Tutorial: Solving Spin-Fermion Model with DQMC

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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 Measurement

3. Some Results of Hubbard Model
   - Kinetic Energy
   - Double Occupancy
   - $S(\pi, \pi)$
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 \( j, i, i_{n-1}, \ldots, i_1, i_0 \),

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

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

\[
p(i, j) = P(X_{n+1} = j | X_n = i)
\]
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

$$\sum_x \pi(x)p(x, y) = \pi(y),$$

or in the matrix form $\pi p = \pi$

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 $\pi$:

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

After a transpose operation, $\pi^T$ is just like eigenvector.
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 $Z = \sum_{\text{all configurations}} e^{-\beta H(C)}$.
How can we get the probability distribution we want?

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

\[ \pi(i) p(i,j) = \pi(j) p(j,i) \]  \hspace{1cm} (3)

Verify as follows:

\[ \sum_i \pi(i) p(i,j) = \sum_i \pi(j) p(j,i) = \pi(j) \sum_i p(j,i) = \pi(j) \]  \hspace{1cm} (4)
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
      \[
      R(x', x_t) = \min \left( 1, \frac{P(x') g(x_t | x')}{P(x_t) g(x' | x_t)} \right);
      \]
   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

$$H = -J \sum_{<i,j>} s_i s_j$$  \hspace{1cm} (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 \( u \leq R(x',x_t) \), accept. Flip the spin successfully.
      ELSE reject, don’t flip the spin.
   d. set \( t = t + 1 \)
What does 'determinant' mean here?

\[
\text{Tr} \left[ e^{-\sum_{i,j} c_i^\dagger A_{i,j} c_j} e^{-\sum_{i,j} c_i^\dagger B_{i,j} c_j} \right] = \text{Det}(1 + e^{-A} e^{-B})
\] (6)
Model: A Spin-Fermion coupled Model

\[ H = H_f + H_s + H_{f-s} \]  

where

\[ H_f = -t_1 \sum_{\langle ij \rangle, \lambda, \sigma} c_{i,\lambda,\sigma}^\dagger c_{j,\lambda,\sigma} - t_2 \sum_{\langle\langle ij \rangle\rangle, \lambda, \sigma} c_{i,\lambda,\sigma}^\dagger c_{j,\lambda,\sigma} \]

\[ - t_3 \sum_{\langle\langle\langle ij \rangle\rangle\rangle, \lambda, \sigma} c_{i,\lambda,\sigma}^\dagger c_{j,\lambda,\sigma} + h.c. - \mu \sum_{i,\lambda,\sigma} n_{i,\lambda,\sigma} \]  

\[ H_s = - J \sum_{\langle ij \rangle} s_i^z s_j^z - h \sum_i s_i^x \]  

\[ H_{f-s} = - \xi \sum_i s_i^z (\sigma_{i,1}^z - \sigma_{i,2}^z), \]  

and \( \sigma_{i,\lambda}^z = \frac{1}{2} (c_{i,\lambda,\uparrow}^\dagger c_{i,\lambda,\uparrow} - c_{i,\lambda,\downarrow}^\dagger c_{i,\lambda,\downarrow}) \) is the fermion spin along \( z \).
Model: A Spin-Fermion coupled Model

Figure:

- fermion site
- Ising site
- Ising spin
- fermion
- coupling

- $\lambda = 2$
- $\lambda = 1$
- $\xi$
- $t_1$
- $t_2$
- $t_3$
- $h$
- $J$
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

\[ Z = \text{Tr} \left[ e^{-\beta \hat{H}} \right] = \text{Tr} \left[ \left( e^{-\Delta \tau \hat{H}} \right)^M \right] \]
To take care of the interaction part, we need do the HS transformation

\[ e^{-\Delta \tau \hat{H}_I} = \prod_i e^{-\Delta \tau U(\hat{n}_{i\uparrow} - \frac{1}{2})(\hat{n}_{i\downarrow} - \frac{1}{2})} = \prod_i \lambda \sum_{s_i,\tau = \pm 1} e^{\alpha s_i,\tau (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})} = \lambda^N \sum_{s_i,\tau = \pm 1} \left( \prod_i e^{\alpha s_i,\tau \hat{n}_{i\uparrow}} \prod_i e^{-\alpha s_i,\tau \hat{n}_{i\downarrow}} \right) \]
We should first trace out the bare transverse field Ising model. We know that

\[ e^{\Delta \tau \hat{h} \hat{s}_{i}^{x}} = \cosh(\Delta \tau h) \mathbf{1} + \sinh(\Delta \tau h) \hat{s}_{i}^{x} \]  
(11)

