# Determinant Quantum Monte Carlo Method

for Simulating Hubbard Model

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# Hubbard model

Hubbard model: the simplest model of interacting particles

- A kinetic term allowing for "hopping" ($t$)
- A potential term consisting of an on-site interaction ($U$)
- Chemical potential ($\mu$)

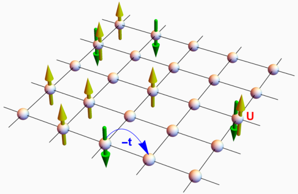



Figure from Huang, E. *et al.* [7]

Hamiltonian:

$$H = -t \sum_{\langle ij \rangle, \sigma} \left( c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_{i} \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_{i} \left( n_{i\uparrow} + n_{i\downarrow} \right)$$

# Traces reduction

- Partition function:

$$Z = \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right)$$

- $4^N$ summations for $N$-particles system
- Dimension reduction (for Hamiltonian of quadratic form):

$$H = \sum_{i,\,j=1}^{N} c_{i\sigma}^{\dagger} h_{ij} c_{j\sigma} \implies \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right) = \det\left(\mathbf{I} + \mathrm{e}^{-\beta \mathbf{h}}\right)$$

- $4^N$-traces $\implies$ $N$-determinants

# Hubbard–Stratonovich transformation

- Potential term in Hubbard model: a quartic term

$$U n_{i\uparrow} n_{i\downarrow} = U c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}$$

- Hubbard–Stratonovich transformation:

$$\mathrm{e}^{-\Delta\tau U\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{1}{2}\mathrm{e}^{-\Delta\tau U/4} \sum_{s_{i,l}=\pm 1} \mathrm{e}^{-\Delta\tau\lambda s_{i,l}\left(n_{i\uparrow}-n_{i\downarrow}\right)}$$

  where

$$\cosh(\Delta\tau\lambda) = \mathrm{e}^{\Delta\tau U/2}$$

  Imaginary time

$$\Delta\tau = \beta/L$$

- $c^4 \implies c^2$ + auxiliary fields$s_{i,l}$

# Final partition function

$$Z = \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right) = \mathrm{Tr}\left(\prod_{l=1}^{L} \mathrm{e}^{-\Delta\tau(K+V)}\right) \simeq \mathrm{Tr}\left(\prod_{l=1}^{L} \mathrm{e}^{-\Delta\tau K}\mathrm{e}^{-\Delta\tau V}\right)$$
$$= \cdots = \det \mathbf{M}^{\uparrow} \cdot \det \mathbf{M}^{\downarrow}$$

where

$$\mathbf{M}^{\sigma} = \mathbf{I} + \mathbf{B}^{\sigma}(L)\,\mathbf{B}^{\sigma}(L-1)\cdots\mathbf{B}^{\sigma}(1), \quad \mathbf{B}^{\sigma}(l) = \mathrm{e}^{-\Delta\tau\mathbf{k}}\,\mathrm{e}^{\mp\Delta\tau\lambda\mathbf{v}(l)}$$

with matrices

$$k_{ij} = -\begin{pmatrix} \mu & t & & \\ t & \mu & t & \\ & t & \mu & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \quad v(l)_{ij} = \begin{pmatrix} s_{1,l} & & & \\ & s_{2,l} & & \\ & & s_{3,l} & \\ & & & \ddots \end{pmatrix}$$

# Monte Carlo algorithm

- $s_{i,l}$: compare with Ising model
- Monte Carlo for Ising:
  1. Initialize spin distribution
  2. Evaluate flip probability $P$ for spin $s_i$
  3. Generate a random number $\xi \in [0, 1]$. If $\xi < P$, then flip $s_i$
  4. Repeat step 2, 3 until equilibrium
  5. Evaluate the ensemble average for physical quantities
- Almost the same for Hubbard model ($s_i \longrightarrow s_{i,l}$)
- Flip probability

$$R_{i,l} = R^{\uparrow}_{i,l} R^{\downarrow}_{i,l}, \qquad R^{\sigma}_{i,l} = \frac{\det \mathbf{M}^{\sigma\prime}}{\det \mathbf{M}^{\sigma}}$$

- Time complexity: $\mathcal{O}(N^3)$

## Equal-time Green function

- Definition:

$$G^{\sigma}(l)_{ij} = \langle \mathcal{T}\left[c_{i\sigma}(l\Delta\tau)\, c^{\dagger}_{i\sigma}(l\Delta\tau)\right]\rangle = \left[\mathbf{I} + \mathbf{A}^{\sigma}(l)\right]^{-1}_{ij}.$$

  where

$$\mathbf{A}^{\sigma}(l) = \mathbf{B}^{\sigma}(l)\cdots\mathbf{B}^{\sigma}(1)\mathbf{B}^{\sigma}(L)\cdots\mathbf{B}^{\sigma}(l+1)$$

