多体問題の計算科学
#9
2017/6/12

Computational Science for Many-Body Problems

Quantum Monte Carlo Methods
1. Grassmann number
2. Path integral for free fermions
3. Hubbard-Stratonovich transformation
4. Path integral QMC for Hubbard model

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)

Preparation for Path Integral QMC

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

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

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

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

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

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

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: $\int \psi d\psi = 1 \quad \int d\psi\psi = -1$

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

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

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

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

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

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

Path Integral for Fermions

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

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

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

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

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

*Valid for any one-body Hamiltonian

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

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

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

$A:\ 2NM \times 2NM$ matrix

$\mu,\nu:$ site index i, spin index σ, 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

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

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

$4NM$ dimensional integral $\rightarrow$ $4N$ 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

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

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

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

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

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

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

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

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).

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

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

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

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

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

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

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

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

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

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

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

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

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

Update

Update configuration of Ising variables

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

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

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

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

Update

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

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

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

When the update is given by a local spin flip

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

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

$$= \prod_{\sigma=\uparrow,\downarrow} \left(G_L^{-1} B_{L-1}\cdots B_1 B_M \cdots B_L\right)_{i\sigma, i\sigma} g_{i\sigma}$$

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

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

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

$\mathcal{O}(N^3 M)$

Next Week

Linear algebra in many-body physics

-Eigenvalue problem for fermions
-Eigenvalue problem for bosons

2nd report about QMC