Tutorial: Solving Spin-Fermion Model with DQMC

Gaopei Pan

Insitute of Physics, CAS
University of Chinese Academy of Sciences

pangaopei14@mails.ucas.ac.cn

October 11, 2019

Overview

1. Monte Carlo simulation method and process
   - Markov Chain Monte Carlo(MCMC)
   - Metropolis–Hastings Algorithm
   - An simple example: Ising model
2. DQMC(Determinant Quantum Monte Carlo)
   - Model
   - Partition Function
   - Sign Problem
   - Update
   - Numerical Stabilization
   - Operator and Measurment
3. Some Results of Hubbard Model
   - Kinetic Energy
   - Double Occupancy
   - $S(\pi, \pi)$

Markov Chain

What is Markov Chain?

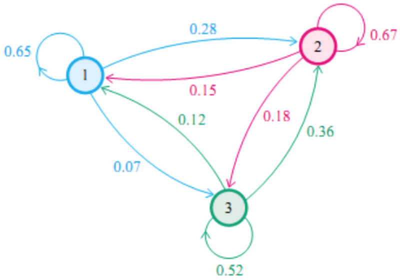
We say that $\{X_0, X_1, \ldots\}$ is a discrete time Markov chain with transition matrix $p(i,j)$ if for any $j, i, i_{n-1}, \ldots, i_1, i_0$,

$$P\left(X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \ldots, X_0 = i_0\right) = p(i,j)$$

Note that the transition probability $p(i,j)$ can also be written as

$$p(i,j) = P\left(X_{n+1} = j | X_n = i\right)$$

Markov Chain



$$p = \begin{bmatrix} 0.65 & 0.28 & 0.17 \\ 0.15 & 0.67 & 0.18 \\ 0.12 & 0.36 & 0.52 \end{bmatrix} \quad (1)$$

Stationary Distribution

Let $p(x,y)$ be the transition matrix of a Markov chain. If $\pi(x)$ is a probability function on the state space of the Markov chain, such that

$$\sum_x \pi(x)p(x,y) = \pi(y), \quad \text{or in the matrix form} \quad \pi p = \pi$$

we say that $\pi(x)$ is a stationary distribution.

Theorem

If the Markov chain is irreducible and aperiodic, then there is a unique stationary distribution . Additionally, in this case p^k converges to a rank-one matrix in which each row is the stationary distribution π:

$$\lim_{k\to\infty} \mathbf{p}^k(i,:) = \pi \tag{2}$$

After a transpose operation, π^T is just like eigenvector.

Markov Chain Monte Carlo(MCMC)

There is a given probability distribution $P(X)$. We hope we can get a markov chain whose stationary distribution is the given $P(X)$, which means after enough sweep steps, obtained sample satisfies $P(X)$.

For example, P is $W(C) = \frac{e^{-\beta H(C)}}{Z}$, where $Z = \sum_{\text{all C1qonfigurations}} e^{-\beta H(C)}$

Detailed Balance Condition

How can we get the probability distribution we want?

Only need to satisfy the **detailed balance condition**

$$\pi(i)p(i,j) = \pi(j)p(j,i) \tag{3}$$

Verify as follows:

$$\sum_i \pi(i)p(i,j) = \sum_i \pi(j)p(j,i) = \pi(j)\sum_i p(j,i) = \pi(j) \tag{4}$$

Metropolis–Hastings Algorithm

1. Pick an initial x_0, set $t = 0$
2. Iterate

a. **Generate**: randomly generate a candidate state x' according to $g(x'|x_t)$;

b. **Calculate**: calculate the acceptance probability $R(x', x_t) = \min\left(1, \frac{P(x')}{P(x_t)} \frac{g(x_t|x')}{g(x'|x_t)}\right)$;

c. **Accept or Reject**: generate a uniform random number $u \in [0, 1]$. IF $u \leq R(x', x_t)$, accept and set $x_{t+1} = x'$. ELSE reject and $x_{t+1} = x_t$

d. set $t = t + 1$

Where $g(x'|x)$ is proposal distribution and $R(x', x)$ is acceptance ratio. (From wiki)

