An Introduction to Determinant Quantum Monte Carlo

Condensed Matter Student Club Talk

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What is DQMC?

Terminology

Determinant Quantum Monte Carlo is a numerical method for interacting fermion systems.

1. **Quantum**: it treats a quantum many-body problem in imaginary time
2. **Monte Carlo**: it samples many auxiliary-field configurations stochastically
3. **Determinant**: after introducing the auxiliary field, the fermions can be integrated out and their weight is written as a determinant

This talk

1. Explain why generic interacting fermion problems are hard numerically
2. Demonstrate the central idea of DQMC: rewrite the interacting problem as a Monte Carlo over non-interacting problem with auxiliary fields; discuss the fermion sign problem
3. Present applications

Many-body numerics

General fermion many-body Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

$$\hat{H}_0 = \sum_{ij} T_{ij} c_i^\dagger c_j, \quad \hat{H}_I = \frac{1}{2} \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_l c_k$$

- Non-interacting: diagonalize the one-body matrix $T = U^\dagger \lambda U$ with cost $O(N^3)$

$$\sum_{ij} T_{ij} c_i^\dagger c_j = c^\dagger T c = d^\dagger \lambda d, \; d = U^\dagger c$$

- Interacting: work in the full many-body Hilbert space, which grows exponentially, so diagonalization quickly becomes impractical

Hilbert space explosion

For spinless fermions on N sites:

$$\dim \mathcal{H} = 2^N.$$

For 4 sites,

$$\mathcal{B} = \{|0000\rangle, |0001\rangle, |0010\rangle, \ldots, |1111\rangle\}.$$

Even a modest system already has an exponentially large basis.

DQMC: decouple interacting problem $\rightarrow$ stochastic non-interacting problem

Classical Ising MCMC

Warm-up: Ising model

$$H_{\text{Ising}} = -J \sum_{\langle ij \rangle} s_i s_j, \qquad s_i = \pm 1$$

$$W[\mathcal{C}] = e^{-\beta H_{\text{Ising}}[\mathcal{C}]}, \quad Z = \sum_{\mathcal{C}} W[\mathcal{C}]$$

- $\mathcal{C} = \{s_i\}$: spin configuration
- $P[\mathcal{C}] = W[\mathcal{C}]/Z$: probability distribution
- Larger $W[\mathcal{C}]$ means the configuration is sampled more often

Local update:

$$s_i \to -s_i.$$

Metropolis rule:

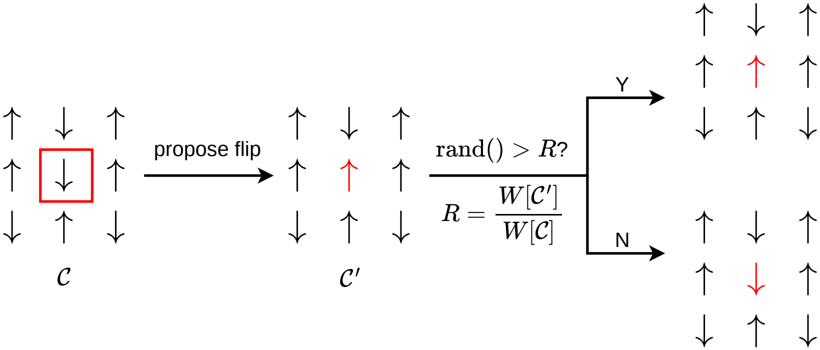
$$R = \frac{W[\mathcal{C}']}{W[\mathcal{C}]} = e^{-\beta(H[\mathcal{C}'] - H[\mathcal{C}])},$$

$$A(\mathcal{C} \to \mathcal{C}') = \min(1, R).$$

1. Propose $\mathcal{C}'$ (local/cluster/global)
2. Accept or reject with A
3. Repeating until converges

DQMC analogy: same structure, but $\mathcal{C} = \{l_{t,i}\}$ and $W[\mathcal{C}] \ngeq 0$ becomes a fermion weight

Metropolis update illustration



DQMC targets

In many-body physics, we are interested in the finite- and zero-T properties.

For finite temperature,

$$Z_\beta = \mathrm{Tr}(e^{-\beta \hat{H}}), \qquad \langle \hat{O} \rangle = \frac{\mathrm{Tr}(\hat{O} e^{-\beta \hat{H}})}{Z_\beta}$$

For ground-state projection,

$$Z_\Theta = \langle \Psi_T | e^{-2\Theta \hat{H}} | \Psi_T \rangle \,, \quad \langle \hat{O} \rangle_0 = \lim_{\Theta \to \infty} \frac{\langle \Psi_T | e^{-\Theta \hat{H}} \hat{O} e^{-\Theta \hat{H}} | \Psi_T \rangle}{Z_\Theta}$$

where $|\Psi_T\rangle$ is a trial state with nonzero ground-state overlap, $\langle \Psi_T | \Psi_0 \rangle \neq 0$.

