多体問題の計算科学

Computational Science for Many-Body Problems

#9 Applications of QMC methods
-Path integral & applications

15:10-16:40 June 15, 2021

Quantum Monte Carlo Methods

1. Path integral for quantum spins
2. Path integral for fermions
   - Grassmann number
   - Path integral for free fermions
   - Hubbard-Stratonovich transformation
   - Path integral QMC for Hubbard model
3. Applications of QMC

Quantum Monte Carlo Methods

Typical examples of QMC

■ Variational MC+diffusion MC/Green's function MC

No sign problems, but depend on variational wave functions

McMillan (^{4}He, 1965)
Ceperley-Chester-Kalos (^{3}He, 1977)

cf.) CASINO https://vallico.net/casinoqmc/

■ Imaginary-time path integral by Suzuki-Trotter decomposition

- D-dimensional Transverse field Ising model:
  Mapped on $(D+1)$-dimensional classical Mote Carlo
- Variation: Continuous-time MC, World line MC…
  (implemented in ALPS)
- Power Lanczos by QMC (projective Monte Carlo)

Serious limitation: Sign *problems*

Bosons and fermions:
Blankenbecler-Scalapino-Sugar (1981)
Hirsch (1985)

Path Integral QMC for Spin Models: Formulation

Feynman’s Path Integral:

Transform calculations of non-commutative operators to ones with commutative numbers or *anticommutative Grassmann numbers*

Path Integral by Suzuki

M. Suzuki, S. Miyashita, & A. Kuroda, PTP 58, 1377 (1977)

Suzuki-Trotter decomposition

-Decomposition of partition function:

$$Z = \mathrm{tr}[e^{-\beta\hat{H}}]$$

$$= \sum_{\{\sigma_j\}} \langle \sigma_0\sigma_1\cdots\sigma_{N-1}|e^{-\beta\hat{H}}|\sigma_0\sigma_1\cdots\sigma_{N-1}\rangle$$

$$= \sum_{\{\sigma_j\}} \langle \sigma_0\sigma_1\cdots\sigma_{N-1}|\left(e^{-\frac{\beta}{M}\hat{H}}\right)^M|\sigma_0\sigma_1\cdots\sigma_{N-1}\rangle$$

-Further decomposition of operators

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

$$e^{-\delta_\tau\hat{H}} = e^{-\delta_\tau\hat{H}_1}e^{-\delta_\tau\hat{H}_2} - \frac{\delta_\tau^2}{2}[\hat{H}_1, \hat{H}_2] + \mathcal{O}(\delta_\tau^3)$$

$$\delta_\tau = \beta/M$$

Path Integral: Checkerboard Decomposition

M. Suzuki, S. Miyashita, & A. Kuroda, PTP 58, 1377 (1977).
As a review, H. G. Evertz, Adv. Phys. 52, 1 (2003).

An example: 1D XXZ model

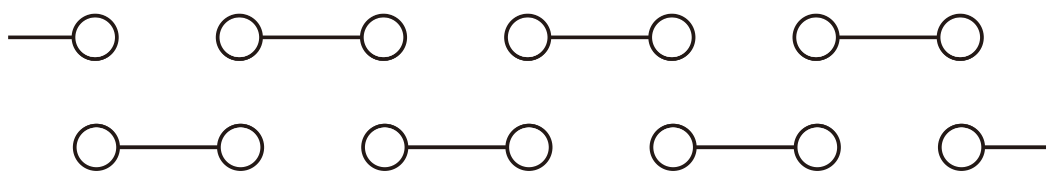
$$\hat{H} = J_x \sum_i (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y) + J_z \sum_i \hat{S}_i^z \hat{S}_{i+1}^z$$

$\hat{H}$

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

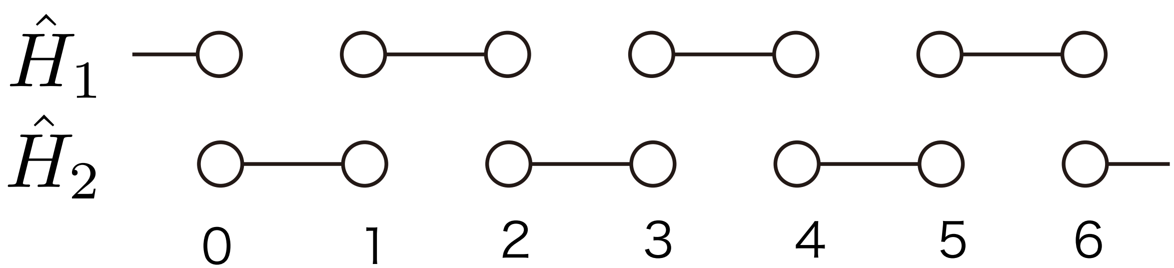
$\hat{H}_1$

$\hat{H}_2$



$$\sum_{\{\sigma_j\}} \langle \sigma_0 \sigma_1 \cdots \sigma_{N-1} | \left(e^{-\frac{\beta}{M} \hat{H}} \right)^M | \sigma_0 \sigma_1 \cdots \sigma_{N-1} \rangle$$

$$\simeq \sum_{\{\sigma_j\}} \langle \sigma_0 \sigma_1 \cdots \sigma_{N-1} | \left(e^{-\delta_\tau \hat{H}_1} e^{-\delta_\tau \hat{H}_2} \right)^M | \sigma_0 \sigma_1 \cdots \sigma_{N-1} \rangle$$



$$e^{-\delta_\tau \hat{H}_2} = e^{-\delta_\tau \hat{H}_{01}} e^{-\delta_\tau \hat{H}_{23}} e^{-\delta_\tau \hat{H}_{45}} \ldots$$

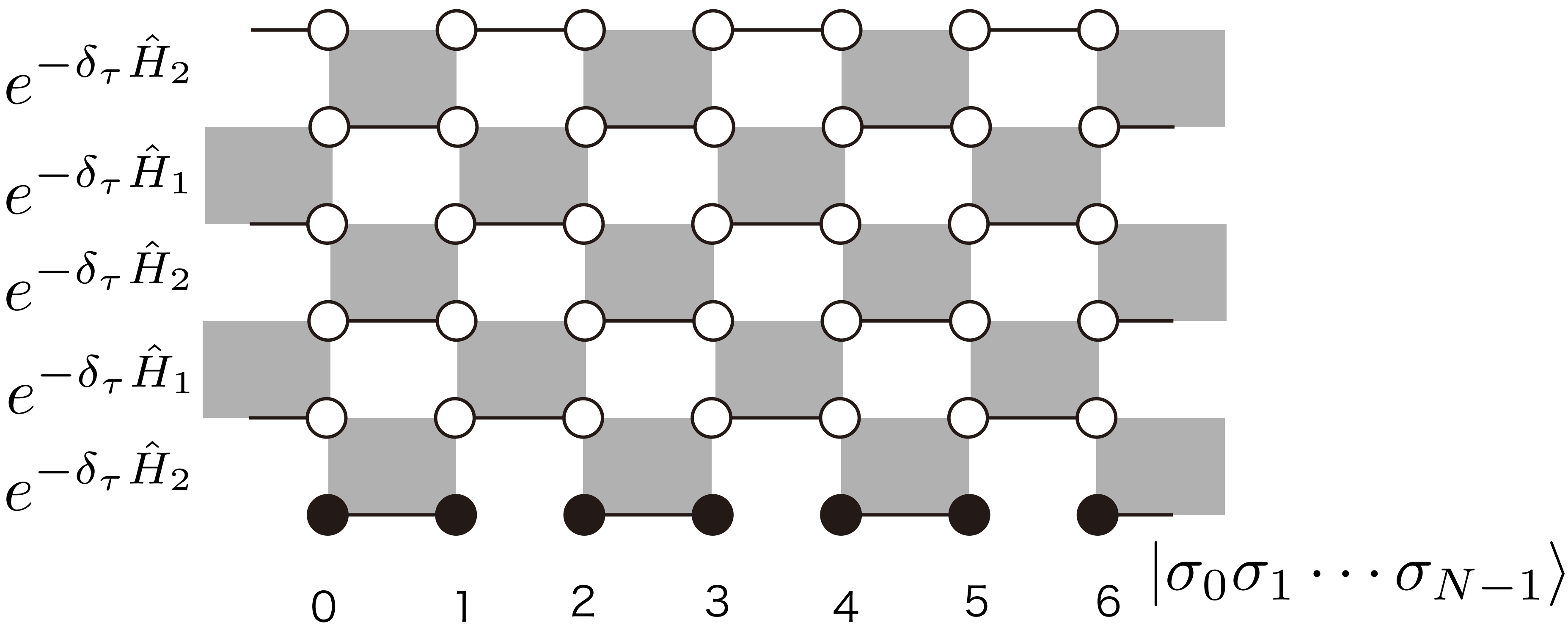
$$e^{-\delta_\tau \hat{H}_1} = e^{-\delta_\tau \hat{H}_{12}} e^{-\delta_\tau \hat{H}_{34}} e^{-\delta_\tau \hat{H}_{56}} \ldots$$

$$\hat{H}_{\ell m} = J_x (\hat{S}^x_\ell \hat{S}^x_m + \hat{S}^y_\ell \hat{S}^y_m) + J_z \hat{S}^z_\ell \hat{S}^z_m$$

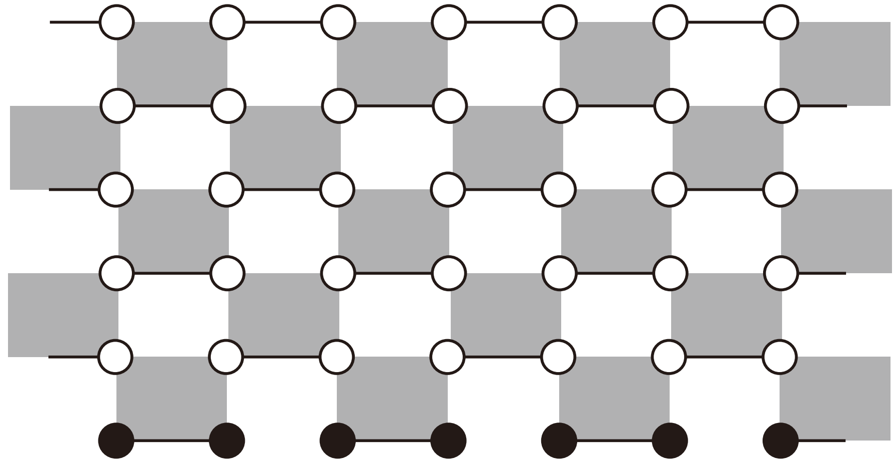
Path Integral: Checkerboard Decomposition

$$e^{-\delta_\tau \hat{H}_2} = e^{-\delta_\tau \hat{H}_{01}} e^{-\delta_\tau \hat{H}_{23}} e^{-\delta_\tau \hat{H}_{45}} \cdots$$

$$e^{-\delta_\tau \hat{H}_1} = e^{-\delta_\tau \hat{H}_{12}} e^{-\delta_\tau \hat{H}_{34}} e^{-\delta_\tau \hat{H}_{56}} \cdots$$



