# Notes for qRBM-AFQMC

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## 1 Introduction

This note is going to introduce a new "variational trial wave function" for CPMC and the following construction as "technical details".

All the discussion below is based on one-band Hubbard

$$H = -t \sum_{\langle i,j\rangle,\sigma} C^{\dagger}_{i,\sigma} C_{j,\sigma} + U \sum_{j} n_{j,up} n_{j,dn}$$

where $C^{\dagger}_{j,\sigma}$ ($C^{\dagger}_{j,\sigma}$) creates (annihilates) an electron with spin $\sigma$ ($\sigma = up, dn$) at lattice site $j$ and $, j\rangle$ connects two nearest neighbor sites, $n_{j,\sigma} \equiv C^{\dagger}_{j,\sigma} C_{j,\sigma}$. and 2-D lattice set with Closed Boundary Condition.

## 2 Trial Wave Function

The trial wave function is

$$|\psi\rangle \equiv \sum_{\{h_k\}} \prod_{k=1}^{M} e^{\sum_{i,j,\sigma} w^{k}_{i,j,\sigma} h_k C^{\dagger}_{i\sigma} C_{j\sigma}} |\phi_0\rangle = \sum_{\{h_k\}} \prod_{k=1}^{M} e^{D^k h_k} |\phi_0\rangle$$

where $D^k \equiv \sum_{i,j,\sigma} w^{k}_{i,j,\sigma} C^{\dagger}_{i\sigma} C_{j\sigma}$, $h_k = \pm 1$ is a set of auxiliary field and $|\phi_0\rangle$ is any single Slater determinate (noted as "DET state").

The reasons we choose it as an trial wave function are:

1. In AFQMC and RBM trial wave function, Auxiliary field can be used to describe the interaction in quantum state.

2. when the number of $h_k$ goes to $2 * Nsites$, it agree with AFQMC. (Where $Nsites$ is the numer of sites in lattice.)

3. In Theory, this trial wave function can approach to any DET states.

# 3 Technical Details

## 3.1 Energy for $|\psi\rangle$

As a variational approach, the expected value of $H$ is supposed to be minimized for the trial wave function.

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{\{h_k\},\{h'_k\}}\langle\phi_0|\prod_{k=1}^{M} e^{D^{k\dagger}h_k} H \prod_{k=1}^{M} e^{D^k h'_k}|\phi_0\rangle}{\sum_{\{h_k\},\{h'_k\}}\langle\phi_0|\prod_{k=1}^{M} e^{D^{k\dagger}h_k} \prod_{k=1}^{M} e^{D^k h'_k}|\phi_0\rangle} = \frac{\sum_{\{h_k\},\{h'_k\}}\langle\phi_0(h)|H|\phi_0(h')\rangle}{\sum_{\{h_k\},\{h'_k\}}\langle\phi_0(h)|\phi_0(h')\rangle}$$

$$\langle\phi_0(h)|\phi_0(h')\rangle = det(\Phi_0(h)^\dagger\Phi_0(h')) = det(A)$$

$$\langle\phi_0(h)|C^\dagger_{i\sigma}C_{j\sigma}|\phi_0(h')\rangle = det(A) * [\Phi_0(h)A^{-1}\Phi_0(h')^\dagger]_{j\sigma,i\sigma}$$

$$\langle\phi_0(h)|n_{i,up}n_{j,dn}|\phi_0(h')\rangle = \frac{\langle\phi_0(h)|n_{i,up}|\phi_0(h')\rangle\langle\phi_0(h)|n_{j,dn}|\phi_0(h')\rangle}{\langle\phi_0(h)|\phi_0(h')\rangle}$$

where $|\phi_0(h)\rangle \equiv \prod_{k=1}^{M} e^{D^k h'_k}|\phi_0\rangle$, $A \equiv \Phi_0(h)^\dagger\Phi_0(h')$ and $\Phi$ is the matrix of DET state $|\phi_0\rangle$.

For a given trial wave function $|\psi\rangle$, $2 \times 2^M \times 2^M$ times matrix ($2 * Nsites$ by $Ntot$) multiplication is needed (without considering any symmetry) where $Ntot$ is the number of electrons in this system.

## 3.2 Derivative of Energy for $|\psi\rangle$

### 3.2.1 Wick's Theorem in single DET state: prove

Claim: for n-body operators in the average of DET states $|\phi_1\rangle$, $|\phi_2\rangle$, Wick's Theorem can be applied. For example:

$$\langle\phi_1|C^\dagger_i C_j C^\dagger_k C_l|\phi_2\rangle\langle\phi_1|\phi_2\rangle = \langle\phi_1|C^\dagger_i C_j|\phi_2\rangle\langle\phi_1|C^\dagger_k C_l|\phi_2\rangle$$

$$+\langle\phi_1|C^\dagger_i C_l|\phi_2\rangle\langle\phi_1|C_j C^\dagger_k|\phi_2\rangle - \langle\phi_1|C^\dagger_i C^\dagger_k|\phi_2\rangle\langle\phi_1|C_j C_l|\phi_2\rangle$$

The proving goes like this:

First prove Wick's Theorem can be applied to empty state $|0\rangle$ and electron creation and annihilation operators on position. $\langle 0|C^\dagger_i \cdots C_j|0\rangle$.

Then prove Wick's Theorem can be applied to empty state $|0\rangle$ and linear combination $\{B_i\}$ of electron creation and annihilation operators on position. $\langle 0|B^\dagger_i \cdots B_j|0\rangle$.

Then prove Wick's Theorem can be applied to DET state $|\phi_1\rangle$, $|\phi_2\rangle$ and electron creation and annihilation operators on position. $\langle B_1 B_2 \cdots B_M|C^\dagger_i \cdots C_j|B'^\dagger_M \cdots B'^\dagger_2 B'^\dagger_1\rangle = \langle\phi_1|C^\dagger_i \cdots C_j|\phi_2\rangle$.

