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In this paper, we show a numerical "decomposition method" to extract information in Green Function (or called Density Matrix) to construct a wave function. Constrain Path Monte Carlo (CPMC) use constraint to control the sign problem in strongly correlated fermion systems. Here, we apply this "decomposition method" to CPMC and with self-consistency we give a new S.C. CPMC algorithm which can systematically improve the constraint from the Green Function of last iteration. The behavior of this new S.C. CPMC is demonstrated in 2-D Hubbard Model. Detailed comparisons are made with exact diagonalization results and other S.C. CPMC. Moreover, some model become possible to calculate which are otherwise beyond reach in CPMC framework.

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I. 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 Quanrum Monte Carlo (QMC)[**?**], which it's possible for classical computer to chase exponential scale and get the estimation of some physical quantities in principle.

However, phase problems in Fermion system prevent the convergence of QMC. The most effective approach to deal with phase problem is by 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, Constrain Path Monte Carlo (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 (or called 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 as a constrain rather than trial wave function. So that, CPMC, as an 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:

$$H = \sum_{j,\delta,\sigma} -t_{j,j+\delta} c^\dagger_{j,\sigma} c_{j+\delta,\sigma} + U \sum_j n_{j,up} n_{j,dn}$$

where $c^\dagger_{j,\sigma}$ ($c^\dagger_{j,\sigma}$) creates (annihilates) an electron with

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

II. 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 HF). 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.

A. Theoretical derivation

Instead of using DET state (Slater Determinate) in normal CPMC, we choose pesudo-BCS state as trial wave function. 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 ($Nsite$ is the number of lattice sites), has some constraints in the definition of BCS state, 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 $pBCS(F)$.

Theory: For any Green Function

$$G_{i,j,\delta} = \frac{<\psi|C^\dagger_{i,\delta} C_{j,\delta}|\psi>}{<\psi|\psi>}$$

with $N_{pin_{up}} = N_{spin_{dn}}$ and 'part of spin symmetry', there exist a pseudo-BCS state $pBCS(F)$ 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

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

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 matrix F, such that the Green Function G' of this pseudo-BCS state $pBCS(F)$ is G or at least the error can be minimized.

For diagonalized matrix F,

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

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

where k is a set of non-repetitive sample of $1, 2, ...Nsite$.

it's easy to see that $C^\dagger_{k_1,up} C^\dagger_{k_1,dn} ... C^\dagger_{k_{Nspin},up} C^\dagger_{k_{Nspin},dn}$ 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 $pBCS(F)$ is:

$$G'_{ij,\delta} \equiv \frac{<pBCS|C^\dagger_{i,\delta} C_{j,\delta}|pBCS>}{<pBCS|pBCS>}$$

If $i \neq j$, then $<pBCS|C^\dagger_{i,\delta} C_{j,\delta}|pBCS> = 0$, since this new paired state

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

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

If $i = j$, then

$$<pBCS|C^\dagger_{i,\delta} C_{i,\delta} (C^\dagger_{k_1,up} C^\dagger_{k_1,dn} ... C^\dagger_{k_{Nspin},up} C^\dagger_{k_{Nspin},dn})|0> \neq 0$$

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

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

For diagonal matrix G and G', $G_{i,i} = G'_{i,i}$ gives us a "$Nsite$ variable equation set". This equation set may have analytic solution with low computation complexity, but is hard to find out. Two 'almost non-cost' approximate solutions are given 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'.

B. 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}, eigenvalue matrix λ (in the system with "part of spin symmetry", $\lambda_{up} = \lambda_{dn} \equiv \lambda$).

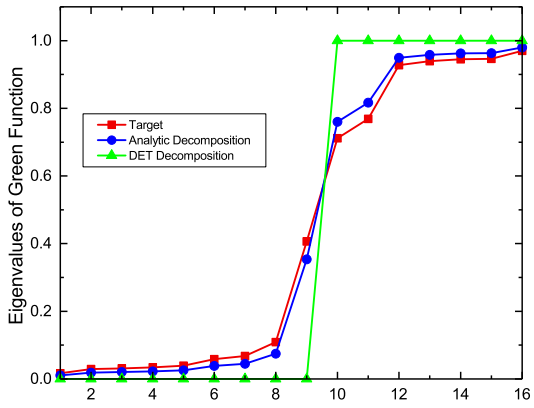
2. The new pseudo-BCS trial wave function F is $F = T^{\dagger}_{up} A T_{dn}$ where $A \equiv f(\lambda)$ is diagonalized matrix.

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. This is the exact decomposition for pseudo-HFB state (with the same definition as pseudo-BCS state), which means in some grand canonical ensemble system, this decomposition is the exact solution for $G = G'$.