An simple example: Ising model

$$H = -J \sum_{<i,j>} s_i s_j \tag{5}$$

1. Pick an initial Configuration $\{s_i\}$, set $t = 0$
2. Iterate

   a. **Generate**: try to randomly flip a spin: $s_i = -s_i$;

   b. **Calculate**: calculate the acceptance probability

$R = \min\left(1, e^{-\beta \Delta H}\right)$;

   c. **Accept or Reject**: generate a uniform random number $u \in [0, 1]$.

IF $u \leq R\left(x', x_t\right)$, accept. Flip the spin successfully.

ELSE reject, don't flip the spin.

   d. set $t = t + 1$

DQMC(Determinant Quantum Monte Carlo)

What does 'determinant' mean here?

$$\mathrm{Tr}\,[e^{-\sum_{i,j} c_i^\dagger A_{i,j} c_j} e^{-\sum_{i,j} c_i^\dagger B_{i,j} c_j}] = \mathrm{Det}(1 + e^{-\mathbf{A}} e^{-\mathbf{B}}) \tag{6}$$

$$H = H_f + H_s + H_{f-s} \tag{7}$$

where

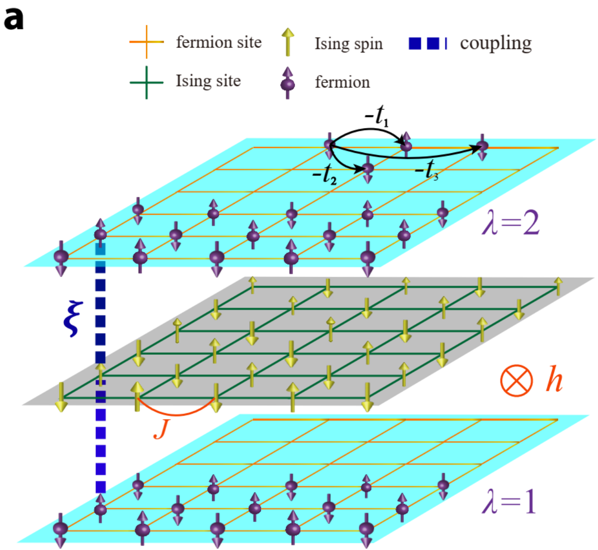
$$\begin{aligned} H_f =& -t_1 \sum_{\langle ij \rangle, \lambda, \sigma} c^\dagger_{i,\lambda,\sigma} c_{j,\lambda,\sigma} - t_2 \sum_{\langle\langle ij \rangle\rangle, \lambda, \sigma} c^\dagger_{i,\lambda,\sigma} c_{j,\lambda,\sigma} \\ & - t_3 \sum_{\langle\langle\langle ij \rangle\rangle\rangle, \lambda, \sigma} c^\dagger_{i,\lambda,\sigma} c_{j,\lambda,\sigma} + h.c. - \mu \sum_{i,\lambda,\sigma} n_{i,\lambda,\sigma} \end{aligned} \tag{8}$$

$$H_s = -J \sum_{\langle ij \rangle} s^z_i s^z_j - h \sum_i s^x_i \tag{9}$$

$$H_{f-s} = -\xi \sum_i s^z_i \left(\sigma^z_{i,1} - \sigma^z_{i,2} \right), \tag{10}$$

and $\sigma^z_{i,\lambda} = \frac{1}{2}(c^\dagger_{i,\lambda,\uparrow} c_{i,\lambda,\uparrow} - c^\dagger_{i,\lambda,\downarrow} c_{i,\lambda,\downarrow})$ is the fermion spin along z.

