X-Method for CPMC

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1 X-Method for CPMC

The problem will be solved in four steps:

1) Pre-analysis

2) Matlab Program Modification

3) Input/Output

4) Discussion

Notice:
Calculation used these parameters below if no special mention:
Lx=4;
Ly=4;
Lz=1;
N_up=7;
N_dn=7;
kx=0;
ky=0;
kz=0;
U=8;
tx=1;
ty=1;
tz=1;
deltau=0.01;
N_wlk=[100:1:107];
N_blksteps=100;
N_eqblk=5;
N_blk=10;
itv_modsvd=5;
itv_pc=10;
itv_Em=20;
N_y=1;

1.1 Pre-analysis

Using X-Method to simulate all the Green Functions of CPMC_Groundstate with one (N_y=1) or more walkers and doing CPMC again with these new Phi_T (walkers).

Model:

$$|\varphi>=\sum_{\overrightarrow{y}} W*\overrightarrow{y}*(e^{\sum_{i,j,k} y_i*a_{i,j,k}*C_j^\dagger C_k}|\phi_{up}>)\bigotimes(e^{\sum_{i,j,k} -y_i*a_{i,j,k}*C_j^\dagger C_k}|\phi_{dn}>)$$

where $|\phi_*>$ is Slater determinant, $C^\dagger$,C is particles creation and annihilation operators and a, w are variational parameters and the number of variational parameters is linear to $N\_sites^2 * N\_y$. (the size of lattice: N_sites, the number of walkers N_y.)

Many symmetry can be used in the calculation to accelerate this algorithm. In this report, "half-filled" is used.

N_y is the number of walkers and here N_y=1, since it's easier to replace Phi_T in CPMC.

1.2 Matlab Program Modification

batchsample_X_G.m;
CPMC_Lab_G.m;
CPMC_Lab_BP_X.m;
halfK_X.m;
initialization_X.m;
initialization_BP_X.m;
measure_BP_G.m;
stepwlk_AP_G.m;
X_Pickup_G.m;
X_RBM_Energy_X_RBM_G.m;
X_RBM_G_dif.m;
X_RBM_Initialization_Pickup.m;
X_RBM_update_Pickup_G.m;
X_Return_G.m;

1.3 Input/Output

1.fig;

1.4 Discussion

1. This method is iterative and related to renormalization group transformation.

2. Effective variational methods can be applied to improve the efficiency.

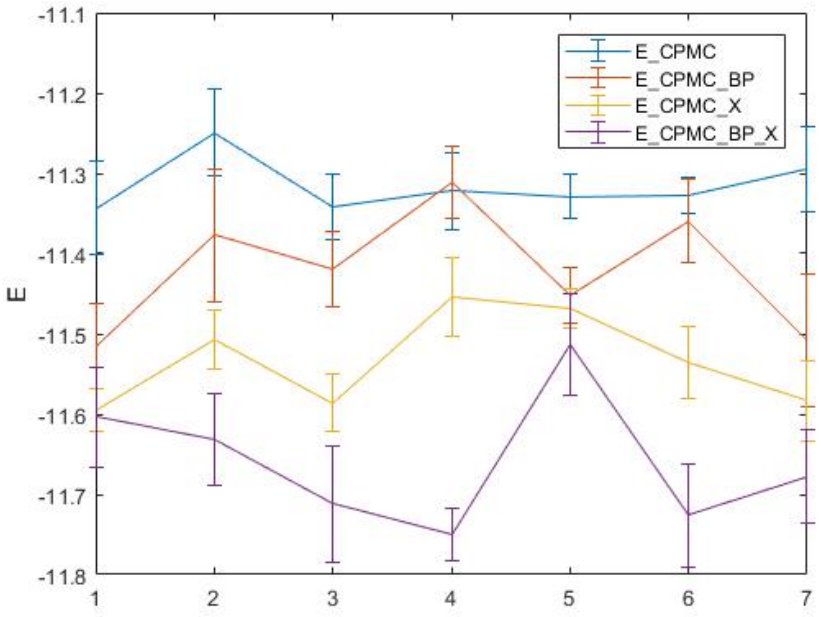

Figure 1: 1.fig; This is 7 times independent calculations of CPMC in 4 different methods; $Lx = 4$,$Ly = 4$,$N\_up = 7$,$N\_dn = 7$,$U = 8$; E_CPMC are the results of normal CPMC, E_CPMC_BP are the results of CPMC with back propagation, E_CPMC_X are the results of CPMC with one-iteration X-Method, E_CPMC_BP_X are the results of CPMC with one-iteration X-Method and back propagation.