Operators independently act on pairs of spins

$$Z =$$ 

$$Z \simeq \sum_{\{\sigma_j\}} \langle \sigma_0 \sigma_1 \cdots \sigma_{N-1} | \left(e^{-\delta_\tau \hat{H}_1} e^{-\delta_\tau \hat{H}_2} \right)^M | \sigma_0 \sigma_1 \cdots \sigma_{N-1} \rangle$$

$$= \sum_{\{\sigma_j\}} \langle \sigma_0 \sigma_1 \cdots \sigma_{N-1} | \prod_{(\ell,m)=(2m+1,2m+2)} \left[\left(\sum_{\sigma_\ell,\sigma_m} |\sigma_\ell \sigma_m\rangle \langle \sigma_\ell, \sigma_m| \right) e^{-\delta_\tau \hat{H}_{\ell m}} \left(\sum_{\sigma'_\ell,\sigma'_m} |\sigma'_\ell \sigma'_m\rangle \langle \sigma'_\ell \sigma'_m| \right) \right]$$

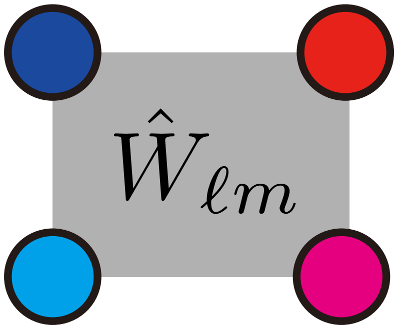
$$\times \prod_{(\ell,m)=(2m,2m+1)} \left[\left(\sum_{\sigma_\ell,\sigma_m} |\sigma_\ell \sigma_m\rangle \langle \sigma_\ell, \sigma_m| \right) e^{-\delta_\tau \hat{H}_{\ell m}} \left(\sum_{\sigma'_\ell,\sigma'_m} |\sigma'_\ell \sigma'_m\rangle \langle \sigma'_\ell \sigma'_m| \right) \right]$$

$$\cdots$$

$$\times \prod_{(\ell,m)=(2m+1,2m+2)} \left[\left(\sum_{\sigma_\ell,\sigma_m} |\sigma_\ell \sigma_m\rangle \langle \sigma_\ell, \sigma_m| \right) e^{-\delta_\tau \hat{H}_{\ell m}} \left(\sum_{\sigma'_\ell,\sigma'_m} |\sigma'_\ell \sigma'_m\rangle \langle \sigma'_\ell \sigma'_m| \right) \right]$$

$$\times \prod_{(\ell,m)=(2m,2m+1)} \left[\left(\sum_{\sigma_\ell,\sigma_m} |\sigma_\ell \sigma_m\rangle \langle \sigma_\ell, \sigma_m| \right) e^{-\delta_\tau \hat{H}_{\ell m}} \left(\sum_{\sigma'_\ell,\sigma'_m} |\sigma'_\ell \sigma'_m\rangle \langle \sigma'_\ell \sigma'_m| \right) \right] |\sigma_0 \sigma_1 \cdots \sigma_{N-1}\rangle$$

Path Integral: Checkerboard Decomposition



$$(\hat{W}_{\ell m})_{\sigma_\ell \sigma_m ; \sigma_\ell \sigma_m} = \langle \sigma_\ell \sigma_m | e^{-\delta_\tau \hat{H}_{\ell m}} | \sigma_\ell \sigma_m \rangle$$

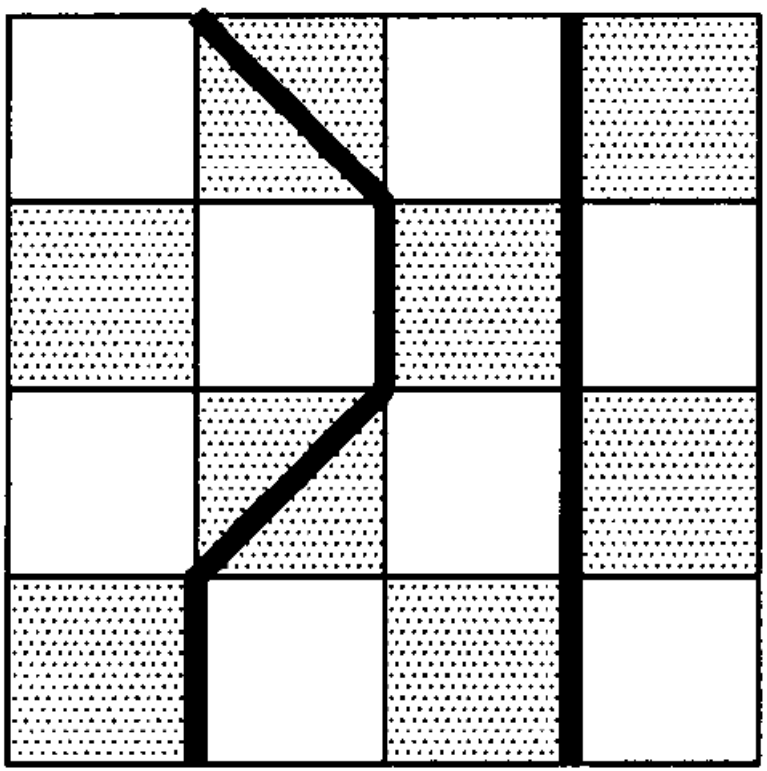
$$\hat{W}_{\ell m} = \begin{pmatrix} \langle \downarrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\downarrow \rangle & 0 & 0 & 0 \\ 0 & \langle \uparrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\downarrow \rangle & \langle \uparrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\uparrow \rangle & 0 \\ 0 & \langle \downarrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\downarrow \rangle & \langle \downarrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\uparrow \rangle & 0 \\ 0 & 0 & 0 & \langle \uparrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\uparrow \rangle \end{pmatrix}$$

$$= \begin{pmatrix} e^{-\delta_\tau J_z/4} & 0 & 0 & 0 \\ 0 & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & -e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & 0 \\ 0 & -e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & 0 \\ 0 & 0 & 0 & e^{-\delta_\tau J_z/4} \end{pmatrix}$$

Path Integral: World Line Representation

As a review, H. G. Evertz, Adv. Phys. 52, 1 (2003).

World line represents (1+1)D spin configurations



0. Bold line connects spin-up sites/virtual sites
1. Bold lines go through only shaded boxes

In XXZ model:

2. Bold lines never overlap each other
3. Bold lines only terminate at the top or bottom of the checkerboard

Usually, sampled and updated by the loop algorithm

(see the Evertz (2003))

Preparation for Fermion Path Integral

Path Integral for Fermions

Path integral

Transform calculations of non-commutative operators to ones with commutative numbers or *anticommutative Grassmann numbers*

By employing coherent state:
An eigenstate of an annihilation operator

Grassman number: $\mathbb{G}$
1. All Grassman numbers are mutually anticommutative, and anticommutative with any fermion operators
2. Squares of all Grassman numbers are zero

$$\text{if } \psi, \phi \in \mathbb{G},\ \psi\phi = -\phi\psi$$
$$\text{therefore } \psi^2 = -\psi^2 = 0$$

R. Shankar, Rev. Mod. Phys. 66, 129 (1994).

Coherent State of Fermions

Coherent state:
An eigenstate of an annihilation operator

Grassman number: $\mathbb{G}$

1. All Grassman numbers are mutually anticommutative, and anticommutative with any fermion operators
2. Squares of all Grassman numbers are zero

$$\boxed{|\psi\rangle = |0\rangle - \psi\hat{c}^\dagger|0\rangle}$$

$$\boxed{\langle\overline{\psi}| = \langle 0| - \langle 0|\hat{c}\ \overline{\psi}}$$

$$\begin{aligned}\hat{c}\ |\psi\rangle &= \psi\hat{c}\ \hat{c}^\dagger|0\rangle \\ &= \psi|0\rangle \\ &= \psi(|0\rangle - \psi\hat{c}^\dagger|0\rangle) \\ &= \psi|\psi\rangle\end{aligned}$$

$$\langle\overline{\psi}|\hat{c}^\dagger = \langle\overline{\psi}|\overline{\psi}$$

$$\psi, \overline{\psi} \in \mathbb{G}$$

R. Shankar, Rev. Mod. Phys. 66, 129 (1994).

Analysis of Grassman Numbers

Function of Grassman number: $f(\psi) = f_0 + f_1\psi$

Relation between Grassman and complex number

Integral of Grassman number: $\int \psi d\psi = 1 \qquad \int d\psi\psi = -1$

$$\int 1 d\psi = 0$$

Closure by Grassman numbers: $\underline{1 = \int |\psi\rangle\langle\overline{\psi}|e^{-\overline{\psi}\psi} d\overline{\psi}d\psi}$

$$\begin{aligned}
\mathrm{Tr}\hat{O} &= \langle 0|\hat{O}|0\rangle + \langle 0|\hat{c}\ \hat{O}\hat{c}^\dagger|0\rangle \\
&= \int \langle 0|\hat{O}|\psi\rangle\langle\overline{\psi}|0\rangle e^{-\overline{\psi}\psi} d\overline{\psi}d\psi + \int \langle 0|\hat{c}\ \hat{O}|\psi\rangle\langle\overline{\psi}|\hat{c}^\dagger|0\rangle e^{-\overline{\psi}\psi} d\overline{\psi}d\psi \\
&= \int \langle -\overline{\psi}|\hat{O}|\psi\rangle e^{-\overline{\psi}\psi} d\overline{\psi}d\psi
\end{aligned}$$

