

Self Consistent CPMC with pseudo-BCS state

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1 Introduction

One of the hardest part to simulate quantum systems, especially those strongly correlated systems, with classical computer is the exponential explosion of Hilbert space. one of the key to solved this problem is stochastic sampling (QMC), which it's possible for classical computer to chase exponential scale and get the estimation of some quantities in principle.

However, phase problems in Fermion system prevent the convergence of QMC. The most effective approach to deal with phase problem is adding bias constraint which has been applied to many kind of fields.

But choosing a suitable constraint is hard and sometimes it leads to some fatal man-made bias. For example, CPMC can provide exact results without phase problem if its trial wave function "phiT" (constraint) is exact ground state. So an trial wave function source is needed. But in some situation, those "wave function results" methods (like Hartree-Fock (HF) or density-functional theory (DFT)) can't provide a good enough approximation of ground state and most importantly, they may lead CPMC run into an wrong way. And those "quantities results" methods (like AFQMC or DMRG) which can give a better approximation, are not able to provide a usable wave function without drastically changing its computational scaling or complexity.

In this paper, we are going to introduce a almost 'non-cost' algorithm which can be used to extract wave function from output Green function (Density Matrix) and input this wave function as trial wave function to CPMC calculation. So that, CPMC, as a input-output algorithm, can be easily applied to self-consistent frame which can improve their results to local or even global optimization with heat bath and luck by iteration.

For concreteness, we will use the Hubbard model to describe the self-consistent CPMC procedure:

2 Self Consistent CPMC Method

To start the self-consistent procedure, we run some numerical calculation first (assume we do CPMC with free electrons trial wave function or UHF). Then

with back propagation, we can get the Green Function G of Ground State.

2.1

Now, we want to construct a wave function which has the same Green Function with Ground State. If such a wave function can be found, this wave function must have almost the same behavior with GS, then it can be a good approximation of GS and it can be a good constraint in CPMC.

Theory: For any Green Function G with $Nspin_{up} = Nspin_{dn}$ and 'part of spin symmetry', there exist and only exist a pseudo-BCS state F which has Green function G' such that $G' - > G$

Proof: For any Green Function G , by eigenvalue decomposition, we can get $G_{up} = T_{up} \lambda_{up} T_{up}^\dagger$ and $G_{dn} = T_{dn} \lambda_{dn} T_{dn}^\dagger$ where λ is diagonalized eigenvalue matrix and T is eigenvectors (with "part of spin symmetry", the $\lambda_{up} = \lambda_{dn} \equiv \lambda$).

Then we claim: for any diagonalized Green function, there is a diagonalized BCS matrix F , such that the Green Function of this BCS state F is G .

For diagonalized BCS state F ,

$$BCS(F) = \prod_{i,j} (\sum f_{i,j} C_{i,up}^\dagger C_{j,dn}^\dagger) = \sum_{k_1, k_2, k_3 \dots k_{Nspin}} (\lambda_{k_1} \lambda_{k_2} \lambda_{k_3} \dots \lambda_{k_{Nspin}} C_{k_1,up}^\dagger C_{k_1,dn}^\dagger C_{k_2,up}^\dagger C_{k_2,dn}^\dagger C_{k_3,up}^\dagger C_{k_3,dn}^\dagger \dots)$$

where k is a set of non-repetitive sample of $1, 2, \dots Nsite$. it's easy to see that $C_{k_1,up}^\dagger C_{k_1,dn}^\dagger C_{k_2,up}^\dagger C_{k_2,dn}^\dagger C_{k_3,up}^\dagger C_{k_3,dn}^\dagger \dots C_{k_{Nspin},up}^\dagger C_{k_{Nspin},dn}^\dagger$ is a DET state with DET matrix