### 3.2.2 Wick's Theorem in single DET state: apply

The derivative of E is:

$$\frac{\partial E}{\partial w^k_{i\sigma,j\sigma}} = \frac{\partial \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}}{\partial w^k_{i\sigma,j\sigma}} = \frac{\partial\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle\partial w^k_{i\sigma,j\sigma}} - \frac{\partial\langle\psi|\psi\rangle}{\langle\psi|\psi\rangle\partial w^k_{i\sigma,j\sigma}}E$$

Suppose $w^k_{i,j}$ are real number and $C^\dagger_i C_j$ (produced from the derivative of $e^{D^k h_k}$ ) can be moved to the middle of $\langle\phi_1|\phi_2\rangle$ (This may suggest $[D^i, D^j] = 0$ and needed to be considered carefully):

$$\frac{\partial\langle\psi|\psi\rangle}{\partial w^k_{i\sigma,j\sigma}} = \sum_{\{h_k\},\{h'_k\}} (\langle\phi(h)|h_k C^\dagger_{j\sigma} C_{i\sigma}|\phi(h')\rangle + \langle\phi(h)|h'_k C^\dagger_{i\sigma} C_{j\sigma}|\phi(h')\rangle)$$

Be careful! The normalization of Wick's Theorem is not showed below:

$$\begin{aligned}\frac{\partial\langle\psi|H|\psi\rangle}{\partial w^q_{i\sigma,j\sigma}} = \sum_{\{h_k\},\{h'_k\}} \{&-t * h_q \sum_{,l\rangle}{}^{\dagger}{}_{j\sigma} C_{l\sigma}\rangle_{i\sigma} C^\dagger_{k\sigma}\rangle + h^\dagger_{qj\sigma} C_{i\sigma}\rangle\rangle \\ &+U * h_q \sum_k {}_{k\sigma'}\rangle^\dagger_{j\sigma} C_{k\sigma}\rangle_{i\sigma} C^\dagger_{k\sigma}\rangle + h^\dagger_{qj\sigma} C_{i\sigma}\rangle\rangle \\ &-t * h'_q \sum_{,l\rangle}{}^{\dagger}{}_{l\sigma} C_{j\sigma}\rangle_{k\sigma} C^\dagger_{i\sigma}\rangle + h'^{\dagger}_{qi\sigma} C_{j\sigma}\rangle\rangle \\ &+U * h'_q \sum_k {}_{k\sigma'}\rangle^\dagger_{k\sigma} C_{j\sigma}\rangle_{k\sigma} C^\dagger_{i\sigma}\rangle + h'^{\dagger}_{qi\sigma} C_{j\sigma}\rangle\rangle\}\end{aligned}$$

where $\rangle,\langle$ are kinetic energy and potential energy,${}^\dagger_{j\sigma} C_{l\sigma}\rangle$ is the simplification of $\langle\phi(h)|C^\dagger_{j\sigma} C_{l\sigma}|\phi(h')\rangle$, $\sigma'$ denote the negative direction of $\sigma$.

Since the Green Function (Density Matrix) is calculated in the process to get Energy, there is nearly no cost to find the derivative of Energy.

## 3.3 Symmetry for $D^k$

In the Closed Boundary Condition, $w^k_{i,j} = w^k_{i-j}$.

In the real case, $\langle\phi(h)|C^\dagger_{j\sigma} C_{l\sigma}|\phi(h')\rangle = \langle\phi(h')|C^\dagger_{l\sigma} C_{j\sigma}|\phi(h)\rangle$. The cost may be reduced by 2.

# 4 Conclusion

In summary, if we request:

1.$w^k_{i,j}$ are real number.

2.$C_i^\dagger C_j$, (produced from the derivative of $e^{D^k h_k}$ ) can be moved to the middle of $\langle\phi_1|\phi_2\rangle$.

The cost of calculating E and derivative of E for a given $|\psi\rangle$ (a given $w_{i,j}^k$) is nearly the cost of $2\times 2^M \times 2^M$ times matrix ($2*Nsites$ by $Ntot$) multiplication.

# 5 Update 11/26/2018

This is an update about my recent work

I have written a C++ code to get the minimal energy state with LBFGSpp from our "qRBM trial wave function" (The RBM-like function in this note) and put the minimal energy state into CPMC as trial wave function. (just like what we are supposed to do.)

But there are several things I want to mention:

0. **The equations for derivative in this note do not work!** (We can not neglect the effects of commutator and the $x$ derivative of $e^(xA+yB)$ wouldn't be $Ae^(xA+yB)$ except $[A,B]=0$ where $A$,$B$ are matrix) So in my code we use the numerical derivative which may cost a lot but work at least for small system.

1. The minimal energy state is not a physical state. (The DET states (Slater Determinants) generated by our qRBM are not normalized), those column vectors in physical DET state must be normalized to 1.

2. No matter if we normalize the qRBM state (the state generated by qRBM) or not:

For 2 by 2 system with 2 $Spin_{up}$, 2 $Spin_{dn}$ U=4, **the minimal energy is nearly** $-5.32$ **for the number of hidden elements to be** 1**,** 2**,** 3**,** 4 (which means we have 2, 4, 8, 16 DET states) and the exact results is 5.6(1) (from S.C.CPMC with a small number (400) of walkers -it's easy and gives a good scale for our results).

Since **the increasing number of our hidden parameter wouldn't change the results** too much (which is not expected) and the normalization becomes a problem, I plan to use imaginary number in our notwork parameters (like real time evolution).

# References