R. Shankar, Rev. Mod. Phys. 66, 129 (1994).

Path Integral for Fermions

Path integral for a single fermion

$$\hat{H}[\hat{c}^\dagger, \hat{c}] = \varepsilon \hat{c}^\dagger \hat{c}$$

Suzuki-Trotter decomposition

$$\begin{aligned}
\mathrm{Tr} e^{-\beta \hat{H}[\hat{c}^\dagger, \hat{c}]} &= \mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}[\hat{c}^\dagger, \hat{c}]}\right)^M \\
&\simeq \int \langle -\overline{\psi}(1)| e^{-\frac{\beta}{M}\hat{H}[-\overline{\psi}(1), \psi(M)]} |\psi(M)\rangle e^{-\overline{\psi}(M)\psi(M)} \\
&\times \langle \overline{\psi}(M)| e^{-\frac{\beta}{M}\hat{H}[\overline{\psi}(M), \psi(M-1)]} |\psi(M-1)\rangle e^{-\overline{\psi}(M-1)\psi(M-1)} \\
&\times \cdots \\
&\times \langle \overline{\psi}(2)| e^{-\frac{\beta}{M}\hat{H}[\overline{\psi}(2), \psi(1)]} |\psi(1)\rangle e^{-\overline{\psi}(1)\psi(1)} \prod_{\ell=1}^{M} d\overline{\psi}(\ell) d\psi(\ell)
\end{aligned}$$

$$\begin{aligned}
\langle \overline{\psi}(L)| e^{-\frac{\beta}{M}\varepsilon \hat{c}^\dagger \hat{c}} |\psi(L-1)\rangle &= \exp\left[\left(e^{-\frac{\beta}{M}\varepsilon}\right)\overline{\psi}(L)\psi(L-1)\right] \\
&= \exp\left[\left(1-\frac{\beta}{M}\varepsilon\right)\overline{\psi}(L)\psi(L-1)\right] + \mathcal{O}\left(\left\{\frac{\beta}{M}\varepsilon\right\}^2\right)
\end{aligned}$$

Path Integral for Fermions

Path integral for a single fermion $\quad \hat{H}[\hat{c}^\dagger, \hat{c}] = \varepsilon \hat{c}^\dagger \hat{c}$

$$\mathrm{Tr} e^{-\beta \hat{H}[\hat{c}^\dagger, \hat{c}]} = \langle 0 | e^{-\beta \hat{H}[\hat{c}^\dagger, \hat{c}]} | 0 \rangle + \langle 0 | \hat{c} e^{-\beta \hat{H}[\hat{c}^\dagger, \hat{c}]} \hat{c}^\dagger | 0 \rangle = 1 + e^{-\beta\varepsilon}$$

$$\begin{aligned}
\mathrm{Tr} e^{-\beta \hat{H}[\hat{c}^\dagger, \hat{c}]} &= \mathrm{Tr} \left(e^{-\frac{\beta}{M} \hat{H}[\hat{c}^\dagger, \hat{c}]} \right)^M \\
&\simeq \int \exp\left[+ \frac{\beta}{M} \varepsilon \overline{\psi}(1)\psi(M) - \overline{\psi}(1)\psi(M) - \overline{\psi}(M)\psi(M) \right] \\
&\quad \times \exp\left[- \frac{\beta}{M} \varepsilon \overline{\psi}(M)\psi(M-1) + \overline{\psi}(M)\psi(M-1) - \overline{\psi}(M-1)\psi(M-1) \right] \\
&\quad \times \cdots \\
&\quad \times \exp\left[- \frac{\beta}{M} \varepsilon \overline{\psi}(2)\psi(1) + \overline{\psi}(2)\psi(1) - \overline{\psi}(1)\psi(1) \right] \prod_{\ell=1}^{M} d\overline{\psi}(\ell) d\psi(\ell) \\
&= 1 + \left(1 - \tfrac{\beta}{M}\varepsilon\right)^M \underset{M \to +\infty}{\to} 1 + e^{-\beta\varepsilon}
\end{aligned}$$

Useful relation: $\langle \overline{\psi} | \psi \rangle = e^{\overline{\psi}\psi}$

Further Steps towards QMC

Path integral for QMC

-Many fermions
Complicated but straightforward

-Hubbard-Stratonovich transformation
Hubbard model mapped onto an ensemble of
free fermions feeling Ising one-body potentials

-Balenkenbecler-Scalapino-Sugar formulation for QMC
MC for Ising variables with weights
calculated by fermionic partition functions

R. Blankenbecler, D. J. Scalapino, & R. L. Sugar, Phys. Rev. D 24, 2278 (1981).
J. E. Hirsch, Phys. Rev. B 31, 4403 (1985).

Path Integral for Many Fermions

Fermions have site and spin indices

$$\hat{H}[\{\hat{c}^{\dagger}_{i\sigma}, \hat{c}_{i\sigma}\}] = -\sum_{i,j,\sigma} t_{i,j}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \sum_{i,\sigma} h_{i\sigma}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$$

*Valid for any one-body Hamiltonian

$$\begin{aligned}
\mathrm{Tr}e^{-\beta\hat{H}[\{\hat{c}^{\dagger}_{i\sigma},\hat{c}_{i\sigma}\}]} &= \mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}[\{\hat{c}^{\dagger}_{i\sigma},\hat{c}_{i\sigma}\}]}\right)^M \\
&= \int \langle\{-\overline{\psi}_{i\sigma}(1)\}|e^{-\frac{\beta}{M}\hat{H}[\{-\overline{\psi}_{i\sigma}(1),\psi_{i\sigma}(M)\}]}|\{\psi_{i\sigma}(M)\}\rangle \\
&\quad \times e^{-\sum_{i,\sigma}\overline{\psi}_{i\sigma}(M)\psi_{\sigma}(M)} \\
&\quad \times\langle\{\overline{\psi}_{i\sigma}(M)\}|e^{-\frac{\beta}{M}\hat{H}[\{\overline{\psi}_{i\sigma}(M),\psi_{i\sigma}(M-1)\}]}|\{\psi_{i\sigma}(M-1)\}\rangle \\
&\quad \times e^{-\sum_{i,\sigma}\overline{\psi}_{i\sigma}(M-1)\psi_{i\sigma}(M-1)} \\
&\quad \times\cdots \\
&\quad \times\langle\{\overline{\psi}_{i\sigma}(2)\}|e^{-\frac{\beta}{M}\hat{H}[\{\overline{\psi}_{i\sigma}(2),\psi_{i\sigma}(1)\}]}|\{\psi_{i\sigma}(1)\}\rangle \\
&\quad \times e^{-\sum_{i,\sigma}\overline{\psi}_{i\sigma}(1)\psi_{i\sigma}(1)} \\
&\quad \times\prod_{\sigma=\uparrow,\downarrow}\prod_{i=1}^{N}\prod_{\ell=1}^{M} d\overline{\psi}_{i\sigma}(\ell)d\psi_{i\sigma}(\ell)
\end{aligned}$$

Path Integral for Many Fermions

Decomposed operators for imaginary-time evolution: B_L

$$B_L:\ 2N\times 2N \text{ matrix}$$

$$\begin{aligned}
&\langle\{\overline{\psi}_{i\sigma}(L)\}|e^{-\frac{\beta}{M}\hat{H}[\{\overline{\psi}_{i\sigma}(L),\psi_{i\sigma}(L-1)\}]}|\{\psi_{i\sigma}(L-1)\}\rangle\\
&= e^{-\frac{\beta}{M}\hat{H}[\{\overline{\psi}_{i\sigma}(L),\psi_{i\sigma}(L-1)\}]+\sum_{i,\sigma}\overline{\psi}_{i\sigma}(L)\psi_{i\sigma}(L-1)}\\
&= \exp\left[+\sum_{i,j}\sum_{\sigma,\tau}\overline{\psi}_{i\sigma}(L)(B_L)_{i\sigma,j\tau}\psi_{j\tau}(L-1)\right]
\end{aligned}$$

$$\begin{aligned}
&\langle\{-\overline{\psi}_{i\sigma}(1)\}|e^{-\frac{\beta}{M}\hat{H}[\{-\overline{\psi}_{i\sigma}(1),\psi_{i\sigma}(M)\}]}|\{\psi_{i\sigma}(M)\}\rangle\\
&= \exp\left[-\sum_{i,j}\sum_{\sigma,\tau}\overline{\psi}_{i\sigma}(1)(B_1)_{i\sigma,j\tau}\psi_{j\tau}(M)\right]
\end{aligned}$$

Here, imaginary-time dependence of the matrices *B*
for later usage for taking interactions into account

Path Integral for Many Fermions

Path integral representation of partition function

$$\mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}[\{\hat{c}^\dagger_{i\sigma},\hat{c}_{i\sigma}\}]}\right)^M \simeq \int e^{-\sum_{L=1}^{M}\overline{\psi}(L)I\psi(L)} \times e^{-\overline{\psi}(1)B_1\psi(M)+\sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)}\left[d\overline{\psi}d\psi\right]$$

$$\left[d\overline{\psi}d\psi\right] \equiv \prod_{\sigma=\uparrow,\downarrow}\prod_{i=1}^{N}\prod_{\ell=1}^{M} d\overline{\psi}_{i\sigma}(\ell)d\psi_{i\sigma}(\ell)$$

$$\overline{\psi}(L)B_L\psi(L-1) = \sum_{i,j}\sum_{\sigma,\tau}\overline{\psi}_{i\sigma}(L)(B_L)_{i\sigma,j\tau}\psi_{j\tau}(L-1)$$

$$\overline{\psi}(L)I\psi(L) = \sum_{i,\sigma}\overline{\psi}_{i\sigma}(L)\psi_{i\sigma}(L)$$

Integration over Many Grassmann Variables

One-step integration

$$\int \exp\left[-\sum_{\mu,\nu}\overline{\psi}_\mu A_{\mu\nu}\psi_\nu\right][d\overline{\psi}d\psi] = \det A$$

$$A: \ 2NM \times 2NM \ \text{matrix}$$

$$\mu,\nu: \ \text{site index } i, \text{spin index } \sigma, \text{imaginary time slice}$$

Localized nature of the action S along imaginary time is not exploited in the *one-step* integration

$$S[\{\overline{\psi}_{i\sigma},\psi_{i\sigma}\}] = \sum_{L=1}^{M}\overline{\psi}(L)I\psi(L) + \overline{\psi}(1)B_1\psi(M) - \sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)$$

