Self Consistent CPMC with pseudo-BCS state

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1 Introduction

One of the important way to understanding quantum system is numerical simulating. 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 solve 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 an almost 'non-cost' algorithm which can be used to extract full information from output Green function (Density Matrix) to construct a wave function and input this wave function as trial wave function to CPMC calculation or in another view point, this new method now allow CPMC to use Green Function (Density Matrix) as a constrain rather than trial wave function. 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 optimized results with heat bath and luck by iteration.

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

$$H = -t \sum_{j,\delta,\sigma} c^{\dagger}_{j,\sigma} c_{j+\delta,\sigma} + U \sum_{j} n_{j,up} n_{j,dn}$$

where $c^\dagger_{j,\sigma}$ ($c^\dagger_{j,\sigma}$) creates (annihilates) an electron with spin σ ($\sigma = up, dn$) at lattice site j and δ connects two nearest neighbor sites or other sites which depends on detailed system, $n_{j,\sigma} \equiv c^\dagger_{j,\sigma} c_{j,\sigma}$.

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.

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.

2.1 Theoretical derivation

Instead of DET state in normal CPMC, we are using BCS state as trial wave function to do it. BCS state pairing wave function with N_{spin} paired particles can be written as

$$BCS(F) = \underbrace{\psi^\dagger ... \psi^\dagger}_{N_{spin}} |0>$$

where

$$\psi^\dagger \equiv \sum_{i,j} f_{i,j} c^\dagger_i(up) c^\dagger_j(dn)$$

and $N_{spin_{up}} = N_{spin_{dn}} \equiv N_{spin}$ is the number of pairs, $|0>$ is empty state.

In principle, $F = \{f_{i,j}\}$, a $Nsite$ by $Nsite$ matrix, has some constraints in BCS definition, for example $f_{i,j} = f_{j,i}$. Now, let's get rid of these constraints (F can be any matrix) and define it as pseudo-BCS state $BCS(F)$.

Theory: For any Green Function $G_{i,j,\delta} = \frac{<BCS|C^\dagger_{i,\delta} C^\dagger_{j,\delta}|BCS>}{<BCS|BCS>}$ with $N_{pin_{up}} = N_{spin_{dn}}$ and 'part of spin symmetry', there exist a pseudo-BCS state F which has Green function G' such that G' can approach or equal to G

Proof: For any Green Function G, by eigenvalue decomposition, we can get

$$G_{i,j,\delta} = \frac{< BCS|C^\dagger_{i,\delta} C^\dagger_{j,\delta}|BCS >}{< BCS|BCS >} = \{T_\delta \lambda_\delta T^\dagger_\delta\}_{i,j}$$

where $\lambda_{up} = \lambda_{dn} \equiv \lambda$ (This additional requirement called "part of spin symmetry") is diagonalized eigenvalue matrix and T is eigenvectors.

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

For diagonalized BCS state F,

$$BCS(F) = \prod (\sum_{i,j} f_{i,j} C^\dagger_{i,up} C^\dagger_{j,dn})$$

$$= \sum_{k_1,k_2...k_{Nspin}} (\lambda_{k_1}\lambda_{k_2}...\lambda_{k_{Nspin}} C^\dagger_{k_1,up} C^\dagger_{k_1,dn} C^\dagger_{k_2,up} C^\dagger_{k_2,dn} ... C^\dagger_{k_{Nspin},up} C^\dagger_{k_{Nspin},dn})|0>$$

where k is a set of non-repetitive sample of $1, 2, ...Nsite$ ($Nsite$: the number of latice sites). it's easy to see that $C^\dagger_{k_1,up} C^\dagger_{k_1,dn} C^\dagger_{k_2,up} C^\dagger_{k_2,dn} ... C^\dagger_{k_{Nspin},up} C^\dagger_{k_{Nspin},dn}$ is a DET state with DET matrix $D_{i,j} = 1$ for every $i = k_j$ and $D_{i,j} = 0$ for others.

Now, the Green Function G' of $BCS(F)$ is: $G'_{ij,\delta} = \frac{<BCS|C^\dagger_{i,\delta} C^\dagger_{j,\delta}|BCS>}{<BCS|BCS>}$

If $i \neq j < BCS|C^\dagger_{i,\delta} C^\dagger_{j,\delta}|BCS >= 0$, since the unpaired state

$$C^\dagger_{i,\delta} C^\dagger_{j,\delta} (C^\dagger_{k_1,up} C^\dagger_{k_1,dn} C^\dagger_{k_2,up} C^\dagger_{k_2,dn} ... C^\dagger_{k_{Nspin},up} C^\dagger_{k_{Nspin},dn})|0>$$

can't be found in $< BCS|$.