Model: A Spin-Fermion coupled Model



Model: Hubbard Model

The half-filling Hubbard model on square lattice can be written as

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + h.c. + U \sum_{i} \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right)$$

To perform the DQMC simulation of this model, we start with representing the partition function as a sum over a configuration space. The partition function writes

$$\begin{aligned} Z &= \mathrm{Tr}\left[e^{-\beta \hat{H}} \right] \\ &= \mathrm{Tr}\left[\left(e^{-\Delta\tau \hat{H}} \right)^{M} \right] \end{aligned}$$

Model: Hubbard Model

To take care of the interaction part, we need do the HS transformation

$$
\begin{aligned}
e^{-\Delta\tau \hat{H}_I} &= \prod_i e^{-\Delta\tau U\left(\hat{n}_{i\uparrow}-\frac{1}{2}\right)\left(\hat{n}_{i\downarrow}-\frac{1}{2}\right)} \\
&= \prod_i \lambda \sum_{s_{i,\tau}=\pm 1} e^{\alpha s_{i,\tau}\left(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow}\right)} \\
&= \lambda^N \sum_{s_{i,\tau}=\pm 1} \left(\prod_i e^{\alpha s_{i,\tau}\hat{n}_{i\uparrow}} \prod_i e^{-\alpha s_{i,\tau}\hat{n}_{i\downarrow}} \right)
\end{aligned}
$$

We should first trace out the bare transverse field Ising model. We know that

$$e^{\Delta\tau h\hat{s}_i^x} = \cosh(\Delta\tau h)\mathbf{1} + \sinh(\Delta\tau h)\hat{s}_i^x \tag{11}$$

And we require:

$$\left\langle S_z' \left| e^{\Delta\tau h\hat{s}_i^x} \right| S_z \right\rangle = \Lambda e^{\gamma s_z' s_z} \tag{12}$$

Just take $S_z = \pm 1$, we can get

$$\begin{aligned}\left\langle S_z \left| e^{\Delta\tau h\hat{s}_i^x} \right| S_z \right\rangle &= \cosh(\Delta\tau h) = \Lambda e^{\gamma} \\ \left\langle -S_z \left| e^{\Delta\tau h\hat{s}_i^x} \right| S_z \right\rangle &= \sinh(\Delta\tau h) = \Lambda e^{-\gamma}\end{aligned} \tag{13}$$

Spin part:

$$Z_{spin} = \text{Tr}\left\{ e^{-\beta H_{\text{spin}}} \right\} = \left(\prod_{\tau} \prod_{\langle ij \rangle} e^{\Delta\tau J \, s^z_{i,\tau} s^z_{j,\tau}} \right) \left(\prod_{i} \prod_{\langle \tau,\tau' \rangle} \Lambda e^{\gamma \, s^z_{i,\gamma} s^z_{j,\tau'}} \right) + O\left(\Delta\tau^2\right) \tag{14}$$

where

$$\begin{aligned} \gamma &= -\frac{1}{2} \ln(\tanh(\Delta\tau h)) \\ \Lambda^2 &= \sinh(\Delta\tau h) \cosh(\Delta\tau h) \end{aligned} \tag{15}$$

Trotter Decomposition

$$
\begin{aligned}
Z = \operatorname{Tr}\left\{e^{-\beta H}\right\} &= \operatorname{Tr}\left\{\left(e^{-\Delta\tau H_I} e^{-\Delta\tau H_0}\right)^M\right\} + O\left(\Delta\tau^2\right) \\
&= \sum_{\mathcal{C}} \mathcal{W}_{\mathcal{C}}^{\mathcal{S}} \operatorname{Tr}\left\{\prod_{\tau=M}^{1} e^{\hat{c}^\dagger V(\mathcal{C})\hat{c}} e^{-\Delta\tau \hat{c}^\dagger T \hat{c}}\right\} + O\left(\Delta\tau^2\right)
\end{aligned} \tag{16}
$$