Hoppings along imaginary time exist always between nearest neighbors

Partition Function of Many Fermions

Partial integration over $\overline{\psi}(1),\psi(1),\overline{\psi}(2),\psi(2),\dots,\overline{\psi}(M-1),\psi(M-1)$

$$\mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}[\{\hat{c}^{\dagger}_{i\sigma},\hat{c}_{i\sigma}\}]}\right)^{M} = \int e^{-\sum_{L=1}^{M}\overline{\psi}(L)I\psi(L)} \times e^{-\overline{\psi}(1)B_1\psi(M)+\sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)}\left[d\overline{\psi}d\psi\right]$$

$$\begin{aligned}
&\int e^{-\sum_{L=1}^{M}\overline{\psi}(L)I\psi(L)-\overline{\psi}(1)B_1\psi(M)+\sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)}\left[d\overline{\psi}d\psi\right]\\
&=\int e^{-\overline{\psi}(M)I\psi(M)}\\
&\times\prod_{i,\sigma}\left[1-\overline{\psi}_{i\sigma}(M-1)\psi_{i\sigma}(M-1)\right]\\
&\times\prod_{i,\sigma}\left[1-\overline{\psi}_{i\sigma}(M-2)\psi_{i\sigma}(M-2)\right]\\
&\times\cdots\\
&\times\prod_{i,\sigma}\left[1-\overline{\psi}_{i\sigma}(1)\psi_{i\sigma}(1)\right]\\
&\times\prod_{i_a,\sigma_a,i,\sigma,j,\tau}\left[1-\overline{\psi}_{i\sigma}(M)(B_M)_{i\sigma,i_1\sigma_1}\psi_{i_1\sigma_1}(M-1)\overline{\psi}_{i_1\sigma_1}(M-1)\right.\\
&\qquad\times(B_{M-1})_{i_1\sigma_1,i_2\sigma_2}\psi_{i_2\sigma_2}(M-2)\overline{\psi}_{i_2\sigma_2}(M-2)\\
&\qquad\times\cdots\\
&\qquad\times(B_2)_{i_{M-2}\sigma_{M-2},i_{M-1}\sigma_{M-1}}\psi_{i_{M-1}\sigma_{M-1}}(1)\overline{\psi}_{i_{M-1}\sigma_{M-1}}(1)\\
&\qquad\left.\times(B_1)_{i_{M-1}\sigma_{M-1},j\tau}\psi_{j\tau}(M)\right]\left[d\overline{\psi}d\psi\right]
\end{aligned}$$

Partition Function of Many Fermions

Partial integration

$$\mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}[\{\hat{c}_{i\sigma}^{\dagger},\hat{c}_{i\sigma}\}]}\right)^{M} = \int e^{-\sum_{L=1}^{M}\overline{\psi}(L)I\psi(L)} \times e^{-\overline{\psi}(1)B_1\psi(M)+\sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)}\left[d\overline{\psi}d\psi\right]$$

$$= \int e^{-\overline{\psi}(M)I\psi(M)-\overline{\psi}(M)B_M B_{M-1}\cdots B_1\psi(M)}d\overline{\psi}(M)d\psi(M)$$

$4NM$ dimensional integral → $4N$ dimensional integral

Partition Function of Many Fermions

Partial integration

$$
\begin{aligned}
\mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}[\{\hat{c}^{\dagger}_{i\sigma},\hat{c}_{i\sigma}\}]}\right)^{M} = & \int e^{-\sum_{L=1}^{M}\overline{\psi}(L)I\psi(L)} \\
& \times e^{-\overline{\psi}(1)B_1\psi(M)+\sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)}\left[d\overline{\psi}d\psi\right]
\end{aligned}
$$

$$
\begin{aligned}
= & \int e^{-\overline{\psi}(M)I\psi(M)-\overline{\psi}(M)B_M B_{M-1}\cdots B_1\psi(M)}d\overline{\psi}(M)d\psi(M) \\
= & \det\left[I+B_M B_{M-1}\cdots B_1\right]
\end{aligned}
$$

Partition Function of Many Fermion

Partial integration

$$
\mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}[\{\hat{c}^{\dagger}_{i\sigma},\hat{c}_{i\sigma}\}]}\right)^{M} = \int e^{-\sum_{L=1}^{M}\overline{\psi}(L)I\psi(L)} \times e^{-\overline{\psi}(1)B_1\psi(M)+\sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)}\left[d\overline{\psi}d\psi\right]
$$

$$
= \int e^{-\overline{\psi}(M)I\psi(M)-\overline{\psi}(M)B_M B_{M-1}\cdots B_1\psi(M)} d\overline{\psi}(M)d\psi(M)
$$

$$
= \det\left[I + B_M B_{M-1}\cdots B_1\right]
$$

The following identity is proven:

$$
\det\begin{bmatrix}
I & 0 & 0 & 0 & \cdots & 0 & +B_1 \\
-B_2 & I & 0 & 0 & \cdots & 0 & 0 \\
0 & -B_3 & I & 0 & \cdots & 0 & 0 \\
0 & 0 & -B_4 & I & \cdots & 0 & 0 \\
\vdots & \vdots & & & \ddots & & \vdots \\
0 & 0 & 0 & 0 & \cdots & I & 0 \\
0 & 0 & 0 & 0 & \cdots & -B_M & I
\end{bmatrix} = \det\left[I + B_M B_{M-1}\cdots B_1\right]
$$

Green's Function by Path Integral

A basic observable: Green's function

$$\langle \hat{c}_{i\sigma}(L_1)\hat{c}^\dagger_{j\tau}(L_2)\rangle = \frac{\int \psi_{i\sigma}(L_1)\overline{\psi}_{j\tau}(L_2)e^{-S[\overline{\psi},\psi]}\left[d\overline{\psi}d\psi\right]}{\int e^{-S[\overline{\psi},\psi]}\left[d\overline{\psi}d\psi\right]}$$

$$M > L_1 > L_2 > 1$$

$$S[\overline{\psi},\psi] = \sum_{L=1}^{M}\overline{\psi}(L)I\psi(L) + \overline{\psi}(1)B_1\psi(M) - \sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)$$

$$\hat{c}_{i\sigma}(L) = e^{+L\frac{\beta}{M}\hat{H}}\hat{c}_{i\sigma}e^{-L\frac{\beta}{M}\hat{H}}$$

$$\int e^{-S[\overline{\psi},\psi]}\left[d\overline{\psi}d\psi\right] = \det\left[I + B_{L_2}\cdots B_1 B_M \cdots B_{L_2+1}\right]$$

Green's Function by Path Integral

Details in evaluation of the numerator

$$
\begin{aligned}
& \int \psi_{i\sigma}(L_1)\overline{\psi}_{j\tau}(L_2)e^{-\sum_{L=1}^{M}\overline{\psi}(L)I\psi(L)} \\
& \times e^{-\overline{\psi}(1)B_1\psi(M)+\sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)}\left[d\overline{\psi}d\psi\right] \\
= \quad & \int \psi_{i\sigma}(L_1)\overline{\psi}_{j\tau}(L_2)e^{-\overline{\psi}(L_1)I\psi(L_1)-\overline{\psi}(L_2)I\psi(L_2)} \\
& \times e^{\overline{\psi}(L_1)B_{L_1}\cdots B_{L_2+1}\psi(L_2)-\overline{\psi}(L_2)B_{L_2}\cdots B_1B_M\cdots B_{L_1+1}\psi(L_1)} \\
& \times \left[d\overline{\psi}d\psi\right] \\
= \quad & \partial_\lambda \int e^{-\lambda\overline{\psi}(L_2)e(j\tau,i\sigma)\psi(L_1)-\overline{\psi}(L_1)I\psi(L_1)-\overline{\psi}(L_2)I\psi(L_2)} \\
& \times e^{\overline{\psi}(L_1)B_{L_1}\cdots B_{L_2+1}\psi(L_2)-\overline{\psi}(L_2)B_{L_2}\cdots B_1B_M\cdots B_{L_1+1}\psi(L_1)} \\
& \times \left[d\overline{\psi}d\psi\right] \\
= \quad & \partial_\lambda \int e^{-\overline{\psi}(L_2)I\psi(L_2)} \\
& \times e^{-\lambda\overline{\psi}(L_2)e(j\tau,i\sigma)B_{L_1}\cdots B_{L_2+1}\psi(L_2)-\overline{\psi}(L_2)B_{L_2}\cdots B_1B_M\cdots B_{L_2+1}\psi(L_2)} \\
& \times \left[d\overline{\psi}d\psi\right] \\
= \quad & \partial_\lambda \det\left[I+\lambda e(j\tau,i\sigma)B_{L_1}\cdots B_{L_2+1}+B_{L_2}\cdots B_1B_M\cdots B_{L_2+1}\right]
\end{aligned}
$$

Mathematical Tools

A useful matirx

$$e(I,J) = \begin{array}{c|ccccccc} & & & & J & & & \\ \hline & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ I & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{array}$$

Cofactor expansion of determinant

$$\boxed{\det A = \sum_K \Delta_{KJ}(A) a_{KJ}} \qquad (A)_{IJ} = a_{IJ}$$

$$\to \ \partial_{a_{IJ}} \det A = \Delta_{IJ}(A)$$

Green's Function by Path Integral

Evaluation by cofactor

$$\partial_\lambda \det\left[I + \lambda e(j\tau, i\sigma) B_{L_1} \cdots B_{L_2+1} + B_{L_2} \cdots B_1 B_M \cdots B_{L_2+1}\right]$$
$$= \left(B_{L_1} \cdots B_{L_2+1}\right)_{i\sigma,k} \Delta_{j\tau,k}(I + B_{L_2} \cdots B_1 B_M \cdots B_{L_2+1})$$

$$\left(\left[I + B_{L_2} \cdots B_1 B_M \cdots B_{L_2+1}\right]^{-1}\right)_{kj} = \frac{\Delta_{jk}(I + B_{L_2} \cdots B_1 B_M \cdots B_{L_2+1})}{\det\left[I + B_{L_2} \cdots B_1 B_M \cdots B_{L_2+1}\right]}$$

Green's function by BSS

$$\langle \hat{c}_{i\sigma}(L_1) \hat{c}^\dagger_{j\tau}(L_2) \rangle = \left(B_{L_1} \cdots B_{L_2+1} \left[I + B_{L_2} \cdots B_1 B_M \cdots B_{L_2+1}\right]^{-1}\right)_{i\sigma,j\tau}$$

Blankenbecler, Scalapino, & Sugar, Phys. Rev. D 24, 2278 (1981).
Hirsch, Phys. Rev. B 31, 4403 (1985).