If $i = j$, then

$$< BCS|C^\dagger_{i*} C^\dagger_{i*} (C^\dagger_{k_1,up} C^\dagger_{k_1,dn} C^\dagger_{k_2,up} C^\dagger_{k_2,dn} ... C^\dagger_{k_{Nspin},up} C^\dagger_{k_{Nspin},dn})|0 >\neq 0$$

if and only if there exist some $k_j = i$, and

$$G_{ii*} = \frac{N_{spin} \sum_{k_1,k_2...k_{Nspin}, \exists k_j = i} (\lambda_{k_1}\lambda_{k_2}...\lambda_{k_{Nspin}})^2}{\sum_{k_1,k_2...k_{Nspin}} (\lambda_{k_1}\lambda_{k_2}...\lambda_{k_{Nspin}})^2}$$

For diagonalized G and G', $G_{i,i} = G'_{i,i}$ gives us a "$Nsite$ variable equation set". this equation set may have analytic or numerical exact solution with low computation complexity, but is hard to find out. So that, we give some almost 'non-cost' approximate solutions which let G approach to G' good enough at most of the cases .

By applying linear transformation T to basis $C^\dagger$ 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 Concrete Steps

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

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

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

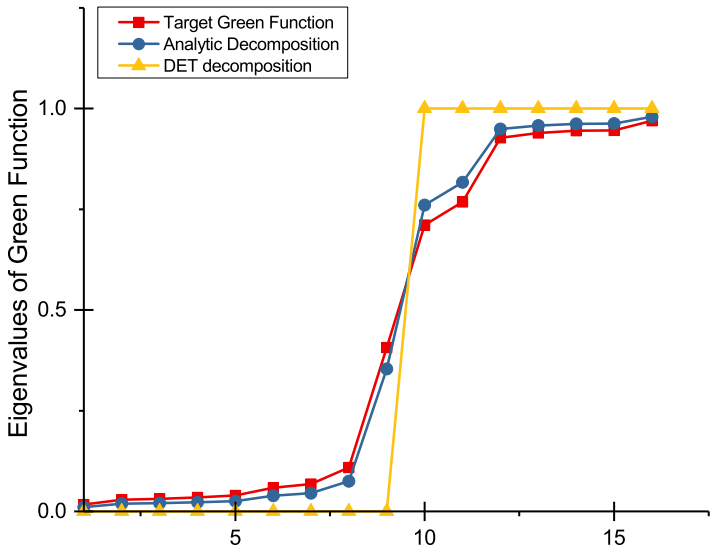
3. There are two kind of f:

1st, DET decomposition: $A_{ii} = 1$ if λ_{ii} is larger or equal to the Nspin-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 , Analytic 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 $G' = G$.

Figure 1: The comparison of two different decomposition methods in trying to fit a Green Function. (From the steps above, they all have the same eigenvectors, so we show their difference in eigenvalues.) This is a real situation for 4 by 4 system. The eigenvalues of green function vs. the order sorted by corresponding eigenvalues.



The decomposition method then become the key of this self-consistent CPMC procedure. if we choose "DET decomposition", the pesudo-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 analytic methods or efficient numerical methods to get an exact decomposition, "Analytic Decomposition" (though is not analytic) is the best decomposition we have now. But it definitely can be improved when this method applied to some detailed system. In FIG.1, we give a briefly comparison for these two decomposition method to give a brief idea about what those decomposition methods going to do and how it works to improve the approximation.

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

2.3 Technical detail

If pesudo-BCS state is applied as trial wave function, there are some changes from "DET trial wave function CPMC" to "pseudo-BCS trial wave function CPMC":

$$< BCS|\phi >= det(A) \equiv det[\phi_{up}^T \cdot F \cdot \phi_{dn}^T]$$

$$\frac{< BCS|c_{(i,up)}c_{(j,up)}^\dagger|\phi >}{< BCS|\phi >} = \delta_{i,j} - [F \cdot \phi_{dn} \cdot A^{-1} \cdot \phi_{up}^T]_{j,i}$$

and Back propagation, $< BCS|n_i n_j|\phi >$ is mentioned in Ettore's recent work.

