Antiferromagnetic State

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1 Antiferromagnetic State

The problem will be solved in five steps:

1) Pre-analysis

2) Matlab Program Modification

3) Input

4) Output

5) Discussion

Notice:
Calculation used these parameters below if no special mention:
Lx=4;
Ly=4;
Lz=1;
N_up=8;
N_dn=8;
kx=0;
ky=0;
kz=0;
tx=1;
ty=1;
tz=1;
deltau=0.01;
N_wlk=300;
N_blksteps=300;
N_eqblk=5;
N_blk=10;
itv_modsvd=5;
itv_pc=5;
itv_Em=30;
N_it=500;
a=0.75;

1.1 Pre-analysis

Model:

$$H = -t \sum_{\{ij\},\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + 0.5 * U \sum_{i} n_{i,\sigma} n_{i,\bar{\sigma}}$$

(This Hubbard Model will present a Antiferromagnetic GroundState, if $U >> t$.)

The normal HF method (Started with Trivial K State) give a bad estimation about GroundState when $U >> t$, so Antiferromagnetic State is used at the beginning of HF method and CPMC.

1.2 Matlab Program Modification

batchsample_itv_Em_BP_s1s_HF.m;
CPMC_Lab_s1s_HF.m;
initialization_HF.m;
stepwlk_AP_s1s.m;

1.3 Input/Output

1.4 Discussion

The difference between $U = 4$ cases is the Trivial State, none of them is exact to the GroundState and gives different results. Both of these two states are eigenstates, since E_BP and E agree with each other (as one of the reasons).

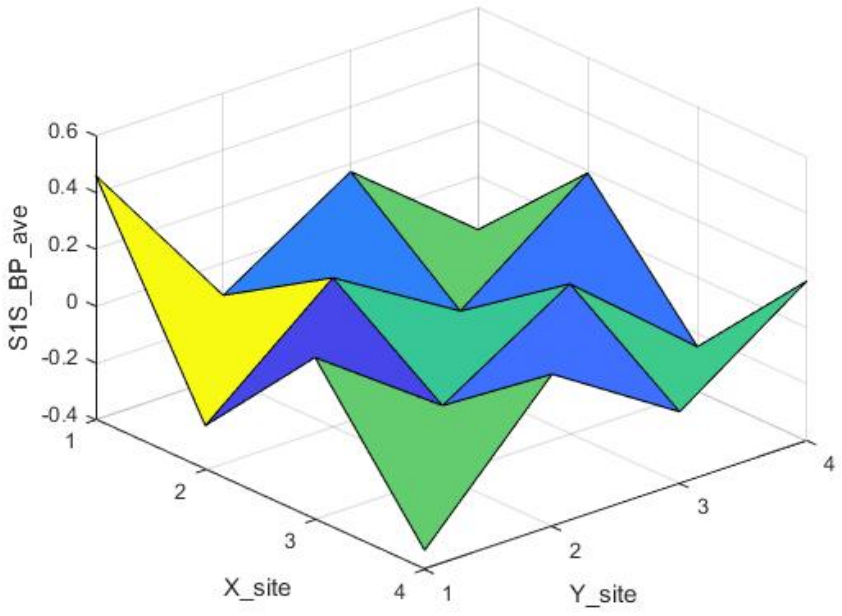

Figure 1: U=4, $< S_1 S_j >$: relative to (1,1), started with Trivial K State. For a small U, localization shows up. E=-12.933, E_BP=-12.977 .

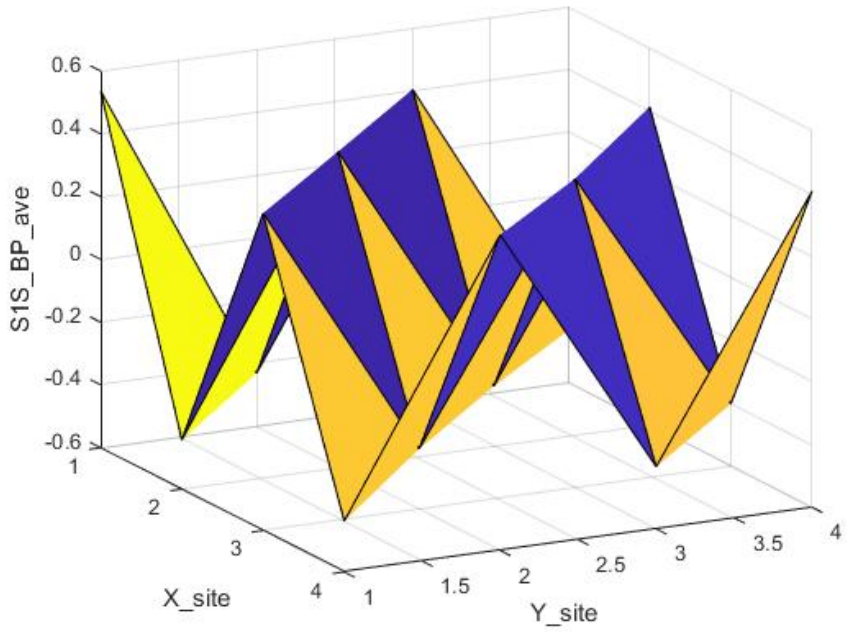

Figure 2: U=4, $< S_1 S_j >$: relative to (1,1), started with Antiferromagnetic State and HF. For a small U, localization shows up. E=-13.488, E_BP=-13.521.
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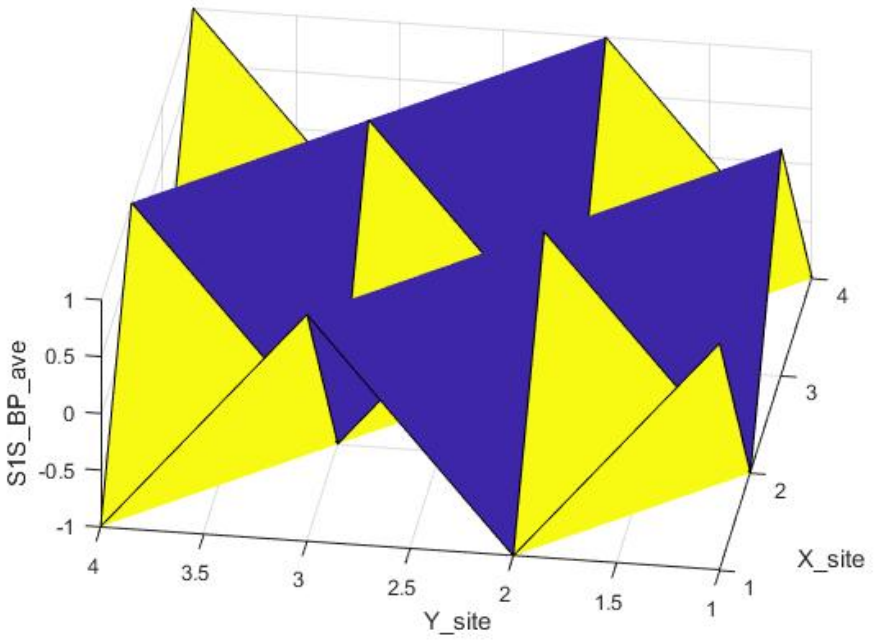

Figure 3: U=99, $< S_1 S_j >$: relative to (1,1), started with Antiferromagnetic State and HF. For a large U, antiferromagnetism shows up. E=-0.652, E_BP=-0.648.