And we require:

\[ \left\langle S_{z}' \mid e^{\Delta \tau \hat{h} \hat{s}_{i}^{x}} \mid S_{z} \right\rangle = \Lambda e^{\gamma s_{z}' s_{z}} \]  
(12)

Just take \( S_{z} = \pm 1 \), we can get

\[ \left\langle S_{z} \mid e^{\Delta \tau \hat{h} \hat{s}_{i}^{x}} \mid S_{z} \right\rangle = \cosh(\Delta \tau h) = \Lambda e^{\gamma} \]  
(13)

\[ \left\langle -S_{z} \mid e^{\Delta \tau \hat{h} \hat{s}_{i}^{x}} \mid S_{z} \right\rangle = \sinh(\Delta \tau h) = \Lambda e^{-\gamma} \]
Spin part:

\[ Z_{\text{spin}} = \text{Tr} \left\{ e^{-\beta H_{\text{spin}}} \right\} \]

\[ = \left( \prod_{\tau} \prod_{\langle ij \rangle} e^{\Delta \tau J_{i,\tau}^z s_{j,\tau}^z} \right) \left( \prod_{i} \prod_{\langle \tau,\tau' \rangle} \Lambda e^{\gamma s_{i,\tau}^z s_{j,\tau'}^z} \right) + O(\Delta \tau^2) \]  

(14)

where

\[ \gamma = -\frac{1}{2} \ln(\tanh(\Delta \tau h)) \]

\[ \Lambda^2 = \sinh(\Delta \tau h) \cosh(\Delta \tau h) \]  

(15)
\[
Z = \text{Tr} \left\{ e^{-\beta H} \right\} = \text{Tr} \left\{ \left( e^{-\Delta \tau H_I} e^{-\Delta \tau H_0} \right)^M \right\} + O(\Delta \tau^2) \\
= \sum C \mathcal{W}_C^S \text{Tr} \left\{ \prod_{\tau=M}^{1} e^{\hat{c}^\dagger V(C) \hat{c}} e^{-\Delta \tau \hat{c}^\dagger T \hat{c}} \right\} + O(\Delta \tau^2) \\
\]

Define
\[
\hat{U}(\tau_2, \tau_1) = \prod_{n=n_1+1}^{n_2} e^{\hat{c}^\dagger V(C) \hat{c}} e^{-\Delta \tau \hat{c}^\dagger T \hat{c}} \\
B(\tau_2, \tau_1) = \prod_{n=n_1+1}^{n_2} e^{V(C)} e^{-\Delta \tau T} \\
\]

Then
\[
Z = \sum C \mathcal{W}_C^S \text{Tr} \{ \hat{U}(\beta, 0) \} = \sum C \mathcal{W}_C^S \det[1 + B(\beta, 0)] \\
\]
Sign Problem

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


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 $\lambda_i$ is an eigenvalue, then $\lambda_i^*$ is also an eigenvalue. If $\lambda_i$ is real, it is twofold degenerate. In this case, the fermion determinant is positive definite,

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

where $H_K$ is imaginary time-independent kinetic energy term and $H_I$ is imaginary time-dependent decoupled interaction term.
\[
\hat{H}_0 = -J \sum_{\langle ij \rangle} \hat{s}_i^z \hat{s}_j^z - t \sum_{\langle ij \rangle \lambda \sigma} \hat{c}_{i \lambda \sigma}^\dagger \hat{c}_{j \lambda \sigma} + \text{h.c.} - \mu \sum_{i \lambda \sigma} \hat{n}_{i \lambda \sigma} - \xi \sum_i s_i^z (\hat{\sigma}_{i1}^z - \hat{\sigma}_{i2}^z)
\]

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

\[
\hat{H}_0 \xrightarrow{\tau} \\
- J \sum_{\langle ij \rangle} \hat{s}_i^z \hat{s}_j^z - t \sum_{\langle ij \rangle \lambda \sigma} \hat{c}_{i \lambda \bar{\sigma}}^\dagger \hat{c}_{j \lambda \bar{\sigma}} + h.c. - \mu \sum_{i \lambda \bar{\sigma}} \hat{n}_{i \lambda \bar{\sigma}} - \xi \sum_i s_i^z (\hat{\sigma}_{i1}^z + \hat{\sigma}_{i2}^z)
\]