Home work: Equal-time Green's function

$$\langle \hat{c}_{i\sigma} \hat{c}^\dagger_{j\tau} \rangle = \langle \hat{c}_{i\sigma}(L) \hat{c}^\dagger_{j\tau}(L) \rangle = \left(\left[I + B_{L_2} \cdots B_1 B_M \cdots B_{L_2+1}\right]^{-1}\right)_{i\sigma,j\tau}$$

Hubbard-Stratonovich Transformation

R. Stratonovich is best known for the Stratonovich integral (stochastic integral)
J. Hubbard, Phys. Rev. Lett. 3, 77 (1959).

$$e^{-\Delta\tau U \hat{n}_\uparrow \hat{n}_\downarrow} = \exp\left[\frac{\Delta\tau U}{2}\left\{(\hat{n}_\uparrow - \hat{n}_\downarrow)^2 - \hat{n}_\uparrow - \hat{n}_\downarrow\right\}\right]$$

$$\hat{n}_\sigma^2 = \hat{n}_\sigma \ \ (\hat{n}_\sigma = \hat{c}_\sigma^\dagger \hat{c}_\sigma)$$

$$\int_{-\infty}^{+\infty} d\phi_{\mathrm{s}} \exp\left[-\frac{\Delta\tau U}{2}\left\{\phi_{\mathrm{s}} - (\hat{n}_\uparrow - \hat{n}_\downarrow)\right\}^2\right] = \sqrt{\frac{2\pi}{\Delta\tau U}}$$

Continuous Hubbard-Stratonovich transformation

$$e^{\frac{\Delta\tau U}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow)^2} = \sqrt{\frac{\Delta\tau U}{2\pi}} \int d\phi_{\mathrm{s}} \exp\left[-\frac{\Delta\tau U}{2}\phi_{\mathrm{s}}^2 + \Delta\tau U \phi_{\mathrm{s}}(\hat{n}_\uparrow - \hat{n}_\downarrow)\right]$$

Hubbard-Stratonovich Transformation

J. E. Hirsch, Phys. Rev. B 28, 4059 (1983).

Discrete Hubbard-Stratonovich transformation

Find an operator that is equivalent to exponential of doublon

$$\begin{aligned} e^{-\Delta\tau U \hat{n}_\uparrow \hat{n}_\downarrow}|0\rangle &= |0\rangle \\ e^{-\Delta\tau U \hat{n}_\uparrow \hat{n}_\downarrow}|\uparrow\rangle &= |\uparrow\rangle \\ e^{-\Delta\tau U \hat{n}_\uparrow \hat{n}_\downarrow}|\downarrow\rangle &= |\downarrow\rangle \\ e^{-\Delta\tau U \hat{n}_\uparrow \hat{n}_\downarrow}|\uparrow\downarrow\rangle &= e^{-\Delta\tau U}|\uparrow\downarrow\rangle \end{aligned}$$

An ansatz inspired by the continuous HS transformation

$$\hat{O}_{\mathrm{HS}}(\Delta\tau U) = \frac{1}{2}\sum_{s=\pm 1} \exp\left[\phi s(\hat{n}_\uparrow - \hat{n}_\downarrow) - \frac{\Delta\tau}{2} U(\hat{n}_\uparrow + \hat{n}_\downarrow)\right]$$

$$e^{\frac{\Delta\tau U}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow)^2} = \sqrt{\frac{\Delta\tau U}{2\pi}} \int d\phi_{\mathrm{s}} \exp\left[-\frac{\Delta\tau U}{2}\phi_{\mathrm{s}}^2 + \Delta\tau U \phi_{\mathrm{s}}(\hat{n}_\uparrow - \hat{n}_\downarrow)\right]$$

Hubbard-Stratonovich Transformation

J. E. Hirsch, Phys. Rev. B 28, 4059 (1983).

Discrete Hubbard-Stratonovich transformation

$$\hat{O}_{\mathrm{HS}}(\Delta\tau U) = \frac{1}{2}\sum_{s=\pm 1} \exp\left[\phi s(\hat{n}_\uparrow - \hat{n}_\downarrow) - \frac{\Delta\tau}{2}U(\hat{n}_\uparrow + \hat{n}_\downarrow)\right]$$

$$\begin{aligned}
\hat{O}_{\mathrm{HS}}(\Delta\tau U)|0\rangle &= |0\rangle \\
\hat{O}_{\mathrm{HS}}(\Delta\tau U)|\uparrow\rangle &= e^{-\frac{\Delta\tau U}{2}}\left(\frac{e^{+\phi}+e^{-\phi}}{2}\right)|\uparrow\rangle \\
\hat{O}_{\mathrm{HS}}(\Delta\tau U)|\downarrow\rangle &= e^{-\frac{\Delta\tau U}{2}}\left(\frac{e^{+\phi}+e^{-\phi}}{2}\right)|\downarrow\rangle \\
\hat{O}_{\mathrm{HS}}(\Delta\tau U)|\uparrow\downarrow\rangle &= e^{-\Delta\tau U}|\uparrow\downarrow\rangle
\end{aligned}$$

$$\begin{aligned}
e^{-\Delta\tau U\hat{n}_\uparrow\hat{n}_\downarrow}|0\rangle &= |0\rangle \\
e^{-\Delta\tau U\hat{n}_\uparrow\hat{n}_\downarrow}|\uparrow\rangle &= |\uparrow\rangle \\
e^{-\Delta\tau U\hat{n}_\uparrow\hat{n}_\downarrow}|\downarrow\rangle &= |\downarrow\rangle \\
e^{-\Delta\tau U\hat{n}_\uparrow\hat{n}_\downarrow}|\uparrow\downarrow\rangle &= e^{-\Delta\tau U}|\uparrow\downarrow\rangle
\end{aligned}$$

$$e^{-\frac{\Delta\tau U}{2}}\left(\frac{e^{+\phi}+e^{-\phi}}{2}\right) = 1$$

$$\phi = 2\ \mathrm{arctanh}\sqrt{\tanh\frac{\Delta\tau U}{4}}$$

$$\left(\tanh\frac{\phi}{2}\right)^2 = \frac{\cosh\phi - 1}{\cosh\phi + 1} = \tanh\frac{\Delta\tau U}{4}$$

$$\rightarrow\quad e^{-\Delta\tau U\hat{n}_\uparrow\hat{n}_\downarrow} = \hat{O}_{\mathrm{HS}}(\Delta\tau U)$$

Path Integral for Hubbard Models

Hubbard model

$$\hat{H}[\{\hat{c}_{i\sigma},\hat{c}^{\dagger}_{i\sigma}\}] = -\sum_{i,j,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

Split step

$$e^{+\Delta\tau\sum_{i,j,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}-\Delta\tau U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}}$$
$$= e^{+\Delta\tau\sum_{i,j,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}} e^{-\Delta\tau U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}} + \mathcal{O}\left(\Delta\tau^2 U^2, \Delta\tau^2 t^2\right)$$

HS transformation

$$e^{-\Delta\tau\hat{H}[\{\hat{c}^{\dagger}_{i\sigma},\hat{c}_{i\sigma},s_i\}]} = \left(\frac{1}{2}\right)^{N}\sum_{\{s_i\}=\pm 1} e^{\Delta\tau\sum_{i,j,\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}}$$
$$\times e^{\phi\sum_i s_i(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})-\frac{\Delta\tau}{2}U\sum_i(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})}$$

Hubbard model is mapped onto
an ensemble of free fermions interacting with Ising variables

Path Integral for Hubbard Models

Split step for kinetic and interaction terms

$$
\begin{aligned}
e^{-\Delta\tau \hat{H}[\{\hat{c}^\dagger_{i\sigma},\hat{c}_{i\sigma},s_i\}]} &= \left(\frac{1}{2}\right)^N \sum_{\{s_i\}=\pm 1} e^{\Delta\tau \sum_{i,j,\sigma} t_{ij}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}} \\
&\quad \times e^{\phi \sum_i s_i(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow}) - \frac{\Delta\tau}{2} U \sum_i (\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})} \\
&= \left(\frac{1}{2}\right)^N \sum_{\{s_i\}=\pm 1} e^{-K[\{\hat{c}^\dagger_{i\sigma},\hat{c}_{i\sigma}\}]} e^{-V[\{\hat{c}^\dagger_{i\sigma},\hat{c}_{i\sigma},s_i\}]}
\end{aligned}
$$

$$
\begin{aligned}
& \langle\overline{\psi}(L)|e^{-K[\{\hat{c}^\dagger_{i\sigma},\hat{c}_{i\sigma}\}]} e^{-V[\{\hat{c}^\dagger_{i\sigma},\hat{c}_{i\sigma},s_i\}]}|\psi(L-1)\rangle \\
= & \int \langle\overline{\psi}(L)|e^{-K[\{\overline{\psi}_{i\sigma}(L),\psi_{i\sigma}(\ell)\}]}|\psi(\ell)\rangle\langle\overline{\psi}(\ell)|e^{-V[\{\overline{\psi}_{i\sigma}(\ell),\psi_{i\sigma}(L-1),s_i\}]}|\psi(L-1)\rangle \\
& \times e^{-\overline{\psi}(\ell) I \psi(\ell)} \prod_{i\sigma} d\overline{\psi}_{i\sigma}(\ell) d\psi_{i\sigma}(\ell) \\
= & \, e^{\overline{\psi}(L)(I-K_L)(I-V[\{s_i(L)\}])\psi(L-1)}
\end{aligned}
$$

$$B_L = (I-K_L)(I-V_L[\{s_i(L)\}])$$

Path Integral for Hubbard Models

$$\langle \hat{O}[\{\hat{c}^{\dagger}_{i\sigma}, \hat{c}_{i\sigma}\}]\rangle = \frac{\left(\frac{1}{2}\right)^{NM} \sum_{\{s_i(L)\}=\pm 1} \int \hat{O}[\{\overline{\psi}_{i\sigma}, \psi_{i\sigma}\}] e^{-S[\{\overline{\psi}_{i\sigma}, \psi_{i\sigma}, s_i\}]} [d\overline{\psi} d\psi]}{\left(\frac{1}{2}\right)^{NM} \sum_{\{s_i(L)\}=\pm 1} \int e^{-S[\{\overline{\psi}_{i\sigma}, \psi_{i\sigma}, s_i\}]} [d\overline{\psi} d\psi]}$$

Weight $\quad Z[\{s_i\}] = \int e^{-S[\{\overline{\psi}_{i\sigma}, \psi_{i\sigma}, s_i\}]} [d\overline{\psi} d\psi]$

$$\langle \hat{O}[\{\hat{c}^{\dagger}_{i\sigma}, \hat{c}_{i\sigma}\}]\rangle = \frac{\sum_{\{s_i\}} Z[\{s_i\}] \frac{\int \hat{O}[\{\overline{\psi}_{i\sigma}, \psi_{i\sigma}\}] e^{-S[\{\overline{\psi}_{i\sigma}, \psi_{i\sigma}, s_i\}]} [d\overline{\psi} d\psi]}{\int e^{-S[\{\overline{\psi}_{i\sigma}, \psi_{i\sigma}, s_i\}]} [d\overline{\psi} d\psi]}}{\sum_{\{s_i\}} Z[\{s_i\}]}$$

Hubbard model is mapped onto
an ensemble of free fermions feeling Ising one-body potentials