Define

$$
\begin{aligned}
\hat{U}\left(\tau_2, \tau_1\right) &= \prod_{n=n_1+1}^{n_2} e^{\hat{c}^\dagger V(\mathcal{C})\hat{c}} e^{-\Delta\tau \hat{c}^\dagger T \hat{c}} \\
B\left(\tau_2, \tau_1\right) &= \prod_{n=n_1+1}^{n_2} e^{V(\mathcal{C})} e^{-\Delta\tau T}
\end{aligned} \tag{17}
$$

Then

$$
Z = \sum_{\mathcal{C}} \mathcal{W}_{\mathcal{C}}^{\mathcal{S}} \operatorname{Tr}\{\hat{U}(\beta, 0)\} = \sum_{\mathcal{C}} \mathcal{W}_{\mathcal{C}}^{\mathcal{S}} \det[\mathbf{1} + B(\beta, 0)] \tag{18}
$$

Sign Problem

Sometimes the weight $W(C)$ is not a real positive number. We say that we meet sign-problem.

Theorem (CJ Wu, SC Zhang, Phys. Rev. B 71, 155115 (2005))

If there exists an antiunitary operator T, such that

$$TH_K T^{-1} = H_K, \quad TH_I T^{-1} = H_I, \quad T^2 = -1$$

then the eigenvalues of the $I + B$ matrix always appear in complex conjugate pairs, i.e., if λ_i is an eigenvalue, then λ_i^* is also an eigenvalue. If λ_i is real, it is twofold degenerate. In this case, the fermion determinant is positive definite,

$$\det(I + B) = \prod_i |\lambda_i|^2 \geqslant 0$$

where H_K is imaginary time-independent kinetic energy term and H_I is imaginary time-dependent decoupled interaction term.

Sign Problem

$$\hat{H}_0 = -J\sum_{\langle ij\rangle}\hat{s}_i^z\hat{s}_j^z - t\sum_{\langle ij\rangle\lambda\sigma}\hat{c}^\dagger_{i\lambda\sigma}\hat{c}_{j\lambda\sigma} + h.c. - \mu\sum_{i\lambda\sigma}\hat{n}_{i\lambda\sigma} - \xi\sum_i s_i^z\left(\hat{\sigma}^z_{i1} - \hat{\sigma}^z_{i2}\right)$$

Note that $\hat{H}_0$ is time reversal (combine with τ_x on orbital space) invariant, then we can simulate any filling case without sign problem

$$\begin{aligned}\hat{H}_0 &\xrightarrow{\mathcal{T}} \\ &- J\sum_{\langle ij\rangle}\hat{s}_i^z\hat{s}_j^z - t\sum_{\langle ij\rangle\lambda\sigma}\hat{c}^\dagger_{i\lambda\bar{\sigma}}\hat{c}_{j\lambda\bar{\sigma}} + \text{h.c.} - \mu\sum_{i\lambda\bar{\sigma}}\hat{n}_{i\lambda\bar{\sigma}} - \xi\sum_i s_i^z\left(-\hat{\sigma}^z_{i1} + \hat{\sigma}^z_{i2}\right) \\ &\xrightarrow{\tau_x \text{ on orbital space}} \\ &- J\sum_{\langle ij\rangle}\hat{s}_i^z\hat{s}_j^z - t\sum_{\langle ij\rangle\lambda\sigma}\hat{c}^\dagger_{i\lambda\bar{\sigma}}\hat{c}_{j\lambda\bar{\sigma}} + h.c. - \mu\sum_{i\lambda\bar{\sigma}}\hat{n}_{i\lambda\bar{\sigma}} - \xi\sum_i s_i^z\left(-\hat{\sigma}^z_{i2} + \hat{\sigma}^z_{i1}\right) \\ &= \hat{H}_0\end{aligned}$$