FIG. 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 nearest-hopping Hubbard system. The eigenvalues of green function vs. the order sorted by corresponding eigenvalues.



The decomposition method is the key of this self-consistent CPMC procedure. if we choose "DET decomposition", the pesudo-BCS reduce to DET state and it is 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 are going to do and how it works to improve the approximation. And In TABLE.II, we shows this improved approximation indeed improve the results of CPMC with Exact Green Function input.

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.

C. 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":

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

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

and Back propagation, $< pBCS|n_i n_j|\phi >$ is mentioned in Ettore's recent work[**?**]. (ϕ is the DET state, F is the matrix in $pBCS(F)$)

III. RESULTS

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.

TABLE.I, 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.

In FIG.2, we zoom in a typical iteration procession which shows the behaviors of this two decomposition methods.

In FIG.3, we give a comparison to Mingpu's work[**?**] in the 4 by 16 system with Pinning Field Boundary Condition [**?**] (In this paper, we choose the same Pinning Field B.C. as Mingpu). DMRG are supposed to give an exact 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.

In FIG.4 we apply our methods to t' Hubbard model[**?**] (t for nearset-hopping and t' for second-nearest hopping) 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

L	(N_{up},N_{dn})	U/t	B.C.	initial input	CPMC	S.C. CPMC	STDEV	Exact	Error %
4*4	(7,7)	4	(0.01,0.02)	FS	-15.8491	-15.73447318	0.009394346	-15.766049	-0.20027921
4*4	(7,7)	4	(0,0)	FS	-15.5905	-15.80229278	0.00579164	-15.744	0.370253929
4*4	(7,7)	8	(0.01,0.02)	FS	-12.2185	-12.05883613	0.039008527	-11.875287	1.545639529
4*4	(7,7)	12	(0.01,0.02)	FS	-10.5287	-9.930954499	0.036520317	-10.054347	-1.22725721
4*8	(14,14)	4	closeopen	FS	-31.7378	-31.84122779	0.008133821	-31.860961	-0.06193586
4*8	(14,14)	6	closeopen	FS	-26.8088	-26.85017159	0.019699276	-26.824331	0.096332543
4*8	(14,14)	8	closeopen	FS	-23.7089	-23.48018192	0.048505975	-23.565985	-0.36409785
4*12	(21,21)	4	closeopen	FS	-48.3804	-48.44568123	0.011594626	-48.4397	0.012347778
4*12	(21,21)	6	closeopen	FS	-40.877	-40.92933387	0.027863773	-40.779	0.368655117
4*12	(21,21)	8	closeopen	FS	-36.119	-35.76470789	0.057420491	-35.8133	-0.13568173

TABLE I. 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.

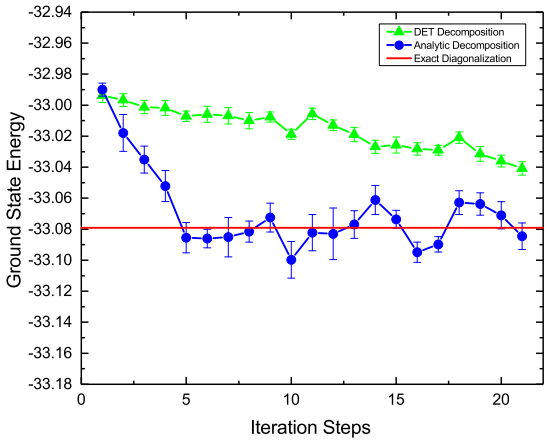


FIG. 2. 4*8, $U = -4$, $Nspin_{up} = Nspin_{dn} = 14$, P.B.C., nearest-hopping Hubbard Model. The comparison between two detail iteration curves from pesudo-BCS S.C. CPMC with two different decomposition methods. Ground state energy vs. the number of iteration steps.

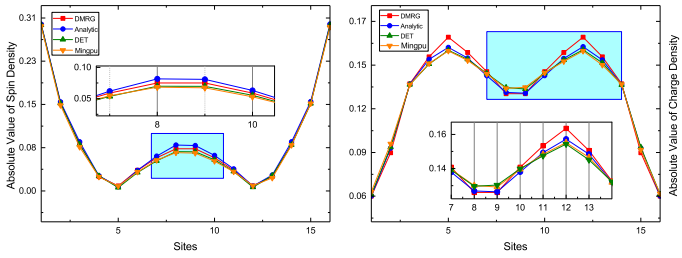


FIG. 3. 4*16, $U = -4$, $Nspin_{up} = Nspin_{dn} = 28$, Pinning Field B.C., nearest-hopping Hubbard Model. The comparison between pesudo-BCS S.C. CPMC and Mingpu's results. Absolute value of spin density ($< n_{i,up} - n_{i,dn} > /2$) along the y-direction vs. site label. The right panel plots the corresponding charge density ($1- < n_{i,up} + n_{i,dn} >$).