Update

Update configuration of Ising variables

$$\Delta_L = \frac{I - V_L[\{s_i'(L)\}]}{I - V_L[\{s_i(L)\}]} \qquad B_L = (I - K_L)(I - V_L[\{s_i(L)\}])$$

$$\frac{Z[\{s_i'\}]}{Z[\{s_i\}]} = \frac{\det\left[I + B_{L-1}\cdots B_1 B_M \cdots B_L \Delta_L\right]}{\det\left[I + B_{L-1}\cdots B_1 B_M \cdots B_L\right]}$$

$$\begin{aligned} & \frac{\det\left[I + B_{L-1}\cdots B_1 B_M \cdots B_L \Delta_L\right]}{\det\left[I + B_{L-1}\cdots B_1 B_M \cdots B_L\right]} \\ = \quad & \frac{\det\left[G_L\{I + G_L^{-1} B_{L-1}\cdots B_1 B_M \cdots B_L(\Delta_L - I)\}\right]}{\det\left[G_L\right]} \\ = \quad & \det\left[I + G_L^{-1} B_{L-1}\cdots B_1 B_M \cdots B_L(\Delta_L - I)\right] \end{aligned}$$

$$I + B_{L-1}\cdots B_1 B_M \cdots B_L = G_L$$

Update

$$
\begin{aligned}
&\frac{\det\left[I + B_{L-1}\cdots B_1 B_M \cdots B_L \Delta_L\right]}{\det\left[I + B_{L-1}\cdots B_1 B_M \cdots B_L\right]} \\
= \quad &\frac{\det\left[G_L\{I + G_L^{-1} B_{L-1}\cdots B_1 B_M \cdots B_L(\Delta_L - I)\}\right]}{\det\left[G_L\right]} \\
= \quad &\det\left[I + G_L^{-1} B_{L-1}\cdots B_1 B_M \cdots B_L(\Delta_L - I)\right]
\end{aligned}
$$

When the update is given by a local spin flip

$$\Delta_L - I = g_{i\uparrow} e(i\uparrow, i\uparrow) + g_{i\downarrow} e(i\downarrow, i\downarrow)$$

$$
\begin{aligned}
&\det\left[I + G_L^{-1} B_{L-1}\cdots B_1 B_M \cdots B_L(\Delta_L - I)\right] \\
= \quad &\prod_{\sigma=\uparrow,\downarrow} \left(G_L^{-1} B_{L-1}\cdots B_1 B_M \cdots B_L\right)_{i\sigma,i\sigma} g_{i\sigma}
\end{aligned}
$$

O(N^2) algorithm for the update of inverse G_L is known

$$\left(I + B_{L-1}\cdots B_1 B_M \cdots B_L\right)^{-1} \to \left(I + B_{L-1}\cdots B_1 B_M \cdots B_L \Delta_L\right)^{-1}$$

Update

Important formula for the update

$$\det\left[I + B_{L-1}\cdots B_1 B_M \cdots B_L\right] = \det\left[I + B_L B_{L-1}\cdots B_1 B_M \cdots B_{L+1}\right]$$

$$\begin{aligned}
&B_L\left(I + B_{L-1}\cdots B_1 B_M \cdots B_L\right)^{-1} B_L^{-1} \\
&= \left(I + B_L B_{L-1}\cdots B_1 B_M \cdots B_L B_L^{-1}\right)^{-1} \\
&= \left(I + B_L B_{L-1}\cdots B_1 B_M \cdots B_{L+1}\right)^{-1}
\end{aligned}$$

Cost for a MC step $\mathcal{O}(N^3 M)$

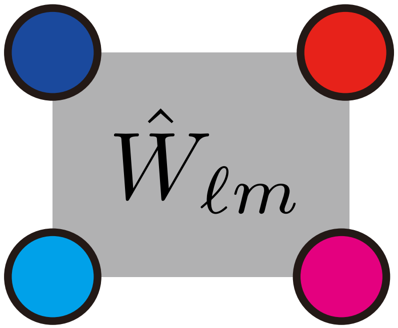
Feynman's Path Integral:

Transform calculations of non-commutative operators to ones with commutative numbers or *anticommutative Grassmann numbers*

Application of QMC

-Problems can be solved by QMC & the sign problem
-Dynamical mean-field theory
-Quantum chemistry

Negative Sign in Suzuki's Path Integral



$$(\hat{W}_{\ell m})_{\sigma_\ell \sigma_m ; \sigma_\ell \sigma_m} = \langle \sigma_\ell \sigma_m | e^{-\delta_\tau \hat{H}_{\ell m}} | \sigma_\ell \sigma_m \rangle$$

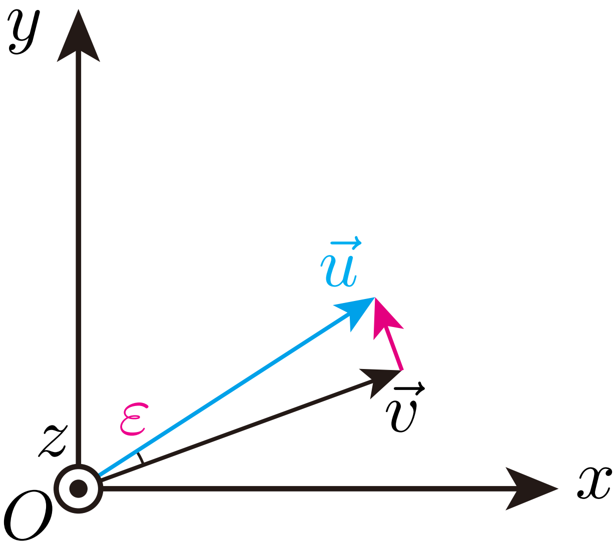
$$\hat{W}_{\ell m} = \begin{pmatrix} \langle \downarrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\downarrow \rangle & 0 & 0 & 0 \\ 0 & \langle \uparrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\downarrow \rangle & \langle \uparrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\uparrow \rangle & 0 \\ 0 & \langle \downarrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\downarrow \rangle & \langle \downarrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\uparrow \rangle & 0 \\ 0 & 0 & 0 & \langle \uparrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\uparrow \rangle \end{pmatrix}$$

$$= \begin{pmatrix} e^{-\delta_\tau J_z/4} & 0 & 0 & 0 \\ 0 & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & -e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & 0 \\ 0 & -e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & 0 \\ 0 & 0 & 0 & e^{-\delta_\tau J_z/4} \end{pmatrix}$$

Rotation of Vector

Infinitesimal rotation ε :

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 1 & -\varepsilon & 0 \\ +\varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$



$$\begin{pmatrix} 1 & -\varepsilon & 0 \\ +\varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - i\varepsilon \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\simeq e^{-i\varepsilon \ell_z}$$

$$\ell_z \equiv \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\ell_x \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\ell_y \equiv \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

Finite Angle Rotation

Finite rotation

$$\vec{u} = e^{-i\theta\vec{n}\cdot\vec{\ell}}\vec{v}$$

$$\lim_{N\to+\infty}\left(1 - i\frac{\theta}{N}\vec{n}\cdot\vec{\ell}\right)^N = e^{-i\theta\vec{n}\cdot\vec{\ell}}$$

Rotations are not commutable:

$$e^{-i\theta_1\ell_z} = \begin{pmatrix} +\cos\theta_1 & -\sin\theta_1 & 0 \\ +\sin\theta_1 & +\cos\theta_1 & 0 \\ 0 & 0 & +1 \end{pmatrix}$$

$$e^{-i\theta_2\ell_x} = \begin{pmatrix} +1 & 0 & 0 \\ 0 & +\cos\theta_2 & -\sin\theta_2 \\ 0 & +\sin\theta_2 & +\cos\theta_2 \end{pmatrix}$$

$$e^{-i\theta_1\ell_z}e^{-i\theta_2\ell_x} \neq e^{-i\theta_2\ell_x}e^{-i\theta_1\ell_z}$$

Infinitesimal Rotation: An Example of Lie Algebra

SU(2) $$[\ell_\alpha, \ell_\beta] = i\epsilon_{\alpha\beta\gamma}\ell_\gamma$$

$[\ell_\alpha, \ell_\beta] \equiv \ell_\alpha\ell_\beta - \ell_\beta\ell_\alpha \qquad \alpha, \beta, \gamma = x, y, z$

Antisymmetric tensor: $$\epsilon_{\alpha\beta\gamma} = \begin{cases} +1 & \text{for } (\alpha,\beta,\gamma) = (x,y,z), (y,z,x), (z,x,y) \\ -1 & \text{for } (\alpha,\beta,\gamma) = (x,z,y), (y,x,z), (z,y,x) \\ 0 & \text{others} \end{cases}$$

3 D representation:

$$\ell_z \equiv \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\ell_x \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\ell_y \equiv \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

2 D representation:

$$s_z = \frac{1}{2}\begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$s_x = \frac{1}{2}\begin{pmatrix} 0 & +1 \\ +1 & 0 \end{pmatrix}$$

$$s_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}$$

有限回転はSO(3)と呼ばれるリー群 $$e^{-i\theta\vec{n}\cdot\vec{\ell}}$$

2D Rep. to 3D Rep.

Wave function to spin components

$$\vec{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

$$\langle s_z \rangle \equiv \vec{u}^\dagger s_z \vec{u}$$

$$\langle s_x \rangle \equiv \vec{u}^\dagger s_x \vec{u}$$

$$\langle s_y \rangle \equiv \vec{u}^\dagger s_y \vec{u}$$

$$\vec{s} = \begin{pmatrix} \langle s_x \rangle \\ \langle s_y \rangle \\ \langle s_z \rangle \end{pmatrix}$$

Rep. & Basis of Rotation Group

“Wave function”

Double rep.

$$e^{-i\phi s_z} e^{-i\theta s_y} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \vec{u} = \begin{pmatrix} \cos\frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \sin\frac{\theta}{2} e^{+i\frac{\phi}{2}} \end{pmatrix}$$

Spin

$$e^{-i\phi \ell_z} e^{-i\theta \ell_y} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \vec{s} = \frac{1}{2} \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}$$

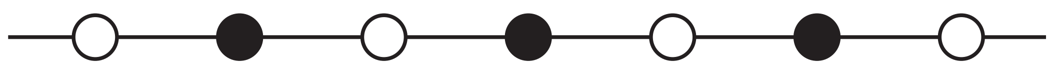
Rotation of Local Spin Coordinate

M. Suzuki, S. Miyashita, & A. Kuroda, PTP 58, 1377 (1977).
As a review, H. G. Evertz, Adv. Phys. 52, 1 (2003).

An example: 1D XXZ model

$$\hat{H} = J_x \sum_i (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y) + J_z \sum_i \hat{S}_i^z \hat{S}_{i+1}^z$$

$\hat{H}$



$$\widetilde{S}_{2\ell}^x = e^{-i\pi \hat{S}_{2\ell}^z} \hat{S}_{2\ell}^x e^{+i\pi \hat{S}_{2\ell}^z} = -\hat{S}_{2\ell}^x$$
$$\widetilde{S}_{2\ell}^y = e^{-i\pi \hat{S}_{2\ell}^z} \hat{S}_{2\ell}^y e^{+i\pi \hat{S}_{2\ell}^z} = -\hat{S}_{2\ell}^y$$

$$\widetilde{S}_{2\ell+1}^x = \hat{S}_{2\ell+1}^x$$
$$\widetilde{S}_{2\ell+1}^y = \hat{S}_{2\ell+1}^y$$

$$\widetilde{H} = -J_x \sum_i (\widetilde{S}_i^x \widetilde{S}_{i+1}^x + \widetilde{S}_i^y \widetilde{S}_{i+1}^y) + J_z \sum_i \hat{S}_i^z \hat{S}_{i+1}^z$$

