\sum_{i=1}^{M} e^{-\beta E_i} \langle \Psi_i | O | \Psi_i \rangle}{\sum_{i=1}^{M} e^{-\beta E_i}} \]

If you are interested in dynamics, full-spectrum diagonalization is often all you can do

- Spectral weight, structure factor
  
  \[ A(k, \omega) \quad S(q, \omega) \]

- Properties of excited states
  - e.g. entanglement in Many-body localization
Numerical Methods for Quantum Systems

- Lanczos diagonalization

Iterative: project out the groundstate (and some low-lying excited states) only

\[ N \approx 40 \]
Numerical Methods for Quantum Systems

• Density Matrix Renormalization Group
  • Reduce the size of the Hilbert space through some clever decimation procedure
  • Keep only the “important” information (entanglement)
  • Perform a Lanczos diagonalization using the remaining Hilbert space

• Tensor Networks

Schollwoeck, Stoudenmire, Orus
Quantum Monte Carlo  

Performs **importance sampling** of state space

Goal: simulate quantum many-body models, particularly those with strong interactions, $D > 1$

- lattice or continuum
- free of systematic errors or bias
- equilibrium properties only
- often done on as large sizes as possible:

Can characterize phases (and phase transitions) $\xi \to \infty$

Condensed matter, materials, atomic systems, quantum information systems, lattice gauge theory, nuclear and particle physics
"Quantum Monte Carlo" in title
A “zoo” of QMC methods, depending on which system you want to study

\[
\hat{H} = -\frac{\hbar^2}{2m} \sum_i \hat{\nabla}_i^2 + \sum_i \hat{V}_{\text{ext}}(\vec{r}_i) + \sum_{i<j} \hat{V}_{\text{int}}(|\vec{r}_i - \vec{r}_j|)
\]

Path Integral Monte Carlo

Ceperly, Del Maestro

\[
H = -J \sum \left( |\uparrow\rangle \langle \uparrow| + \text{H.c.} \right) + V \sum \left( |\uparrow\rangle \langle \uparrow| + |\downarrow\rangle \langle \downarrow| \right)
\]

Diffusion Monte Carlo

Syljuåsen

\[
\hat{H} = J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j \quad \hat{H} = J \sum_{\langle ij \rangle} \left( b_i^\dagger b_j + b_i b_j^\dagger \right)
\]

Continuous world–line, Stochastic Series Expansion

Prokof’ev, Sandvik

\[
\hat{H} = -t \sum_{\langle ij \rangle, \sigma} \left( c_i^\dagger, \sigma c_j, \sigma + \text{h.c.} \right) + U \sum_{i=1}^{N} n_{i,\uparrow} n_{i,\downarrow}
\]

Auxiliary field Monte Carlo

Assaad, Evertz
What unifies these methods as “Quantum” Monte Carlo?

- A $D$–dimensional quantum model has a $D+1$ dimensional representation on the computer

- The presence of some form of sign problem:

Not all quantum models are amenable to efficient simulation by QMC. Something very fundamental precludes certain (very interesting) models.
Quantum Monte Carlo consists of three ingredients

- A $D+1$ dimensional “representation” on the computer
- A procedure for updating configurations of the representation
- A way of devising measurements

The first thing you need is a choice of basis:

\[
S^z = \pm \frac{1}{2} \quad \uparrow \downarrow
\]

\[
\mathbb{1} = \frac{1}{\sqrt{2}} (\uparrow \downarrow - \downarrow \uparrow)
\]

\[
|R\rangle = |\vec{r}_1, \ldots \vec{r}_N\rangle
\]
Stochastic Series Expansion QMC

A simple to implement, powerful QMC method for lattice models

\[ \hat{H} = J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j \quad \hat{H} = J \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_i b_j^\dagger) \]