3 Result

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

First we use the one-band two-dimensional Hubbard model at density $n = 0.875$ as a general test case. The hopping matrix element δ is t for nearest neighbors and 0 otherwise. These parameters regime suffer a severe fermion sign problems and its ground state in the thermodynamic limit still remains unknown.

In FIG.2 we shows our results in different system size, U, boundary condition and initial trial wave function where exact diagonalization can be done to produce a effective comparison. In most of the situation, especially in small U system, these iterations give a significant improvement with no need to worry about trial wave function and some high accuracy has never been achieved before.

system	twist	input	decomposition method	BK/FW	walker	First step Energy	last 10 Ave Energy (20)	STDEV	Exact Energy	Error %
4477 u=4	(0.01,0.02)	FS	Analytic	BK	5*20*400	-15.84913641	-15.73447318	0.00939435	-15.7660493	-0.200279211
4477 u=4	(0,0)	FS	Analytic	BK	5*20*400	-15.59054106	-15.80229278	0.00579164	-15.744	0.370253929
4477 u=8	(0.01,0.02)	FS	Analytic	BK	5*20*400	-12.21852041	-12.05883613	0.03900853	-11.875287	1.545639529
4477 u=12	(0.01,0.02)	FS	Analytic	BK	5*20*400	-10.52874468	-9.930954499	0.03652032	-10.0543472	-1.2275721
481414 u=4	(0,0)	FS	Analytic	BK	5*20*400	-32.98997521	-33.07668737	0.01128522	-33.07906	-0.007172596
481414 u=4	(0,0)	HF	Analytic	BK	5*20*400	-32.92587081	-33.08020118	0.01004941	-33.07906	0.003449868
481414 u=8	(0,0)	FS	Analytic	BK	5*20*400	-24.71696699	-24.5391534	0.05011579	-24.6466022	-0.435957817
481414 u=12	(0,0)	FS	Analytic	BK	5*20*400	-21.01461539	-20.38908399	0.14362547	-20.7342593	-1.664758335
481414 u=12	(0,0)	HF	Analytic	BK	5*20*400	-20.11042073	-20.50122603	0.14387467	-20.7342593	-1.123904484
481414 u=4	closeopen	FS	Analytic	BK	5*20*400	-31.73779671	-31.84122779	0.00813382	-31.8609612	-0.061935865
481414 u=6	closeopen	FS	Analytic	BK	5*20*400	-26.80875277	-26.85017159	0.01969928	-26.824331	0.096332543
481414 u=8	closeopen	FS	Analytic	BK	5*20*400	-23.70888722	-23.48018192	0.04850598	-23.5659952	-0.364097846
4122121 u=4	closeopen	FS	Analytic	BK	5*20*400	-48.38039308	-48.44568123	0.01159463	-48.4397	0.012347778
4122121 u=6	closeopen	FS	Analytic	BK	5*20*400	-40.87697676	-40.92933387	0.02786377	-40.779	0.368655117
4122121 u=8	closeopen	FS	Analytic	BK	5*20*400	-36.11903901	-35.76470789	0.05742049	-35.8133	-0.135681734

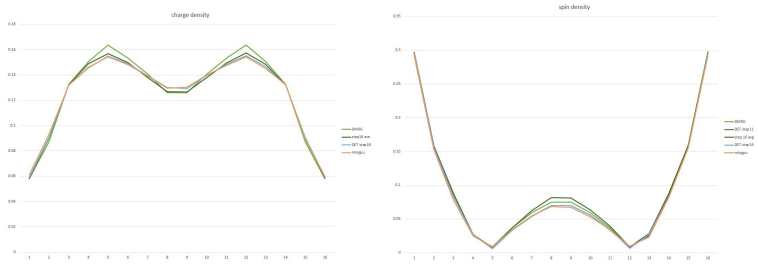
Figure 2: The comparison between "exact ground state energy", results from normal CPMC (first step results), results from pesudo-BCS S.C. CPMC in different system size, U, twist Boundary Condition 2D nearest hopping one band Hubbard model.

In FIG.3, we zoom in a typical iteration procession which shows the behaviors of this two decomposition methods.

In FIG.4, we give a comparison to Mingpu's work before in the 4 by 16 system with the same pinning field . DMRG are supposed to give a exact

Figure 3: The comparison between two detail iteration curves from pesudo-BCS S.C. CPMC with two different decomposition methods. Ground state energy vs. the number of iteration steps.

results about this system's magnetic order. DET decomposition and Mingpu's methods converge to each other but still can't gives a good approximation for the saddle part of charge density. Analytic Decomposition improve the results and match this saddle point well.



