cc-sc-gdqmc

icf

January 2018

1 Green Function Self Consistent for CPMC

The problem will be solved in four steps:

1) Pre-analysis

2) Fortran Program Modification

3) Input/Output

4) Discussion

Notice:
Calculation used these parameters below if no special mention:
Lx=16;
Ly=4;
Lz=1;
N_up=28;
N_dn=28;
kx=0;
ky=0;
kz=0;
U=8;
Nsamples=20 !Nsamples number of sampling do we need in MC process.
Nwalkers=360 * 100 cores !Nwalkers number of walkers
blockstep=1 !blockstep Block number which inidcate the basic size
Thermblock=800 !Thermblock number of blocks do we need in thermal process.
Neqblock=10 !Neqblock number of blocks do we need in equilibrium step(update and measure)

1.1 Pre-analysis

Pinning Field Added.

Using Eigenvector Method to simulate all the Green Functions of CPMC Groundstate with one (Dtot=1) determinate and doing CPMC again with this new Phi_T.:

$$(|PhiT>_{n+1\ n+1}<PhiT|)_{i,j} \approx_n <Phi|C_iC_j|Phi>_n$$

where $|Phi>_n$ is the 'Ground-state' after n_{th} CPMC calculation, $|PhiT>_{n+1}$ is the Slater Determinate with the biggest N_{up} or N_{dn} eigenvectors from Green Function of $|Phi_n>$

1.2 Fortran Program Modification

gdqmc_icf_pin1.2b
gdqmc_icf_pin1.21b

1.3 Input/Output

1.fig;

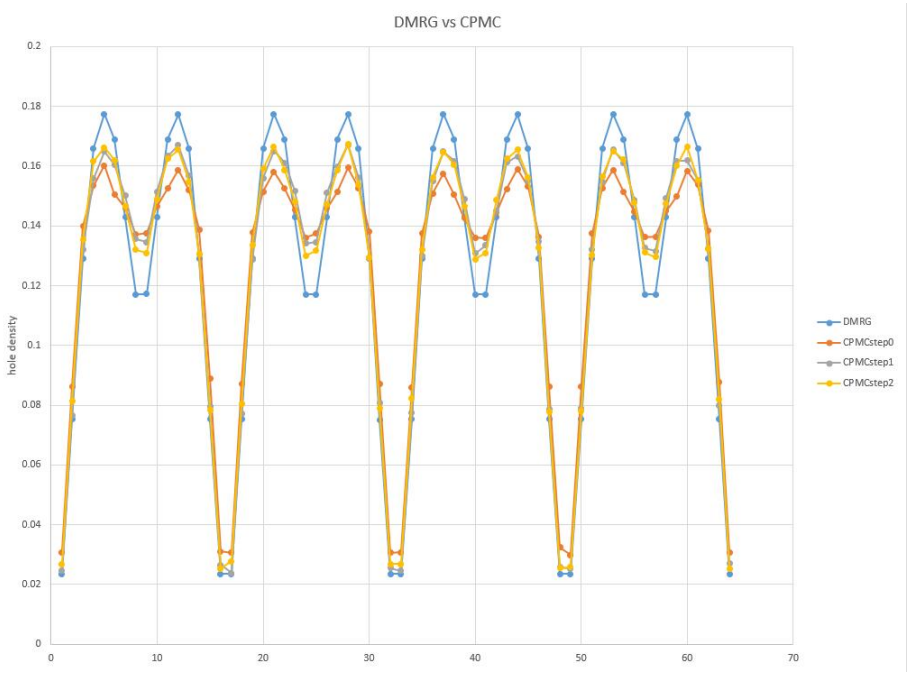

Figure 1: Hole Density $(1 - n_{up} - n_{dn})$: DMRG are referred as standard result; step 0 is a normal cpmc calculation with free electron state $|PhiT>$;step i is the results after i_{th} iteration (self-consist) steps.