Sign Problem

Another point of view: The Hamiltonian is block diagonal as four orbitals, which is

$$(\tau_z, \sigma_z) = [\uparrow 1, \downarrow 1, \uparrow 2, \downarrow 2]$$

We can see $H_{\uparrow 1} = H_{\downarrow 2}, H_{\uparrow 2} = H_{\downarrow 1}$. Regroup four orbitals into two superposition

$$(\alpha_1, \alpha_2) = [(\uparrow 1, \downarrow 2), (\uparrow 2, \downarrow 1)] \ .$$

In the two regroup orbitals, $H_{\alpha_1} = H_{\alpha_2}$, so

$$\det(1 + B(\beta, 0)) = \prod_{i=1}^{2} \det\left(1 + B_{\alpha_i}(\beta, 0)\right) = \left|\det\left(\mathbf{1} + B_{\alpha_1}(\beta, 0)\right)\right|^2$$

So our designer model is free of sign problem.

Accept Ratio

We have known that

$$\begin{aligned}\omega_{\mathcal{C}} =& \phi(\mathcal{C}) \det(\mathbf{1} + \mathbf{B}(\beta,\tau)\mathbf{B}(\tau,0)) \\ =& \phi(\mathcal{C}) \det(\mathbf{G}(0,0))^{-1}\end{aligned}$$

After fliping a spin, the accept ratio(ratio of weight) is

$$\mathcal{R} = \frac{\mathcal{W}^{\mathcal{S}}_{\mathcal{C}'} \det\left(\mathbf{1} + B_{C'}(\beta,0)\right)}{\mathcal{W}^{\mathcal{S}}_{\mathcal{C}} \det\left(\mathbf{1} + B_{\mathcal{C}}(\beta,0)\right)} = \frac{\mathcal{W}^{\mathcal{S}}_{\mathcal{C}'}}{\mathcal{W}^{\mathcal{S}}_{\mathcal{C}}}\mathcal{R}_f \tag{19}$$

And

$$\begin{aligned}\mathcal{R}_f =& \frac{\det\left(\mathbf{1} + B'_C(\beta,0)\right)}{\det\left(1 + B_C(\beta,0)\right)} \\ =& \frac{\det\left(\mathbf{1} + B_C(\beta,\tau)(1+\Delta)B_C(\tau,0)\right)}{\det\left(1 + B_C(\beta,0)\right)} \\ =& \det\left[\mathbf{1} + \Delta\left(\mathbf{1} - \left(\mathbf{1} + B_C(\tau,0)B_{\mathcal{C}}(\beta,\tau)\right)^{-1}\right)\right] \\ =& \det\left[\mathbf{1} + \Delta\left(\mathbf{1} - G_{\mathcal{C}}(\tau,\tau)\right)\right]\end{aligned} \tag{20}$$

Update Green Function

$$
\begin{aligned}
G_{\mathcal{C}'}(\tau,\tau) &= [\mathbf{1} + (\mathbf{1}+\mathbf{\Delta})B_{\mathcal{C}}(\tau,0)B_{\mathcal{C}}(\beta,\tau)]^{-1} \\
&= [\mathbf{1} + B_{\mathcal{C}}(\tau,0)B_{\mathcal{C}}(\beta,\tau)]^{-1} \times \\
&\quad \left[(\mathbf{1} + (\mathbf{1}+\Delta)B_{\mathcal{C}}(\tau,0)B_{\mathcal{C}}(\beta,\tau))\left((\mathbf{1} + B_{\mathcal{C}}(\tau,0)B_{\mathcal{C}}(\beta,\tau))^{-1}\right)\right]^{-1}
\end{aligned} \tag{21}
$$

as $G_{\mathcal{C}}(\tau,\tau) = [\mathbf{1} + B_{\mathcal{C}}(\tau,0)B_{\mathcal{C}}(\beta,\tau)]^{-1}$, we denote

$$
A_{\mathcal{C}} \equiv B_{\mathcal{C}}(\tau,0)B_{\mathcal{C}}(\beta,\tau) \equiv G_{\mathcal{C}}^{-1} - \mathbf{1}
$$