\(\tau_x\) on orbital space

\[
- J \sum_{\langle ij \rangle} \hat{s}_i^z \hat{s}_j^z - t \sum_{\langle ij \rangle \lambda \sigma} \hat{c}_{i \lambda \bar{\sigma}}^\dagger \hat{c}_{j \lambda \bar{\sigma}} + h.c. - \mu \sum_{i \lambda \bar{\sigma}} \hat{n}_{i \lambda \bar{\sigma}} - \xi \sum_i s_i^z (\hat{\sigma}_{i2}^z - \hat{\sigma}_{i1}^z)
\]

\[
= \hat{H}_0
\]
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

\[\det(1 + B(\beta, 0)) = \prod_{i=1}^{2} \det (1 + B_{\alpha_i}(\beta, 0)) = |\det (1 + B_{\alpha_1}(\beta, 0))|^2\]

So our designer model is free of sign problem.
Accept Ratio

We have known that

\[ \omega_C = \phi(C) \det(1 + B(\beta, \tau)B(\tau, 0)) \]
\[ = \phi(C) \det(G(0, 0))^{-1} \]

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

\[ \mathcal{R} = \frac{\mathcal{W}_C^S}{\mathcal{W}_C^S \det(1 + B(\beta, 0))} = \frac{\mathcal{W}_C^S}{\mathcal{W}_C^S} \mathcal{R}_f \]

(19)

And

\[ \mathcal{R}_f = \frac{\det(1 + B'_C(\beta, 0))}{\det(1 + B_C(\beta, 0))} \]
\[ = \frac{\det(1 + B_C(\beta, \tau)(1 + \Delta)B_C(\tau, 0))}{\det(1 + B_C(\beta, 0))} \]
\[ = \det \left[ 1 + \Delta \left( 1 - (1 + B_C(\tau, 0)B_C(\beta, \tau))^{-1} \right) \right] \]
\[ = \det \left[ 1 + \Delta \left( 1 - G_C(\tau, \tau) \right) \right] \]
Update Green Function

\[ G_C'(\tau, \tau) = [1 + (1 + \Delta)B_C(\tau, 0)B_C(\beta, \tau)]^{-1} \]

\[ = [1 + B_C(\tau, 0)B_C(\beta, \tau)]^{-1} \times \left[ (1 + (1 + \Delta)B_C(\tau, 0)B_C(\beta, \tau)) \left( (1 + B_C(\tau, 0)B_C(\beta, \tau))^{-1} \right) \right]^{-1} \]

(21)

as \( G_C(\tau, \tau) = [1 + B_C(\tau, 0)B_C(\beta, \tau)]^{-1} \), we denote

\[ A_C \equiv B_C(\tau, 0)B_C(\beta, \tau) \equiv G_C^{-1} - 1 \]

\[ G_C'(\tau, \tau) = G_C \left[ (1 + (1 + \Delta)A_C) G_C \right]^{-1} \]

\[ = G_C \left[ (1 + (1 + \Delta) (G_C^{-1} - 1)) G_C \right]^{-1} \]

\[ = G_C \left[ 1 + \Delta (1 - G_C) \right]^{-1} \]

(22)
Using the Sherman-Morrison formula

\[(I + UV)^{-1} = I - U(I_k + VU)^{-1}V\]  \hspace{1cm} (23)

we have that

\[\mathcal{R}_f = 1 + \Delta_{ii} (1 - G_c^c)\]

\[G_c'(\tau, \tau) = G_c(\tau, \tau) + \alpha_i G_c(:,i)(G_c(i,:) - e_i)\]  \hspace{1cm} (24)

where

\[\alpha_i = \Delta_{ii} / \mathcal{R}_f\]  \hspace{1cm} (25)

\[O(N^3) \rightarrow O(N^2)\]
Condition Numbers

Condition number of a matrix $A$ is

$$\kappa(A) = \|A^{-1}\| \|A\|$$  \hspace{1cm} (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

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0.1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -0.17 \\ 0.22 \end{bmatrix}$$
The Green function propagating process

\[
G^\sigma(\tau + 1, \tau + 1) = B^\sigma(\tau + 1, \tau)G^\sigma(\tau, \tau)B^\sigma(\tau + 1, \tau)^{-1}
\]  

(27)