2.fig;

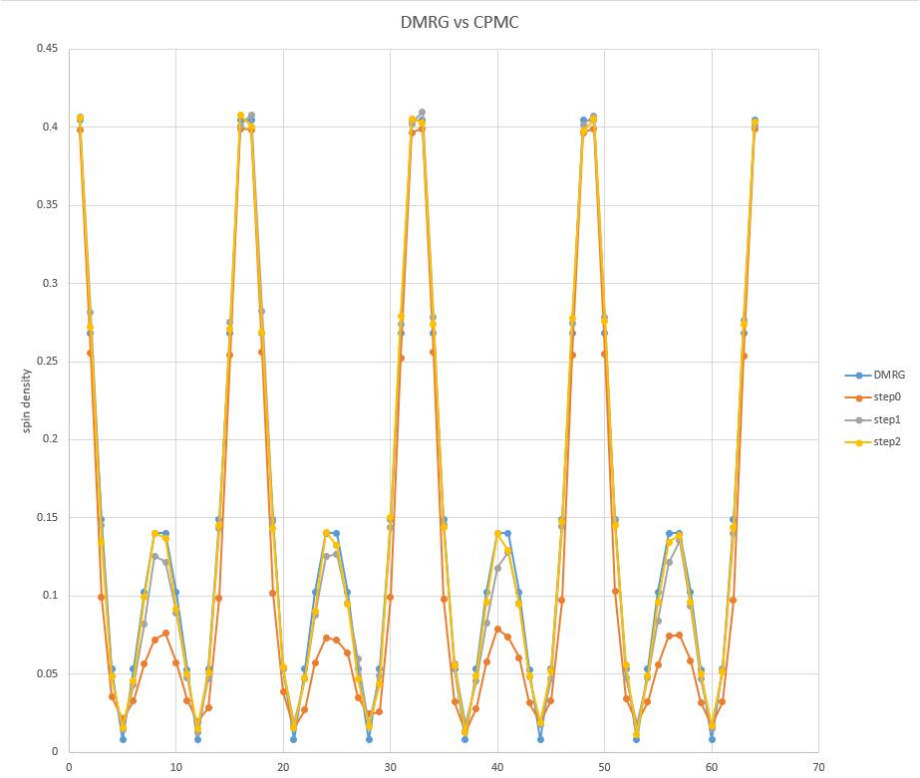

Figure 2: Spin Density ($(-1)^{sitex+sitey} * (n_{up} - n_{dn})$): DMRG are referred as standard result; step 0 is a normal cpmc calculation with free electron state $|PhiT>$;step i is the results after i_{th} iteration (self-consist) steps.

1.4 Discussion

1. There are three methods can be used to get multi-determinate approximation to Green Function

   1) mixed state (with eigenvectors of Green Function)

   2) get an Machine Learning representation of PhiT

   3) pure state variation

2. S.C. CPMC can be used as an adhesive to working with other algorithms

3. S.C. CPMC can be used to get an approximate solution to bigger system with less walkers Example: 4.fig;

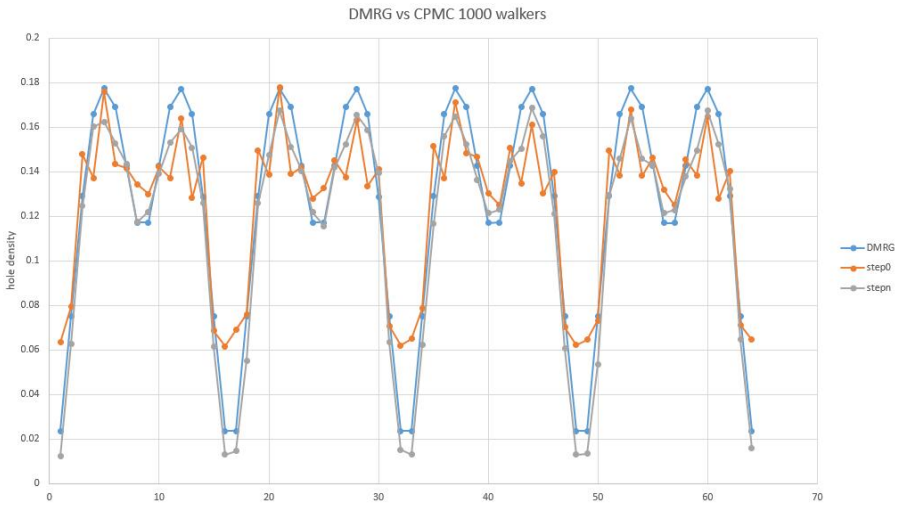

Figure 3: Spin Density $((-1)^{sitex+sitey} * (n_{up} - n_{dn}))$: DMRG are referred as standard result; step 0 is a normal cpmc calculation with free electron state $|PhiT>$;step i is the results after i_{th} iteration (self-consist) steps.

4. In S.C. CPMC all Green Functions have the same eigenvalues!