$$
\begin{aligned}
G_{\mathcal{C}'}(\tau,\tau) &= G_{\mathcal{C}}\left[(\mathbf{1} + (\mathbf{1}+\Delta)A_{\mathcal{C}})\, G_{\mathcal{C}}\right]^{-1} \\
&= G_{\mathcal{C}}\left[\left(\mathbf{1} + (\mathbf{1}+\Delta)\left(G_{\mathcal{C}}^{-1} - \mathbf{1}\right)\right) G_{\mathcal{C}}\right]^{-1} \\
&= G_{\mathcal{C}}\left[\mathbf{1} + \Delta\left(\mathbf{1} - G_{\mathcal{C}}\right)\right]^{-1}
\end{aligned} \tag{22}
$$

Update Green Function

Using the Sherman-Morrison formula

$$(\mathbf{I}+\mathbf{UV})^{-1}=\mathbf{I}-\mathbf{U}\left(\mathbf{I}_k+\mathbf{VU}\right)^{-1}\mathbf{V} \tag{23}$$

we have that

$$\begin{aligned}\mathcal{R}_f &= 1+\Delta_{ii}\left(1-G^{c}_{ii}\right)\\ G_{c'}(\tau,\tau) &= G_c(\tau,\tau)+\alpha_i G_{\mathcal{C}}(:,i)\left(G_{\mathcal{C}}(i,:)-\mathbf{e}_i\right)\end{aligned} \tag{24}$$

where

$$\alpha_i=\Delta_{ii}/\mathcal{R}_f \tag{25}$$

$$O(N^3)\rightarrow O(N^2)$$

Condition Numbers

Condition number of a matrix A is

$$\kappa(A) = \left\|A^{-1}\right\| \|A\| \tag{26}$$

where $\|\cdot\|$ is norm of a matrix.
If condition number is very large, the results may be untrusted.
For example

$$\begin{bmatrix} 5 & 7 \\ 7 & 10 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0.7 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 5 & 7 \\ 7 & 10 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0.69 \\ 1.01 \end{bmatrix}$$

Solutions are

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0.1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -0.17 \\ 0.22 \end{bmatrix}$$

Numerical Stabilization

The Green function propagating process

$$\mathbf{G}^{\sigma}(\tau+1,\tau+1)=\mathbf{B}^{\sigma}(\tau+1,\tau)\mathbf{G}^{\sigma}(\tau,\tau)\mathbf{B}^{\sigma}(\tau+1,\tau)^{-1} \tag{27}$$

will accumulate numerical errors. We need to do numerical stabilization after several steps of propagating.

Numerical Stabilization

$$B(n\tau_w,0) = U_n \underbrace{\begin{bmatrix} \mathrm{X} & & & \\ & \mathrm{X} & & \\ & & \mathrm{X} & \\ & & & \mathrm{x} \end{bmatrix}}_{D_n} V_n$$

$$\begin{aligned}
B((n+1)\tau_w,0) &= B((n+1)\tau_w,n\tau_w)B(n\tau_w,0) \\
&= B((n+1)\tau_w,n\tau_w)U_n \underbrace{\begin{bmatrix} \mathrm{X} & & & \\ & \mathrm{X} & & \\ & & \mathrm{X} & \\ & & & \mathrm{x} \end{bmatrix}}_{D_n} V_n \\
&= \underbrace{\begin{bmatrix} \mathrm{X} & \mathrm{X} & \mathrm{X} & \mathrm{x} \\ \mathrm{X} & \mathrm{X} & \mathrm{X} & \mathrm{x} \\ \mathrm{X} & \mathrm{X} & \mathrm{X} & \mathrm{x} \\ \mathrm{X} & \mathrm{X} & \mathrm{X} & \mathrm{x} \end{bmatrix}}_{B((n+1)\tau_w,n\tau_w)U_n D_n} V_n = U_{n+1} \underbrace{\begin{bmatrix} \mathrm{X} & & & \\ & \mathrm{X} & & \\ & & \mathrm{X} & \\ & & & \mathrm{x} \end{bmatrix}}_{D_{n+1}} V' V_n \\
&= U_{n+1} D_{n+1} V_{n+1}
\end{aligned}$$