- Scales linearly in system size (and inverse temperature)
- Free of systematic Trotter error
- Finite and Zero-temperature representations available

\[ \langle \mathcal{O} \rangle = \frac{1}{Z} \text{Tr}\{\mathcal{O} e^{-\beta H}\} \quad \langle \mathcal{O} \rangle = \frac{1}{Z} \langle \Psi | \mathcal{O} | \Psi \rangle \]
SSE Finite-T representation

\[ \langle \mathcal{O} \rangle = \frac{1}{Z} \text{Tr}\{\mathcal{O}e^{-\beta H}\} \]

\[ \langle \mathcal{O} \rangle = \frac{\sum_x \mathcal{O}_x W(x)}{\sum_x W(x)} \]

partition function \quad \quad Z = \sum_x W(x) = \text{Tr}\{e^{-\beta H}\}

Taylor expand the exponential:

\[ Z = \text{Tr}\{e^{-\beta H}\} = \sum_{\alpha_0} \left\langle \alpha_0 \right| \sum_{n=0}^{\infty} \frac{\beta^n}{n!} (-H)^n \left| \alpha_0 \right\rangle \]
Insert \( n-1 \) resolutions of the identity

\[
Z = \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha_0 | - H | \alpha_1 \rangle \langle \alpha_1 | - H | \alpha_2 \rangle \cdots \langle \alpha_{n-1} | - H | \alpha_n \rangle
\]

\( \alpha_0 = \alpha_n \) to keep the trace nonzero

i.e. periodic in “imaginary time” (the propagation direction)

The weight \( W(x) \) is derived from this;

- proportional to the product of \( n \) matrix elements
- each \( \langle \alpha_i | - H | \alpha_{i+1} \rangle \) is a real number
- must be positive to be interpreted as a probability for use in a Metropolis condition: otherwise get the “sign problem”
The Hamiltonian is broken into elementary lattice operators

\[ H = - \sum_t \sum_a H_{t,a} \]

“type” lattice unit (e.g. bond)

\[ Z = \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \sum_{S_n} \beta^n \frac{n!}{n!} \prod_{i=1}^{n} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle \]

sequence of operator indices

\[ S_n = [t_1, a_1], [t_2, a_2], \ldots, [t_n, a_n] \]

We sample (using Monte Carlo) the operator sequence, basis state, and expansion power \( n \)
A final (practical) step: truncate the length of the operator list

\[ M > n_{\text{max}} \]

Keeping \( M \) fixed but sampling different \( n \): need to introduce \( M-n \) null operators \( H_{0,0} \equiv \mathbb{I} \)

Statistically, the number of different way of picking the placement of the null operators in the expansion list is given by the binomial coefficient

\[
\binom{M}{n} = \frac{M!}{(M-n)!n!}
\]

\[
Z = \sum_{\alpha} \sum_{S_M} \frac{(\beta)^n (M-n)!}{M!} \prod_{i=1}^{M} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle
\]
SSE Zero–T representation (projector)

\[ \langle \mathcal{O} \rangle = \frac{1}{Z} \langle \Psi | \mathcal{O} | \Psi \rangle \quad \text{and} \quad Z = \langle \Psi | \Psi \rangle \]

\[ \langle \mathcal{O} \rangle = \frac{\sum_x O_x W(x)}{\sum_x W(x)} \]

The ground state wavefunction is estimated by a procedure where a large power of the Hamiltonian is applied to a “trial” state \( |\alpha\rangle \)

First, write in terms of energy eigenstates: \( |\alpha\rangle = \sum_n c_n |n\rangle \)

\[
(-H)^m |\alpha\rangle = c_0 |E_0|^m \left[ |0\rangle + \frac{c_1}{c_0} \left( \frac{E_1}{E_0} \right)^m |1\rangle \cdots \right],
\]

\[
\rightarrow c_0 |E_0|^m |0\rangle \quad \text{as} \quad m \rightarrow \infty
\]
\[ Z = \langle 0 | 0 \rangle \quad \text{is then} \quad Z = \langle \alpha | (-H)^m (-H)^m | \alpha \rangle \]

using a Hamiltonian breakup:

\[ H = - \sum_t \sum_a H_{t,a} \]

insert a resolution of the identity between each operator

\[
Z = \sum_{\{\alpha\}} \sum_{S_m} \prod_{j=1}^{2m} \langle \alpha_\ell | H_{t_j,a_j} | \alpha_r \rangle
\]

essentially identical to the finite-T representation, except:

- a fixed value of \( m \) is always used
- the simulation cell is not periodic: \( |\alpha_\ell\rangle \neq |\alpha_r\rangle \)
SSE QMC: Representations