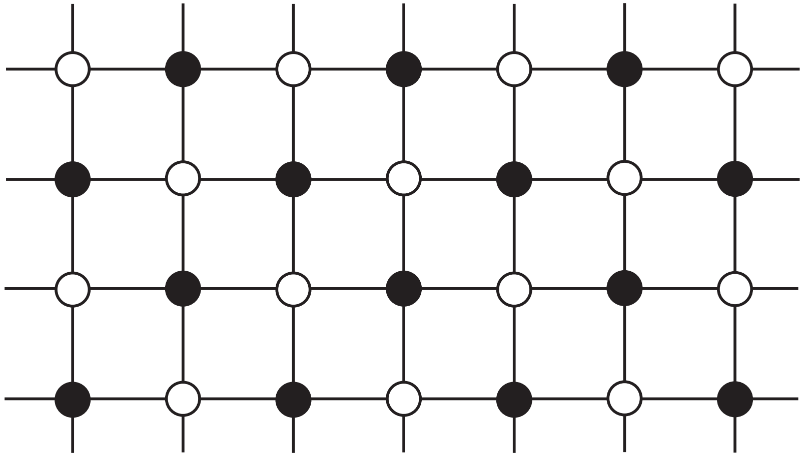
Removal of Negative Weight

$$\widetilde{H} = -J_x \sum_i (\widetilde{S}_i^x \widetilde{S}_{i+1}^x + \widetilde{S}_i^y \widetilde{S}_{i+1}^y) + J_z \sum_i \hat{S}_i^z \hat{S}_{i+1}^z$$

$$\widetilde{W}_{\ell m} = \begin{pmatrix} \langle \downarrow\downarrow | e^{-\delta_\tau \widetilde{H}_{\ell m}} | \downarrow\downarrow \rangle & 0 & 0 & 0 \\ 0 & \langle \uparrow\downarrow | e^{-\delta_\tau \widetilde{H}_{\ell m}} | \uparrow\downarrow \rangle & \langle \uparrow\downarrow | e^{-\delta_\tau \widetilde{H}_{\ell m}} | \downarrow\uparrow \rangle & 0 \\ 0 & \langle \downarrow\uparrow | e^{-\delta_\tau \widetilde{H}_{\ell m}} | \uparrow\downarrow \rangle & \langle \downarrow\uparrow | e^{-\delta_\tau \widetilde{H}_{\ell m}} | \downarrow\uparrow \rangle & 0 \\ 0 & 0 & 0 & \langle \uparrow\uparrow | e^{-\delta_\tau \widetilde{H}_{\ell m}} | \uparrow\uparrow \rangle \end{pmatrix}$$

$$= \begin{pmatrix} e^{-\delta_\tau J_z/4} & 0 & 0 & 0 \\ 0 & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & +e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & 0 \\ 0 & +e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & 0 \\ 0 & 0 & 0 & e^{-\delta_\tau J_z/4} \end{pmatrix}$$

Applicable to bipartite lattice



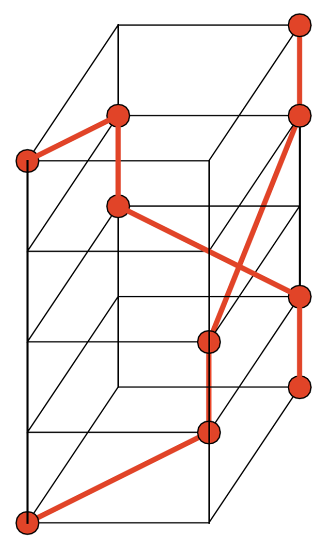
Negative Sign in Fermions

M. Troyer and U.-J. Wiese, Phys. Rev. Lett. 94, 170201 (2005).

Another formulation of path integral

$$Z = \mathrm{tr}[e^{-\beta\hat{H}}] = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \mathrm{tr}[\hat{H}^n]$$

$$= \sum_{n=0}^{\infty} \sum_{\nu_1,\nu_2,\ldots,\nu_n} \frac{(-\beta)^n}{n!} \langle\nu_1|\hat{H}|\nu_2\rangle\langle\nu_2|\hat{H}|\nu_3\rangle\cdots\langle\nu_n|\hat{H}|\nu_1\rangle$$



Negative Sign in Fermions

M. Troyer and U.-J. Wiese, Phys. Rev. Lett. 94, 170201 (2005).

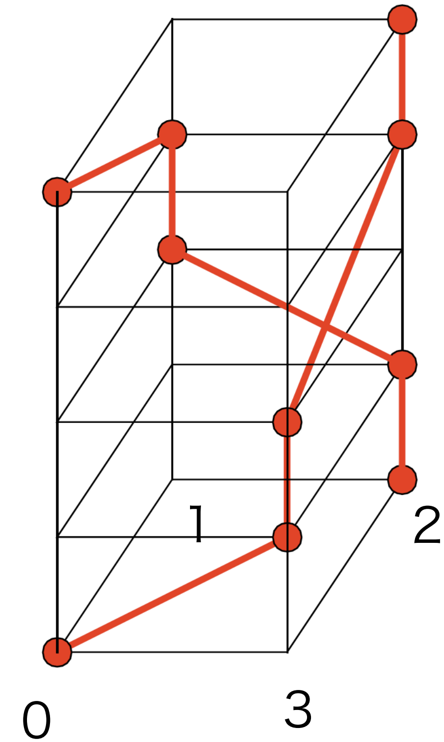
$$|\nu_1\rangle = \hat{c}_2^\dagger \hat{c}_0^\dagger |0\rangle$$

$$|\nu_4\rangle = \hat{c}_2^\dagger \hat{c}_1^\dagger |0\rangle$$

$$|\nu_3\rangle = \hat{c}_3^\dagger \hat{c}_1^\dagger |0\rangle$$

$$|\nu_2\rangle = \hat{c}_3^\dagger \hat{c}_2^\dagger |0\rangle$$

$$|\nu_1\rangle = \hat{c}_2^\dagger \hat{c}_0^\dagger |0\rangle$$



$$\hat{H} = \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i)$$ nearest-neighbor hopping

$$\langle \nu_1 | \hat{H} | \nu_2 \rangle \langle \nu_2 | \hat{H} | \nu_3 \rangle \langle \nu_3 | \hat{H} | \nu_4 \rangle \langle \nu_4 | \hat{H} | \nu_1 \rangle = -1$$

Definition of Averaged Sign

$$Z = \mathrm{tr}[e^{-\beta \hat{H}}] = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \mathrm{tr}[\hat{H}^n]$$

$$= \sum_{n=0}^{\infty} \sum_{\nu_1,\nu_2,\ldots,\nu_n} \frac{(-\beta)^n}{n!} \langle \nu_1 | \hat{H} | \nu_2 \rangle \langle \nu_2 | \hat{H} | \nu_3 \rangle \cdots \langle \nu_n | \hat{H} | \nu_1 \rangle$$

$$= \sum_{n=0}^{\infty} \sum_{\nu_1,\nu_2,\ldots,\nu_n} p(\nu_1, \nu_2, \ldots, \nu_n) = \sum_c p(c)$$

M. Troyer and U.-J. Wiese, Phys. Rev. Lett. 94, 170201 (2005).

$$\langle \mathrm{sign} \rangle = \frac{\sum_c p(c)}{\sum_c |p(c)|} = \frac{Z_\mathrm{f}}{Z_\mathrm{b}} = e^{-V\beta(f_\mathrm{f} - f_\mathrm{b})}$$

-Basis dependent

For example, H. Shinaoka *et al.*, Phys. Rev. B 92, 195126 (2015).

Symmetry Removes Negative Sign

BSS QMC for Hubabrd model

$$\hat{H} = \sum_{\langle i,j \rangle, \sigma} (\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}) + U \sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}$$

Weight for each Ising configuration: $Z = Z_\uparrow Z_\downarrow$

$$Z_\sigma = \det\left[I + B^\sigma_M B^\sigma_{M-1} \cdots B^\sigma_1\right]$$

Atractive Hubbard model $U < 0$

-Ising valuables are spin independent $Z_\uparrow = Z_\downarrow$

Repulsive Hubbard model $U > 0$

-Particle-hole symmetry $Z_\uparrow = cZ_\downarrow \; (c > 0)$

J. E. Hirsch, Phys. Rev. B 28, 4059 (1983).

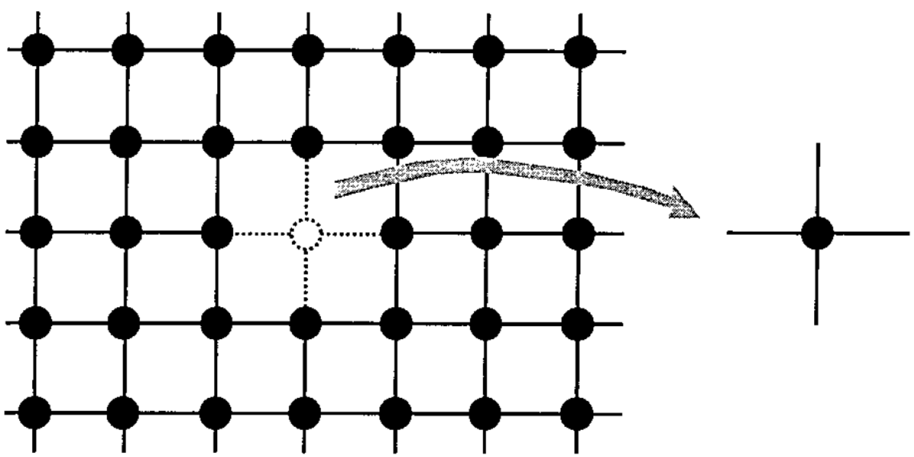
cf.) symmetry of Kane-Mele-Hubbard model

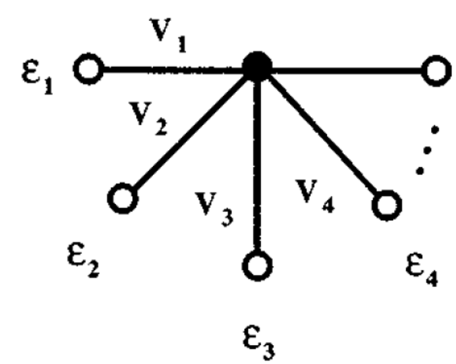
Dynamical Mean Field and Impurity Model

As a review, A. Georges, G. Kotliar, W. Krauth, and Marcelo J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).