In both cases, the key object is a long imaginary-time propagator: $e^{-\beta \hat{H}}$ or $e^{-2\Theta \hat{H}}$.

Step 1: imaginary time slicing

Break the long propagator into many short pieces:

$$e^{-\beta \hat{H}} = \left(e^{-\Delta\tau \hat{H}}\right)^{N_\tau}, \qquad \beta = N_\tau \Delta\tau$$

Then use a Suzuki–Trotter decomposition:

$$e^{-\Delta\tau(\hat{H}_0+\hat{H}_I)} \approx e^{-\Delta\tau \hat{H}_0} e^{-\Delta\tau \hat{H}_I}$$

Interpretation:

- N_τ is the number of imaginary-time slices
- smaller $\Delta\tau$ means smaller Trotter error
- after this step, the hard part is still the interaction piece $e^{-\Delta\tau \hat{H}_I}$

Step 2: decouple the interaction

The idea is to replace a two-body quadratic interaction by an average of one-body interaction over new field (Hubbard-Stratonovich transformation).

Suppose $\hat{H}_I = \sum_i \lambda_i \hat{A}_i^2$ where $\hat{A}_i = c^\dagger A c$

$$e^{\frac{1}{2}A^2} = \frac{1}{\sqrt{2\pi}} \int dq \, e^{-q^2/2} e^{qA}$$

$$\Rightarrow e^{-\Delta\tau \hat{H}_I} = \prod_i e^{-\lambda \Delta\tau \hat{A}_i^2} = \prod_i \left[\sum_{l_i = \pm 1, \pm 2} \gamma_{l_i} e^{\eta_{l_i} \sqrt{-\lambda_i \Delta\tau} \hat{A}_i} \right] + O(\Delta\tau^4)$$

- the interaction is traded for a coupling to an **auxiliary field** q or l_i (continuous/discrete)
- once q is fixed, the fermions only see a one-body problem
- on a lattice, we introduce one field variable for each site and each imaginary-time slice
- fermions propagating with **interaction** $\rightarrow$ **non-interacting** fermions propagating in a **fluctuating background field**

Stochastic summation of propagator

Now let's assemble two things up: discritization and decoupling

$$\underbrace{e^{-\Delta\tau\hat{H}}e^{-\Delta\tau\hat{H}}\cdots e^{-\Delta\tau\hat{H}}}_{N_\tau \text{ copies in total}} = \sum_{\{l_{t,i}\}}\prod_{t=1}^{N_\tau}\left\{e^{-\Delta\tau\hat{H}_0}\left[\gamma_{l_i}e^{\eta_{l_i}\sqrt{-\lambda_i\Delta\tau}\hat{A}_i}\right]\right\} + O(\Delta\tau)$$
$$= \sum_{\mathcal{C}} U_{\mathcal{C}} + O(\Delta\tau)$$

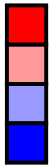
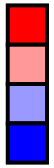
Configuration $\mathcal{C} = \{l_{t,i}\}$ where

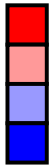
- t: imaginary-time slice
- i: spatial site or interaction-vertex index
- $l_{t,i}$: auxiliary field on site i and time slice t

So DQMC samples a *space-time field history*, not a many-body basis state.

Stochastic summation of propagator: an illustration

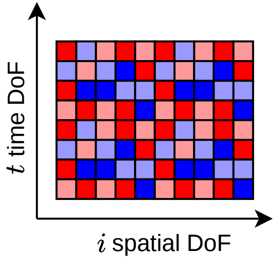
$$\boxed{e^{-\beta\hat{H}} \text{ or } e^{-2\Theta\hat{H}}} = \boxed{e^{-\Delta\tau\hat{H}}}\times\boxed{e^{-\Delta\tau\hat{H}}}\times\boxed{e^{-\Delta\tau\hat{H}}}\times\boxed{e^{-\Delta\tau\hat{H}}}\cdots$$

$=\boxed{e^{-\Delta\tau\hat{H}_0}}\times$  $\times\boxed{e^{-\Delta\tau\hat{H}_0}}\times$  $\times\cdots$