- Finite–T and zero–T representations available
- Both result in very similar practical implementations
- Both can have very similar updating schemes

Thermal Expectation value

\[
\langle \mathcal{O} \rangle = \frac{\text{Tr} \ e^{-\beta \hat{H}} \mathcal{O}}{\text{Tr} \ e^{-\beta \hat{H}}}
\]

T=0 Expectation Value

\[
\langle \mathcal{O} \rangle = \langle \Psi | \mathcal{O} | \Psi \rangle
\]

To understand in more detail, we should examine a specific example.
SSE QMC: Spin–1/2 Heisenberg Model

\[ H = J \sum_{ij} S_i \cdot S_j \]

Let’s examine the finite–T representation:

\[ Z = \sum_\alpha \sum_{S_M} \frac{(\beta)^n (M - n)!}{M!} \prod_{i=1}^{M} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle \]

First: choose a basis \( |\alpha\rangle \)

\[ S^z = \pm \frac{1}{2} \]

Next: specify a specific lattice decomposition:

\[ H = - \sum_t \sum_a H_{t,a} \]
Choose a “bond” decomposition

\[ H = - \sum_t \sum_a H_{t,a} \]

null

\[ H_{0,0} = I, \]

diagonal

\[ H_{1,a} = \frac{1}{4} - S_i^z S_j^z, \]

off–diagonal

\[ H_{2,a} = \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+). \]

- A constant term \(1/4\) is added to the diagonal operator
- Spin operators are rotated by \(\pi/2\) around the z–axis on one of the sublattices

All bond operators are positive
\[ H_{1,a} = \frac{1}{4} - S_i^z S_j^z \]

\[ H_{2,a} = \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \]

\[ n = 6 \quad M = 13 \]

\[ S_n = [0, 0], [2, 0], [0, 0], [2, 2], [0, 0], [1, 4], [0, 0], [2, 0], [0, 0], [1, 3], [0, 0], [2, 2], [0, 0] \]
resembles a world line picture:
The weight $W(x)$ of a sampled configuration $x$ is proportional to the product of the positive matrix elements.

\[
\langle \; \bullet \; \circ \; | H_{1,a} | \; \bullet \; \circ \; \rangle = \langle \; \circ \; \bullet \; | H_{1,a} | \; \circ \; \bullet \; \rangle = \frac{1}{2}
\]

\[
\langle \; \bullet \; \circ \; | H_{2,a} | \; \circ \; \bullet \; \rangle = \langle \; \circ \; \bullet \; | H_{2,a} | \; \bullet \; \circ \; \rangle = \frac{1}{2}
\]

We now have a representation. From this we design updates:

- Local updates can be used to sample diagonal operators $H_{1,a} \leftrightarrow H_{0,0}$

- Non-local updates needed to sample off-diagonal operators $H_{2,a} \leftrightarrow H_{1,a}$
SSE “Diagonal” Updates

• Cycle through the operator list

• If a null operator is encountered, attempt to put a diagonal operator on a random bond \( H_{0,0} \rightarrow H_{1,a} \)

• If a diagonal operator is encountered, attempt to remove it (resulting in a null operator) \( H_{1,a} \rightarrow H_{0,0} \)

Like in classical Monte Carlo, we calculate the ratio of weights:

\[
\frac{W(x')}{W(x)}
\]

The transition probability is then obtained from detailed balance:

\[
W(x)P(x \rightarrow x') = W(x')P(x' \rightarrow x),
\]
SSE “Diagonal” Updates
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\[ Z = \sum_{\alpha} \sum_{S_M} \frac{(\beta)^n(M-n)!}{M!} \prod_{i=1}^{M} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle \]

Transition probabilities for a Metropolis algorithm

\[ P(n \to n + 1) = \min \left( \frac{1}{2} \frac{N_b \beta}{(M - n)}, 1 \right) \]

- a lattice bond must be chosen at random for the insertion

- factor of 1/2 is the matrix element

\[ P(n \to n - 1) = \min \left( \frac{2(M - n + 1)}{N_b \beta}, 1 \right) \]
SSE “Diagonal” Updates

- Sample the power of the expansion effectively
- Easy to implement, local updates
- Do not result in an ergodic simulation: off-diagonal operators are not sampled

we require a method to change the type of more than one operator at once, if we are to preserve the periodic boundaries
SSE “Operator–Loop” Updates

The fact that all non-trivial matrix elements are $1/2$ means that operator types can be changed without a change in weight.