Numerical Stabilization

We recalculate the equal time Green function after several steps of propagating using following equation.

$$
\begin{aligned}
\mathbf{G}(\tau,\tau) &= [\mathbf{1} + \mathbf{B}(\tau,0)\mathbf{B}(\beta,\tau)]^{-1} \\
&= [\mathbf{1} + \mathbf{U}_R\mathbf{D}_R\mathbf{V}_R\mathbf{V}_L\mathbf{D}_L\mathbf{U}_L]^{-1} \\
&= \mathbf{U}_L^{-1}\left[(\mathbf{U}_L\mathbf{U}_R)^{-1} + \mathbf{D}_R\left(\mathbf{V}_R\mathbf{V}_L\right)\mathbf{D}_L\right]^{-1}\mathbf{U}_R^{-1} \\
&= \mathbf{U}_L^{-1}\left[(\mathbf{U}_L\mathbf{U}_R)^{-1} + \mathbf{D}_R^{\max}\mathbf{D}_R^{\min}\left(\mathbf{V}_R\mathbf{V}_L\right)\mathbf{D}_L^{\min}\mathbf{D}_L^{\max}\right]^{-1}\mathbf{U}_R^{-1} \\
&= \mathbf{U}_L^{-1}\left(\mathbf{D}_L^{\max}\right)^{-1}\left[\left(\mathbf{D}_R^{\max}\right)^{-1}\left(\mathbf{U}_L\mathbf{U}_R\right)^{-1}\left(\mathbf{D}_L^{\max}\right)^{-1} + \mathbf{D}_R^{\min}\mathbf{V}_R\mathbf{V}_L\mathbf{D}_L^{\min}\right]^{-1}\left(\mathbf{D}_R^{\max}\right)^{-1}\mathbf{U}_R^{-1}
\end{aligned}
\tag{28}
$$

The ensemble average of physical observable:

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}\left\{e^{-\beta\hat{H}}\hat{O}\right\}}{\mathrm{Tr}\left\{e^{-\beta\hat{H}}\right\}} = \sum_c \mathcal{P}_c \langle \hat{O} \rangle_c + O\left(\Delta\tau^2\right) \tag{29}$$

where

$$\begin{aligned}\mathcal{P}_\mathcal{C} &= \frac{\mathcal{W}_\mathcal{C}^\mathcal{S} \det[\mathbf{1} + B(\beta,0)]}{\sum_\mathcal{C} \mathcal{W}_\mathcal{C}^\mathcal{S} \det[\mathbf{1} + B(\beta,0)]} \\ \langle \hat{O} \rangle_\mathcal{C} &= \frac{\mathrm{Tr}\{\hat{U}(\beta,\tau)\hat{O}\hat{U}(\tau,0)\}}{\mathrm{Tr}\{\hat{U}(\beta,0)\}}\end{aligned} \tag{30}$$

Operator and Measurment

Equal time Green's function:

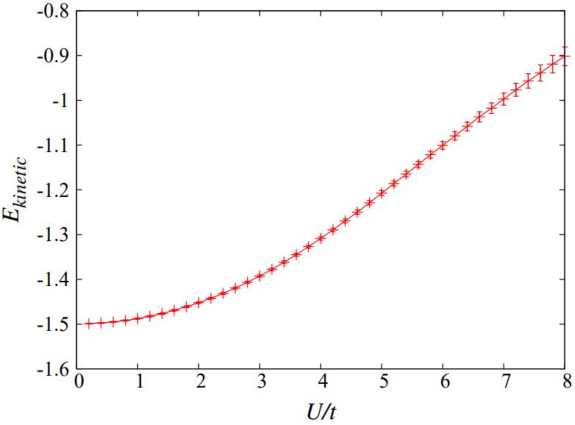
$$(G_{ij})_{\mathcal{C}} = \left\langle \hat{c}_i \hat{c}_j^{\dagger} \right\rangle_{\mathcal{C}} = (\mathbf{1} + B(\tau, 0)B(\beta, \tau))_{ij}^{-1} \tag{31}$$