 $= \sum_i \left(\boxed{-2}+\boxed{-1}+\boxed{+1}+\boxed{+2}\right)$

$$\boxed{l_i} = \gamma_{l_i} e^{\eta_i\sqrt{-\lambda_i\Delta\tau}\hat{A}_i}$$

An Example $\mathcal{C}$



Fermion weights

Once the long propagator is rewritten as a sum over auxiliary-field histories, the partition function becomes a sum over configurations:

$$Z_\beta = \sum_{\mathcal{C}} W[\mathcal{C}], \qquad W[\mathcal{C}] = \operatorname{Tr} U_{\mathcal{C}} = \left(\prod_{t,i} \gamma_{l_{t,i}} e^{\eta_{l_{t,i}} v_i} \right) \det[I + B_{\mathcal{C}}]$$

$$Z_\Theta = \sum_{\mathcal{C}} W[\mathcal{C}], \qquad W[\mathcal{C}] = \langle \Psi_T | U_{\mathcal{C}} | \Psi_T \rangle = \left(\prod_{t,i} \gamma_{l_{t,i}} e^{\eta_{l_{t,i}} v_i} \right) \det[P^\dagger B_{\mathcal{C}} P]$$

For a fixed configuration $\mathcal{C} = \{l_{t,i}\}$, $U_{\mathcal{C}}$ is a non-interacting many-fermion propagator.

- The fermions are integrated out analytically, resulting a weight expressed by a **determinant** (**D** in DQMC)
- Just like Ising MC, we sample configurations with weight $W[\mathcal{C}]$, except now $W[\mathcal{C}]$ need not be nonnegative; evaluating it is still polynomial-cost: $O(N_\tau N^3)$

Ising MC and DQMC: comparison

	Ising MC	**DQMC**
Field configuration $\mathcal{C}$	$\{s_i\}$: space DoFs	$\{l_{t,i}\}$: time and space DoFs
Update complexity	$O(N)$ per sweep	$O(N_\tau N^3)$
Weight	$W[\mathcal{C}] \geq 0$	$W[\mathcal{C}] \ngeq 0$

For readers comfortable with coherent-state path integrals, the same step can be written as

$$\int \mathcal{D}[\bar{c}, c]\, e^{\int d\tau \left[-\bar{c}(\partial_\tau - T)c + \hat{A}^2\right]} = C \int \mathcal{D}[\bar{c}, c]\mathcal{D}[q]\, e^{\int d\tau \left[-\bar{c}(\partial_\tau - T)c + q\hat{A} - q^2/2\right]}$$

Here $q = q_i(\tau)$ is the continuous auxiliary field; once q is fixed, the fermion action is quadratic. At saddle point, $q = \langle A \rangle$ gives the mean-field approximation.

Sign problem

In classical Monte Carlo, $W[\mathcal{C}]$ is nonnegative.

In DQMC, the determinant weight is not guaranteed to be positive:

$$W[\mathcal{C}] < 0 \qquad \text{or even} \qquad W[\mathcal{C}] \in \mathbb{C}.$$

Then

$$P[\mathcal{C}] = \frac{W[\mathcal{C}]}{\sum_{\mathcal{C}} W[\mathcal{C}]}.$$

is no longer a valid probability distribution.

Practical fix: sample with $|\mathrm{Re}\, W[\mathcal{C}]|$ instead, and keep the reweighting sign factor as part of the measurement.

Sign problem: reweighting

With reweighting

$$Z' = \sum_{\mathcal{C}} |\mathrm{Re}\, W[\mathcal{C}]|, \qquad P[\mathcal{C}] = \frac{|\mathrm{Re}\, W[\mathcal{C}]|}{Z'},$$

$$\mathsf{sign}[\mathcal{C}] = \frac{W[\mathcal{C}]}{|\mathrm{Re}\, W[\mathcal{C}]|}, \quad \langle \hat{O} \rangle = \frac{\sum_{\mathcal{C}} |\mathrm{Re}\, W[\mathcal{C}]|\, \mathsf{sign}[\mathcal{C}]\ \langle \hat{O} \rangle_{\mathcal{C}}}{\sum_{\mathcal{C}} |\mathrm{Re}\, W[\mathcal{C}]|\, \mathsf{sign}[\mathcal{C}]} = \frac{\langle \hat{O}\, \mathsf{sign} \rangle_{|\mathrm{Re}\, W|}}{\langle \mathsf{sign} \rangle_{|\mathrm{Re}\, W|}}.$$