Closed “loops” are identified (in a linked list), then flipped with a Swendsen–Wang algorithm.
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Closed “loops” are identified (in a linked list), then flipped with a Swendsen–Wang algorithm.
Other SSE updates:

- Spin-flips: required at high temperature

- Other more sophisticated operator loops possible

- Can be used in conjunction with Parallel Tempering, etc.
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SSE T=0 representation

\[ H = J \sum_{\langle ij \rangle} S_i \cdot S_j \]

Remarkably, a very different representation can have essentially the same updating procedure

\[ Z = \langle \alpha | (-H)^m (-H)^m | \alpha \rangle \]
another example: Transverse Field Ising Model

\[ H = -J \sum_{\langle i,j \rangle} \sigma^z_i \sigma^z_j - h \sum_i \sigma^x_i \]

A convenient Hamiltonian decomposition: \( H = - \sum_t \sum_a H_{t,a} \)

\[ H_{0,0} = I, \]
\[ H_{-1,a} = h(\sigma^+_a + \sigma^-_b), \]
\[ H_{0,a} = h, \]
\[ H_{1,a} = J(\sigma^z_i \sigma^z_j + 1). \]

The index \( a \) can label a bond, or a single lattice site. Note:

\[ \langle \bullet \mid H_{-1,a} \mid \circ \rangle = \langle \circ \mid H_{-1,a} \mid \bullet \rangle = h, \]
\[ \langle \bullet \mid H_{0,a} \mid \bullet \rangle = \langle \circ \mid H_{0,a} \mid \circ \rangle = h. \]
\[ \langle \bullet \bullet \mid H_{1,a} \mid \bullet \bullet \rangle = \langle \circ \circ \mid H_{1,a} \mid \circ \circ \rangle = 2J. \]
another example: Transverse Field Ising Model

Finite-T representation

\[ H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x \]
another example: Transverse Field Ising Model

zero-T representation

\[ H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x \]
The Sign Problem in SSE

• Any constant term can be added to diagonal operators

• Spin operators are rotated by $\pi/2$
  around the z–axis on one of the sublattices ...

\[
Z = \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha_0 | - H | \alpha_1 \rangle \langle \alpha_1 | - H | \alpha_2 \rangle \cdots \langle \alpha_{n-1} | - H | \alpha_n \rangle
\]

Alternatively, we can keep the matrix element unchanged, if we are confident that off–diagonal operators always occur in even numbers

\[
H = - \sum_t \sum_a H_{t,a} \quad H_{2,a} = -\frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)
\]
The Sign Problem in SSE

In the finite-T representation, periodic boundary condition in imaginary time enforce this:
The Sign Problem in SSE

In the finite–T representation, periodic boundary condition in imaginary time enforce this:
Measurements in the SSE:

In general – expectation values of operators either:

- Diagonal in the basis $\langle S^z_i S^z_j \rangle$ $S(q)$

- Associated with the Hamiltonian

  $$\langle B_i B_j \rangle \quad B_i = S^+_i S^-_j + S^-_i S^+_j$$

example:

$$Z = \sum_{\alpha_0} \left\langle \alpha_0 \right| \sum_{n=0}^{\infty} \frac{\beta^n}{n!} (-H)^n \left| \alpha_0 \right\rangle$$

$$E = -\frac{\partial \ln Z}{\partial \beta}$$

$$E = -\frac{1}{Z} \sum_{\alpha_0} \left\langle \alpha_0 \right| \sum_{n=0}^{\infty} \frac{n\beta^{(n-1)}}{n!} (-H)^n \left| \alpha_0 \right\rangle$$

$$E = -\frac{\langle n \rangle}{\beta}$$
Quantum Monte Carlo

- A large class of Metropolis based Monte Carlo methods in $D+1$ dimension

- Extremely powerful, work well in higher $D$

- Inhibited by the “sign problem” for frustrated spins and fermions

- Algorithms are not static: new models, measurements, and tricks are discovered frequently

- At least one Nobel Prize lurking around...