- Probability in Green function:

$$R^{\sigma}_{i,\,l} = 1 + \left[1 - G^{\sigma}(l)_{ii}\right]\Delta^{\sigma}(i,\,l)_{ii}, \quad \Delta^{\sigma}(i,\,l)_{ii} = \mathrm{e}^{\pm 2\Delta\tau\lambda s_{i,\,l}} - 1$$

- Change of Green function as $s_{i,\,l} \longrightarrow -s_{i,\,l}$:

$$\mathbf{G}^{\sigma}(l)' = \mathbf{G}^{\sigma}(l) - \frac{\mathbf{G}^{\sigma}(l)\,\mathbf{\Delta}^{\sigma}(i,\,l)\left[\mathbf{I} - \mathbf{G}^{\sigma}(l)\right]}{R^{\sigma}_{i,\,l}}$$

- Update for next imaginary time:

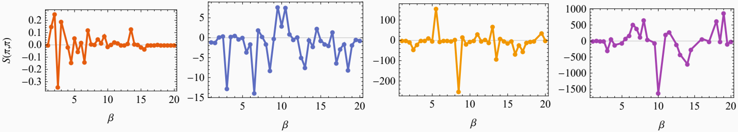
$$\mathbf{G}^{\sigma}(l+1) = \mathbf{B}^{\sigma}(l+1)\,\mathbf{G}^{\sigma}(l)\,\mathbf{B}^{\sigma}(l+1)^{-1}$$

# Full DQMC algorithm

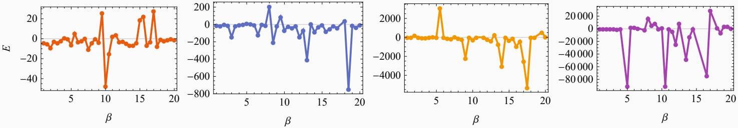
1. Initialize Hubbard–Stratonovich spin field $s_{i,l}$, and calculate Green function at $l = 1$
2. At imaginary time $l$:
   - 2.1 Evaluate flip probability $R_{i,l} = R^{\uparrow}_{i,l} R^{\downarrow}_{i,l}$
   - 2.2 Generate a random number $\xi \in [0, 1]$
   - 2.3 If $\xi < R_{i,l}$, then flip $s_{i,l}$ and update $\mathbf{G}^{\sigma}(l)$
   - 2.4 Evaluate Green function for next time, i.e. $\mathbf{G}^{\sigma}(l+1)$
   - 2.5 Recompute $\mathbf{G}^{\sigma}(l)$ *ab initio* every $l_{\text{stab}}$
3. Return $\mathbf{G}^{\sigma}(l)$ for $l = 1, 2, \cdots, L$
4. Evaluate the ensemble average for physical quantities with Green function

# Our results

- Anti-ferromagnetic structure factor $S^{zz}(\pi, \pi)$:

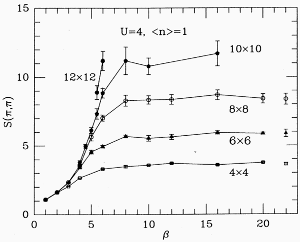



- Energy $E$:




- Size = 4, 8, 16, 32 (1D) from left to right
- Parameters: $t = 1$, $U = 4$, $\mu = 2$, $\Delta\tau = 0.125$, batch = 5
- ~~No physics can be found here :(~~

# What they should be?



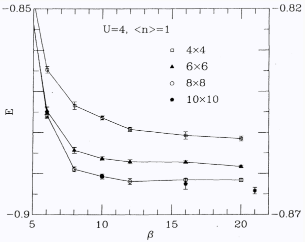




Figure from White, S. *et al.* [8]

- Ground state at low temperature
- $S^{zz}(\pi, \pi)$ increases with size

# Discussion

- Precision is finite in real world
  - Updating Green function: rebuild periodically
  - Inverting ill-conditioned matrices: matrix product stabilization methods (sequential QR-decompositions with column pivoting)
- Fermion sign problem
  - Probability density

$$Z^{-1} \det \mathbf{M}^{\uparrow} \cdot \det \mathbf{M}^{\downarrow}$$

    can be negative
  - Okay for "half-filling" lattice ($\mu = U/2$)

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Thank you!