(a) (b)

Figure 4: The comparison between pesudo-BCS S.C. CPMC and Mingpu's results. Absolute value of charge density along the y-direction vs. site label. The right panel plots the corresponding spin density.

In FIG.5 we apply our methods to t' model %% which can't be touched by CPMC before (can't even give a description of what state it is). The consensus about its phase transition behavior in the thermodynamic limit still going on and the key point is there is no good enough numerical algorithm can locate a accurate phase transition point within the range of 0.5. DMRG is supposed to give a good approximation in small one-Dimension-like system, so results of DMRG is used as Exact results, and we compare it with Analytic Decomposition, DET decomposition to shows it is now possible for us to use S.C. CPMC in this problem. The following formal research about this t' problem with S.C. CPMC will come out later.

4 dicussion

When this method be applied into large U system, the most important reason why it won't work well like small u system is because CPMC can't give an exact enough estimation of Green Function in large U system which in most of this situation, some of the eigenvalues may be larger than 1. And in some of this large U system, DET decomposition work better than Analytical decomposition

And since it is not a exact decomposition, in FIG.6, an exact input Green Function won't give an exact result. So there is always an error for this iteration.

Fortunately, there are many ways to improve this S.C. CPMC if it is applied in some detailed system, for example: releasing the constrain for a while, modifying Green Function due to certain symmetry or other information and finding a better decomposition method.

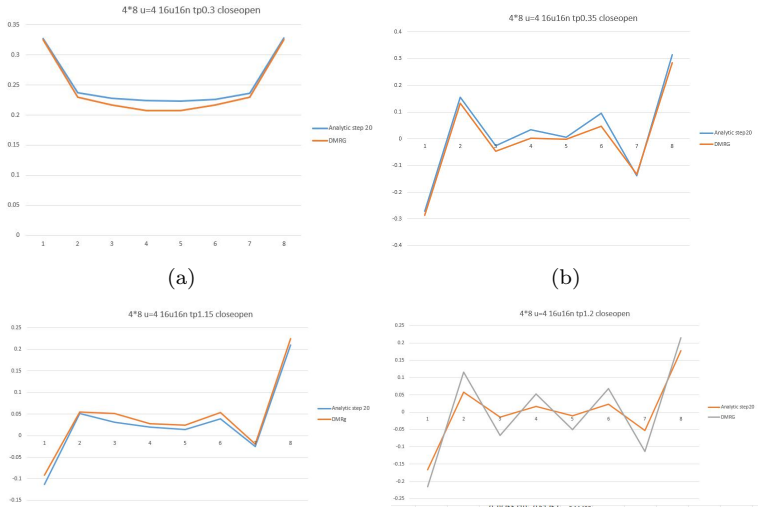


Figure 5: The absolute value of spin density in $U = 4$ half-filling t' model treated by normal CPMC, pesudo-BCS S.C. CPMC with different decomposition method and DMRG (supposed to be exact results). Spin density along the y-direction vs. site label.

system	twist	input	decomposition method	BK/FW	walker	Energy	STDEV	Exact Energy	Error %	converge (20)
4477 u=4	(0,0)	non_twist Exact first=0.44 other 0.4375	Analytic	BK	5×20×400	-15.76565116	0.021297804	-15.744	-0.13752008	-15.80694989
4477 u=4	(0,0)	non_twist Exact first=0.44 other 0.4375	DET	BK	5×20×400	-15.65028647	0.012408288	-15.744	0.595233307	-15.64890772
4477 u=8	(0.01,0.02)	twist Exact first=0.44 other 0.4375	Analytic	BK	5×20×400	-11.87328862	0.070350113	-11.875287	0.016828014	-12.05354462
4477 u=8	(0.01,0.02)	twist Exact first=0.44 other 0.4375	DET	BK	5×20×400	-11.75788655	0.034641026	-11.875287	0.988611459	-11.97751391
4477 u=12	(0.01,0.02)	twist Exact first=0.44 other 0.4375	Analytic	BK	5×20×400	-10.04566011	0.126862648	-10.054347	0.086401341	-9.85424718

Figure 6: an exact input Green Function won't give you a exact result and here a little modification about the Exact Green Function is needed to maybe break the degenercy

5 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.