When $\tau_1 > \tau_2$, we can obtain:

$$\begin{aligned}
(G_{ij}(\tau_1, \tau_2))_{\mathcal{C}} &= \left\langle \hat{c}_i(\tau_1) \hat{c}_j^{\dagger}(\tau_2) \right\rangle_C \\
&= \frac{\mathrm{Tr}\left\{ \hat{U}(\beta, \tau_1) \hat{c}_i \hat{U}(\tau_1, \tau_2) \hat{c}_j^{\dagger} \hat{U}(\tau_2, 0) \right\}}{\mathrm{Tr}\{\hat{U}(\beta, 0)\}} \\
&= \frac{\mathrm{Tr}\left\{ \hat{U}(\beta, \tau_2) \hat{U}^{-1}(\tau_1, \tau_2) \hat{c}_i \hat{U}(\tau_1, \tau_2) \hat{c}_j^{\dagger} \hat{U}(\tau_2, 0) \right\}}{\mathrm{Tr}\{\hat{U}(\beta, 0)\}} \\
&= [B(\tau_1, \tau_2) G_{\mathcal{C}}(\tau_2, \tau_2)]_{ij}
\end{aligned} \tag{32}$$

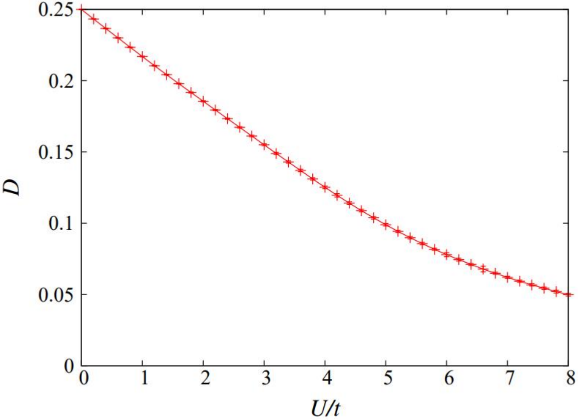
Kinetic Energy

The calculation parameters is $L = 4, \beta = 4$



Double Occupancy

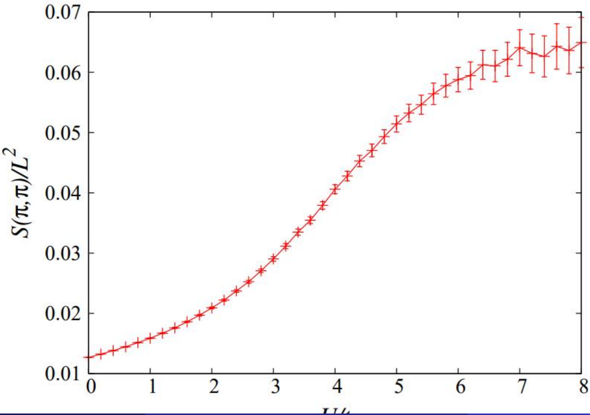
We can define double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ as the order parameter for Mott transition. Here we show the results with parameters $L = 4, \beta = 4$ and U varying from $0.0\mathrm{t}$ to $8.0\mathrm{t}$.



$S(\pi,\pi)$

We measure the z-component antiferromagnetic structure factor $S(\pi,\pi)$ which is defined as

$$S(\mathbf{Q}) = \frac{1}{L^2} \sum_{ij} e^{-i\mathbf{Q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \left\langle \hat{s}_i^z \hat{s}_j^z \right\rangle$$



Thanks