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

\[
B(n\tau_w, 0) = U_n \begin{bmatrix} X & X \end{bmatrix} V_n
\]

\[
B((n+1)\tau_w, 0) = B((n+1)\tau_w, n\tau_w)B(n\tau_w, 0)
\]

\[
= B((n+1)\tau_w, n\tau_w)U_n \begin{bmatrix} X & X \end{bmatrix} V_n
\]

\[
= \begin{bmatrix} X & X & X & x \\
X & X & X & x \\
X & X & X & x \\
X & X & X & x \\
\end{bmatrix}_{D_n} V_n = U_{n+1} \begin{bmatrix} X & X \\
X & x \\
\end{bmatrix}_{D_{n+1}} V'V_n
\]

\[
= U_{n+1}D_{n+1}V_{n+1}
\]
We recalculate the equal time Green function after several steps of propagating using following equation.

\[
G(\tau, \tau) = \left[ 1 + B(\tau, 0)B(\beta, \tau) \right]^{-1} \\
= [1 + U_R D_R V_R V_L D_L U_L]^{-1} \\
= U_L^{-1} \left[ (U_L U_R)^{-1} + D_R (V_R V_L) D_L \right]^{-1} U_R^{-1} \\
= U_L^{-1} \left[ (U_L U_R)^{-1} + D_R^{\text{max}} D_R^{\text{min}} (V_R V_L) D_L^{\text{min}} D_L^{\text{max}} \right]^{-1} U_R^{-1} \\
= U_L^{-1} (D_L^{\text{max}})^{-1} \left[ (D_R^{\text{max}})^{-1} (U_L U_R)^{-1} (D_L^{\text{max}})^{-1} + D_R^{\text{min}} V_R V_L D_L^{\text{min}} \right]^{-1} (D_R^{\text{max}})^{-1} U_R^{-1} \\
(28)
\]
The ensemble average of physical observable:

\[
\langle \hat{O} \rangle = \frac{\text{Tr} \left\{ e^{-\beta \hat{H}} \hat{O} \right\}}{\text{Tr} \left\{ e^{-\beta \hat{H}} \right\}} = \sum_c P_c \langle \hat{O} \rangle_c + O(\Delta \tau^2)
\]  

where

\[
P_c = \frac{\mathcal{W}_c \det[1 + B(\beta, 0)]}{\sum_c \mathcal{W}_c \det[1 + B(\beta, 0)]}
\]

\[
\langle \hat{O} \rangle_c = \frac{\text{Tr}\{\hat{U}(\beta, \tau) \hat{O} \hat{U}(\tau, 0)\}}{\text{Tr}\{\hat{U}(\beta, 0)\}}
\]
Equal time Green's function:

\[ (G_{ij})_C = \langle \hat{c}_i \hat{c}^\dagger_j \rangle_C = (1 + B(\tau, 0)B(\beta, \tau))^{-1}_{ij} \]  \hspace{1cm} (31)

When \( \tau_1 > \tau_2 \), we can obtain:

\[ (G_{ij}(\tau_1, \tau_2))_C = \langle \hat{c}_i(\tau_1) \hat{c}^\dagger_j(\tau_2) \rangle_C \]

\[ \begin{align*}
&= \text{Tr} \left\{ \hat{U}(\beta, \tau_1) \hat{c}_i \hat{U}(\tau_1, \tau_2) \hat{c}^\dagger_j \hat{U}(\tau_2, 0) \right\} \\
&= \frac{\text{Tr}\{\hat{U}(\beta, 0)\}}{\text{Tr}\{\hat{U}(\beta, 0)\}} \\
&= \text{Tr} \left\{ \hat{U}(\beta, \tau_2) \hat{U}^{-1}(\tau_1, \tau_2) \hat{c}_i \hat{U}(\tau_1, \tau_2) \hat{c}^\dagger_j \hat{U}(\tau_2, 0) \right\} \\
&= \frac{\text{Tr}\{\hat{U}(\beta, 0)\}}{\text{Tr}\{\hat{U}(\beta, 0)\}} \\
&= [B(\tau_1, \tau_2) G_C(\tau_2, \tau_2)]_{ij} \hspace{1cm} (32)
\]
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 $0.0t$ to $8.0t$. 

![Graph showing the relationship between D and U/t]
We measure the z-component antiferromagnetic structure factor $S(\pi, \pi)$ which is defined as

$$S(Q) = \frac{1}{L^2} \sum_{ij} e^{-iQ \cdot (r_i - r_j)} \langle \hat{s}_i^z \hat{s}_j^z \rangle$$
Thanks