Now, the Green Function G' of $BCS(F)$ is: $G'_{ij*} = \langle BCS | C_{i*}^\dagger C_{j*} | BCS \rangle$ and $G'_{ij} = 0$ if $i \neq j < BCS | C_{i*}^\dagger C_{j*} | BCS \rangle = 0$ since the unpaired state $C_{i*}^\dagger C_{j*} (C_{k_1,up}^\dagger C_{k_1,dn}^\dagger C_{k_2,up}^\dagger C_{k_2,dn}^\dagger C_{k_3,up}^\dagger C_{k_3,dn}^\dagger \dots C_{k_{Nspin},up}^\dagger C_{k_{Nspin},dn}^\dagger) | 0 \rangle$ can't be found in $\langle BCS |$. If $i = j$, then $C_{i*}^\dagger C_{i*} (C_{k_1,up}^\dagger C_{k_1,dn}^\dagger C_{k_2,up}^\dagger C_{k_2,dn}^\dagger C_{k_3,up}^\dagger C_{k_3,dn}^\dagger \dots C_{k_{Nspin},up}^\dagger C_{k_{Nspin},dn}^\dagger) | 0 \rangle \neq 0$ if and only if there exist some $k = i$, so $G_{ii*} = \sum_{k_1, k_2, k_3 \dots k_{Nspin}, \exists k=i} (\lambda_{k_1} \lambda_{k_2} \lambda_{k_3} \dots \lambda_{k_{Nspin}})^2$.

So for diagonalized G and G' , $G = G'$ gives us a Nsite variable equation set. this equation set may have analytic or numerical exact solution, but is hard to find them. However, we can give some "approximate solution" which let $G - > G'$.

By applying linear transformation T to basis C and C , this results can be generalized exactly to any Green Function G with $Nspin_{up} = Nspin_{dn}$ and 'part of spin symmetry'.

2.2

For any Green Function G we can follow steps below to construct a BCS state has nearly the same Green Function G' with G . steps

1. Get the target Green Function "G" and its eigenvectors G_{up} , G_{dn} , eigenvalues λ_{up} , λ_{dn} (with spin symmetry, $\lambda \equiv \lambda_{up} = \lambda_{dn}$).

2. The new pseudo-BCS trial wave function F is $F = G_{up}^\dagger A G_{dn}$ where A is diagonalized matrix and $A = f(\lambda)$

3. There are two kind of f :

1st, DET decomposition: $A_{ii} = 1$ if λ_{ii} is larger or equal to the N_{spin} -th largest value in λ or $A_{ii} = 0$ (when this decomposition is applied, the pseudo-BCS state reduced to DET state and this is the S.C. CPMC mentioned by Mingpu)

2nd , Analytical decomposition: $A_{ii} = \sqrt{\lambda_{ii}/(1 - \lambda_{ii})}$, which work better. And this is the exact decomposition for pseudo-HFB state, which means in some grand canonical ensemble system, this decomposition is the exact solution for $G' = G$.

The decomposition method then become the key of this self-consistent CPMC procedure. if we choose "DET decomposition", the pseudo-BCS reduce to DET state and it's easy to see why DET state is not good to be used as trial wave function. Since there is no analytical methods or efficient numerical methods to get an exact decomposition, "Analytical Decomposition" (though is not analytic) is the best decomposition we have now. But it definitely can be improved when this method applied to other detailed system.

Another thing we want to mention is that due to the proof above, this new pseudo-BCS S.C. CPMC only work in $N_{spin_{up}} = N_{spin_{dn}}$ and 'part of spin symmetry' system.

2.3

If pseudo-BCS state is applied as trial wave function, there is some change form DET trial wave function CPMC:

%%
and Back propagation is mentioned in Ettore's recent work.
%%

3 Result

There are some results to show the behavior of pseudo-BCS S.C. CPMC.

%%compare with Shi Hao's results (work better at low U system, exact input can't leads to exact results)

%%compare with Mingpu's results (may also work at symmetry break system, independent of initial input and converge soon)

%%results in t' model

4 Summery

In summary, we have developed a new "Green Function to wave function" method which allowed many "wave function input-quantities output algorithm" to be applied to a self-consistent frame. By doing this to CPMC, many results has been improved and this new S.C. CPMC allowed us to touch farther field which we can't do before.

The decomposition method is not optimal, which means many other optimal method like Machine Learning may improve it and lead to better results. So this paper also gives a new optimal problem, solving this problem will give a meaningful improvement to many numerical algorithm.