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 dealing with this problem. The following formal research about this t' problem with S.C. CPMC will come out later.

IV. 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. In some of this large U system, DET decomposition work better than Analytical decomposition

And since it is not a exact decomposition, in TABLE.II, an exact input Green Function won't give an exact result. So error always exist 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.

V. SUMMERY

In summary, we have developed a new "Green Function to wave function" method which allowed many "wave function input-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 optimal problem, solving this problem will give a meaningful improvement to many numerical algorithm.

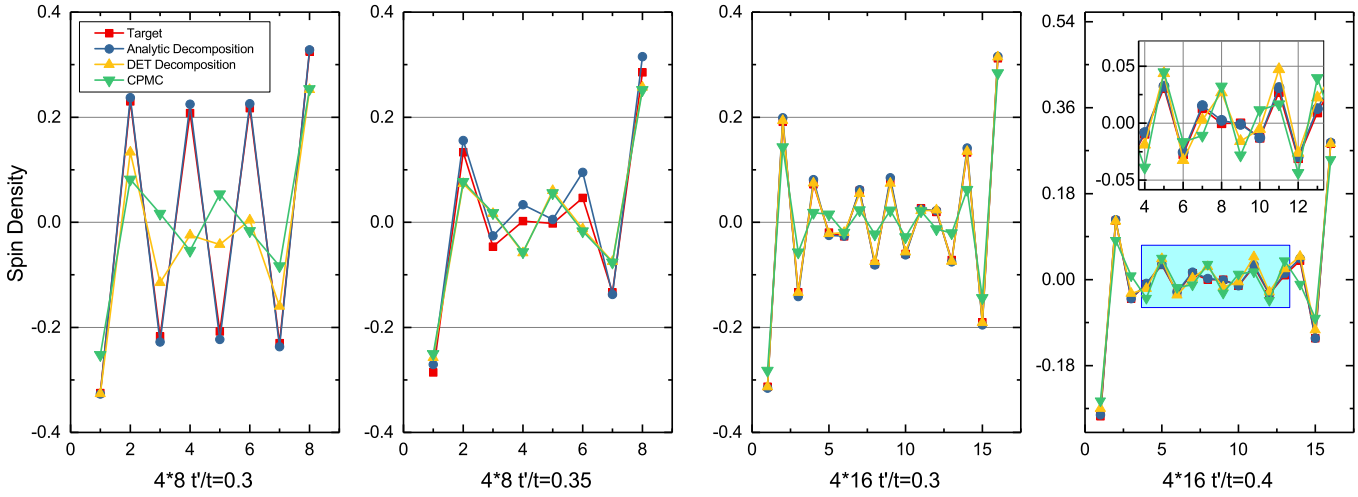


FIG. 4. 4*8 and 4*16, $U = -4$, $Nspin_{up} = Nspin_{dn}$ half-filling, Pinning Field B.C., t' Hubbard Model. Spin density treated by pesudo-BCS S.C. CPMC with different decomposition method and DMRG. Spin density along the y-direction vs. site label.

L	(N_{up},N_{dn})	U/t	Twist B.C.	Decomposition Method	First Step Energy	S.C. CPMC	Exact Energy
4*4	(7,7)	4	(0.01,0.02)	Analytic	-15.7909	-15.70698469	-15.7660493
4*4	(7,7)	4	(0.01,0.02)	DET	-15.68	-15.67964298	-15.7660493
4*4	(7,7)	4	(0,0)	Analytic	-15.7657	-15.80694989	-15.744
4*4	(7,7)	4	(0,0)	DET	-15.6503	-15.64890772	-15.744
4*4	(7,7)	8	(0.01,0.02)	Analytic	-11.8733	-12.05354462	-11.875287
4*4	(7,7)	8	(0.01,0.02)	DET	-11.7579	-11.97751391	-11.875287
4*4	(7,7)	12	(0.01,0.02)	Analytic	-10.0457	-9.85424718	-10.0543472

TABLE II. "First Step Energy" are the results from the first step CPMC calculation in S.C. CPMC with pBCS state as the trial wave function which decomposed from Exact Ground State Green Function by different "Decomposition Method" and "S.C. CPMC" is the converged results in this S.C. calculation. A small modification at Exact Green Function is needed to break the degeneracy.

A. Citations and References

A citation in text uses the command `\cite{#1}` or `\onlinecite{#1}` and refers to an entry in the bibliography. An entry in the bibliography is a reference to another document.