If the average sign becomes very small:

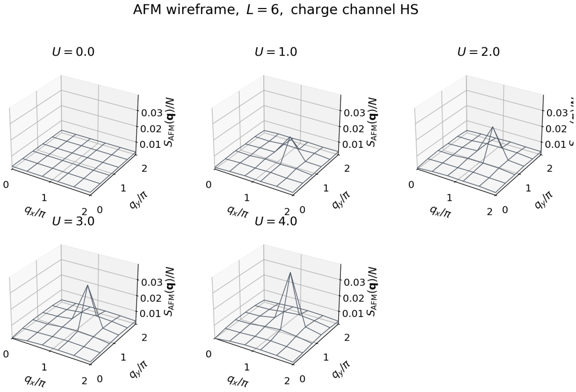
- numerator and denominator are both noisy, so error bars blow up
- the average sign often decreases roughly exponentially with β, system size, or model-dependent frustration/doping

Summary of DQMC algorithm

1. Slice the long propagator into N_τ imaginary-time steps
2. Decouple $\hat{H}_I$ with auxiliary fields and build $\mathcal{C} = \{l_{t,i}\}$
3. For each $\mathcal{C}$, construct the one-body propagator $U_\mathcal{C}$ and weight $W[\mathcal{C}]$
4. Sample $\mathcal{C}$ with a Metropolis update and measure $\langle \hat{O} \rangle_\mathcal{C}$
5. If needed, reweight with $\mathrm{sign}[\mathcal{C}]$ under $|\mathrm{Re}\, W[\mathcal{C}]|$

Example 1: AFM order in the 2D Hubbard model

Half-filled square-lattice Hubbard model: as U/t increases, the spin structure factor develops a pronounced (π, π) peak, signaling antiferromagnetic order.
Here $S(\mathbf{q}) = \frac{1}{N} \sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \langle S_i^z S_j^z \rangle$ with $S_i^z = \frac{1}{2}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$.



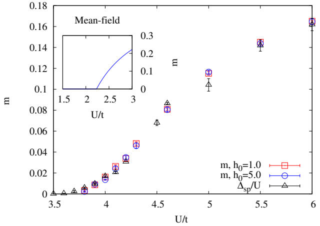
AFM structure factor $S(\mathbf{q})$ across momentum as a function of interaction strength

Example 2: Hubbard model on the honeycomb lattice

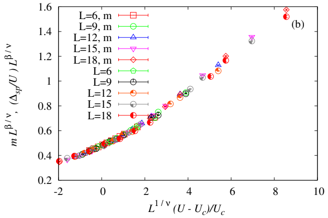
Assaad and Herbut, arXiv:1304.6340

Direct evidence against an intermediate spin-liquid regime:

- the staggered moment and the single-particle gap turn on together
- both quantities are consistent with the same critical scaling near $U_c/t \approx 3.78$



Gap and order turn on together

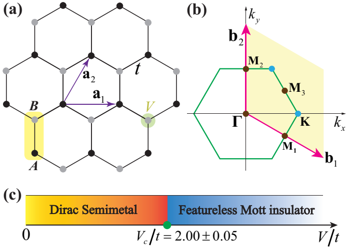


Same universal scaling near U_c

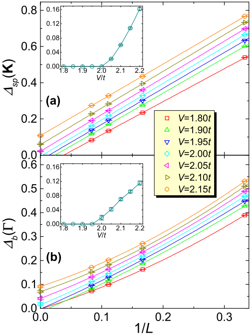
Example 3: symmetric mass generation of Dirac fermions

He et al., arXiv:1603.08376

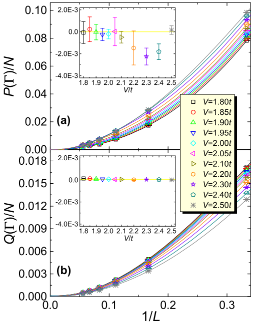
DSM $\to$ FMI transition near $V_c/t \approx 2.0$, with no observed symmetry breaking.



Phase diagram



Gap opening near V_c



$O(6)$ orders remain absent

References and useful resources

Tutorials

- TowardQMC: video introduction to finite-T DQMC
- DQMC at quantummc.xyz: concise Hubbard-model tutorial

Technical review

- Assaad and Evertz, *World line and determinantal Quantum Monte Carlo methods for spins, phonons, and electrons*

Software

- ALF: comprehensive auxiliary-field QMC package
- SmoQyDQMC.jl: Julia package for lattice-fermion QMC simulations