BCS sc cpmc

icf

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1 BCS 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:
kx=0;
ky=0;
kz=0;
Nsamples=20 !Nsamples number of sampling do we need in MC process.
Nwalkers=400 * 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

Periodic Boundary Condition
Simulating all the Green Functions of CPMC Groundstate with BCS state and doing CPMC again with this new Phi_T.:

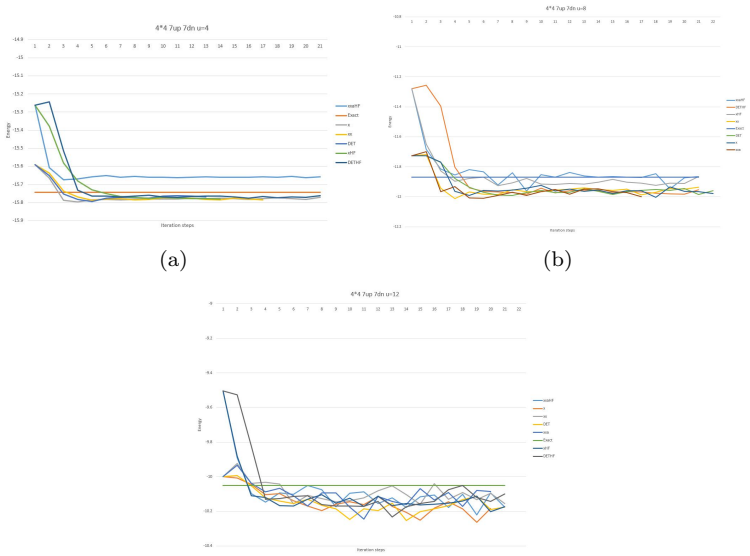
$$< BCS|C_i^\dagger C_j|BCS > \approx_n < Phi|C_i^\dagger C_j|Phi >_n$$

where $|Phi >_n$ is the 'Ground-state' after n_{th} CPMC calculation, $|BCS >$ is the BCS state with specific definition.

1.2 Fortran Program Modification

cpqmc_bcs1.2DET
cpqmc_bcs1.2DETHF
cpqmc_bcs1.2xxa
cpqmc_bcs1.2xxaHF

1.3 Input/Output



(a) (b)

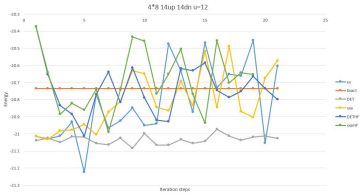
(c)

Figure 1: a) b) c) are results from different SC-CPMC Algorithm "x, xx, xxa, DET" (start with Free Electron State) and "HF" means the SC-CPMC Algorithm start with Hartree-Fock State

1.4 Discussion

1. SC-CPMC have a better behavior at low U system.
2. Different start state will effect the convergence of SC-CPMC.
3. A better approximation will give "at least not worse" results except one case.
4. In S.C. CPMC all Green Functions have the same eigenvalues?

(a) (b)



(c)

Figure 2: a) b) c) are results from different SC-CPMC Algorithm "x, xx, xxa, DET" (start with Free Electron State) and "HF" means the SC-CPMC Algorithm start with Hartree-Fock State