Mapping from lattice model to impurity model

$$\hat{H} = \sum_{\langle i,j \rangle,\sigma} (\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}) + U\sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}$$





$$\hat{H} = \sum_{j,\sigma} \epsilon_j \hat{c}^\dagger_{j\sigma}\hat{c}_{j\sigma} + \sum_{j,\sigma} v_j(\hat{c}^\dagger_{j\sigma}\hat{d}_\sigma + \hat{d}^\dagger_\sigma \hat{c}_{j\sigma}) + U\hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow$$

Dynamical Mean Field and Impurity Model

As a review, A. Georges, G. Kotliar, W. Krauth, and Marcelo J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).

Self-consistent impurity model

$$\hat{H} = \sum_{j,\sigma} \epsilon_j \hat{c}^\dagger_{j\sigma} \hat{c}_{j\sigma} + \sum_{j,\sigma} v_j (\hat{c}^\dagger_{j\sigma} \hat{d}_\sigma + \hat{d}^\dagger_\sigma \hat{c}_{j\sigma}) + U \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow$$

-Green's function of impurity model

$$G^{\mathrm{imp}}(\omega) = \frac{1}{\omega + i\delta + \mu - \Sigma^{\mathrm{imp}}(\omega) - \Delta(\omega)}$$

-Dynamical mean-field

$$\Delta(\omega) = \omega + i\delta + \mu - \Sigma^{\mathrm{imp}}(\omega) - \left[\frac{1}{N} \sum_{\vec{k}} \frac{1}{\omega + i\delta + \mu - \epsilon(\vec{k}) - \Sigma^{\mathrm{imp}}(\omega)} \right]^{-1}$$

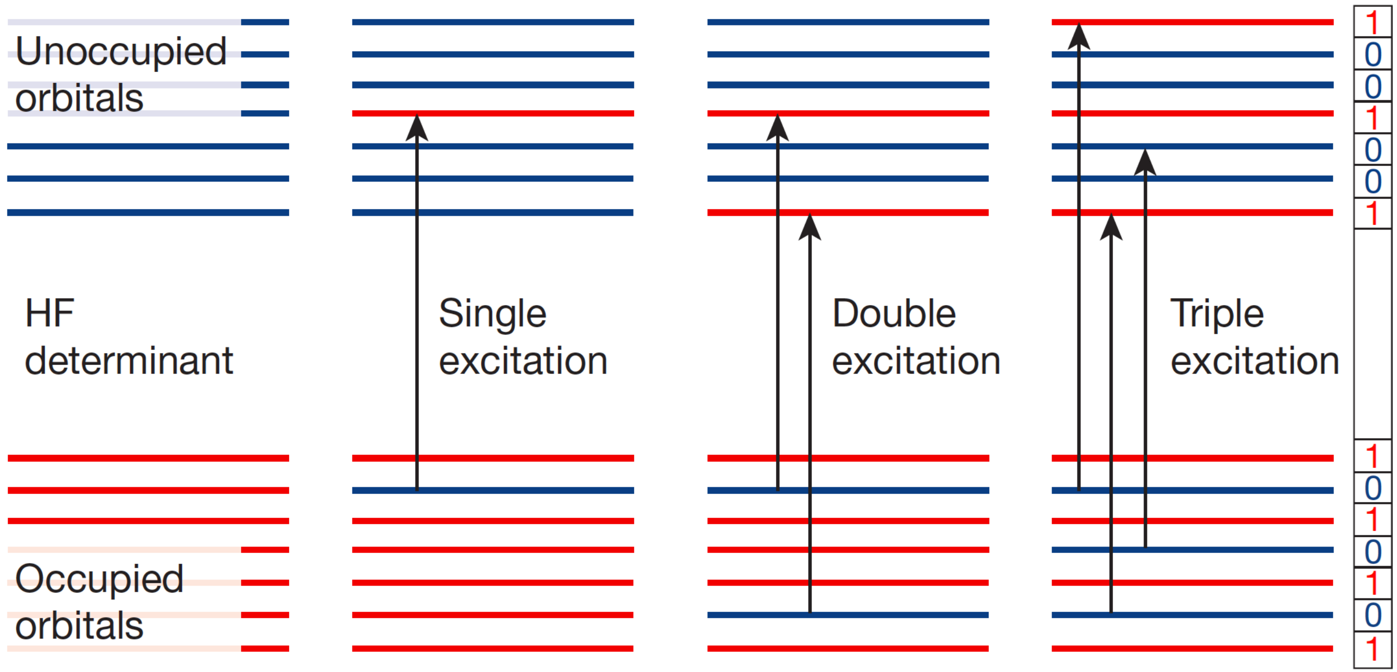
$$= \sum_j \frac{|v_j|^2}{\omega + i\delta - \epsilon_j}$$

You can find applications of DMFT in G. Kotliar, *et al.*, Rev. Mod. Phys. 78, 865 (2006).

Configuration Interaction Monte Carlo

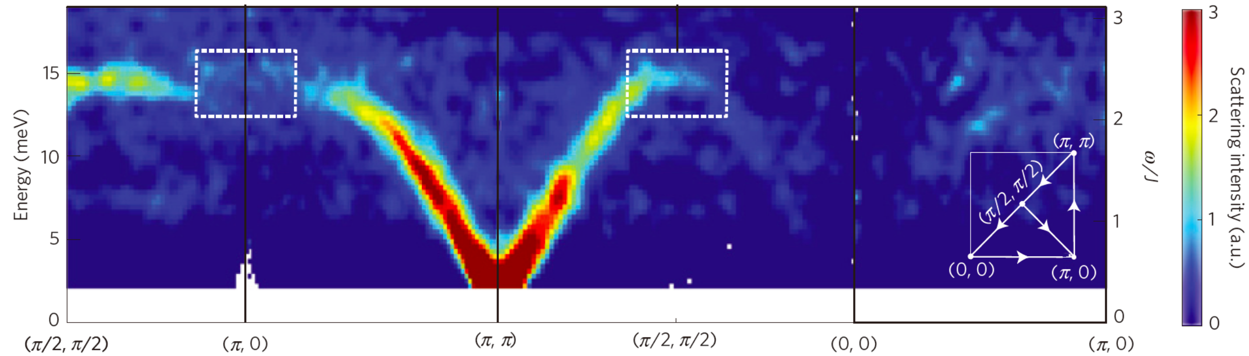
G. H. Booth, A. Grüneis, G. Kresse, A. Alavi, Nature 493, 365 (2013).

Sampling basis set



Example of Applications: Spin Excitations in Square Lattice Heisenberg model

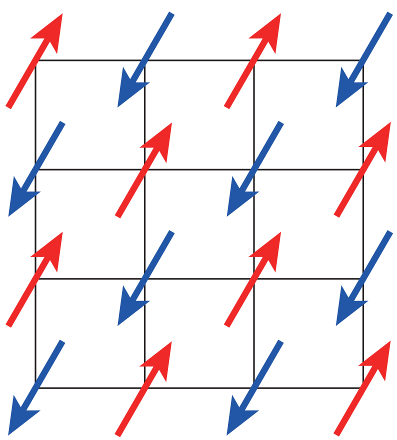
$Cu(DCOO)_2 \cdot 4D_2O$

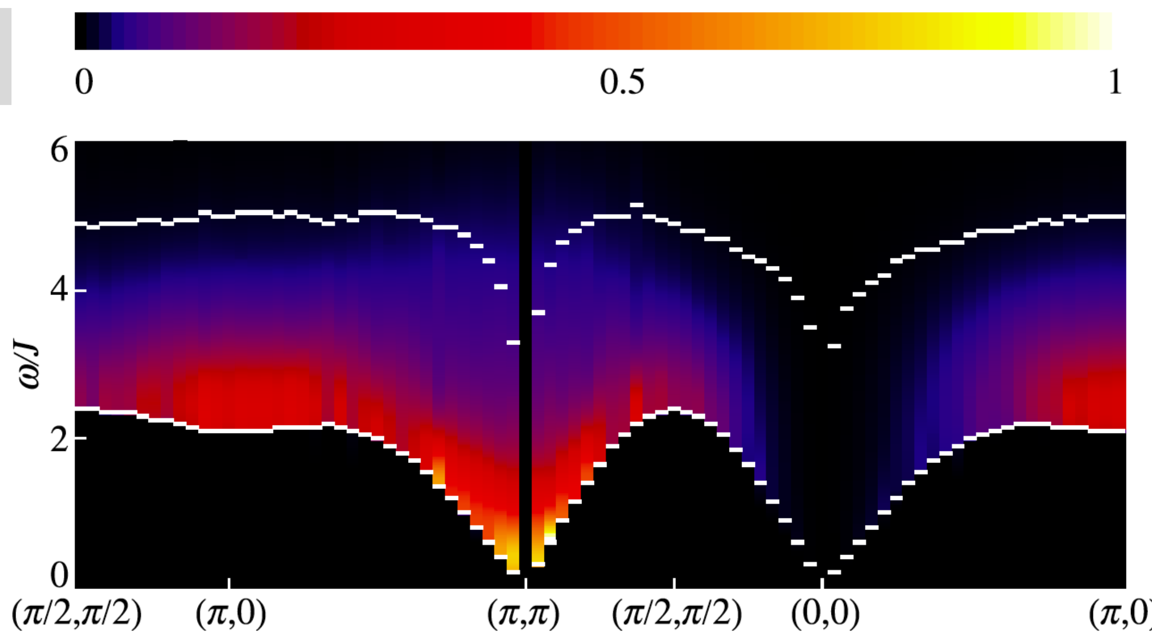


B. Dalla Piazza, *et al.*, Nat. Phys. 11, 62 (2015)

S=1/2 Heisenberg

Ground state





H. Shao, *et al.*, Phys, Rev, X 7, 041072 (2017)

References

-Dynamical mean-field theory

A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg,
Rev. Mod. Phys. 68, 13 (1996).
T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler,
Rev. Mod. Phys. 77, 1027 (2005).
G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. Marianetti,
Rev. Mod. Phys. 78, 865 (2006).

Next Week

Linear algebra in many-body physics

-Eigenvalue problem for fermions
-Eigenvalue problem for bosons

Lecture Schedule

Classical

Quantum

#1 Many-body problems in physics
#2 Why many-body problem is hard to solve
#3 Classical statistical model and numerical simulation
#4 Classical Monte Carlo method and its applications
#5 Molecular dynamics and its application
#6 Extended ensemble method for Monte Carlo methods
#7 Quantum lattice models and numerical approaches
#8 Quantum Monte Carlo methods
#9 Applications of quantum Monte Carlo methods
  -Path integral & applications
#10 Linear algebra of large and sparse matrices for
  quantum many-body problems
#11 Krylov subspace methods and their applications to
  quantum many-body problems
#12 Large sparse matrices and quantum statistical mechanics
#13 Parallelization for many-body problems