X-Method Variational Function

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1 X-Method Variational Function

The problem will be solved in five steps:

1) Pre-analysis

2) Matlab Program Modification

3) Input/Output

4) Discussion

Notice:
Calculation used these parameters below if no special mention:
kx=0;
ky=0;
kz=0;
tx=1;
ty=1;
tz=1;
U=4;

1.1 Pre-analysis

Model:

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

where $|\phi_*>$ is Slater determinant, n_i is particles number operators and a, w are variational parameters and the number of variational parameters is linear to $N\_sites*N\_y$. (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" (Spin symmetry) is used.

N_y is the number of walkers and the number of walkers in all Normal Variational Method results below is 4 .

1.2 Matlab Program Modification

X_2.m;
Energy_X_RBM3_2.m;
X_RBM_update2_2.m;
X_RBM_Initialzation_2.m;
H_K.m;

1.3 Input/Output

21.jpg;
22.jpg;
23.jpg; 24.jpg;

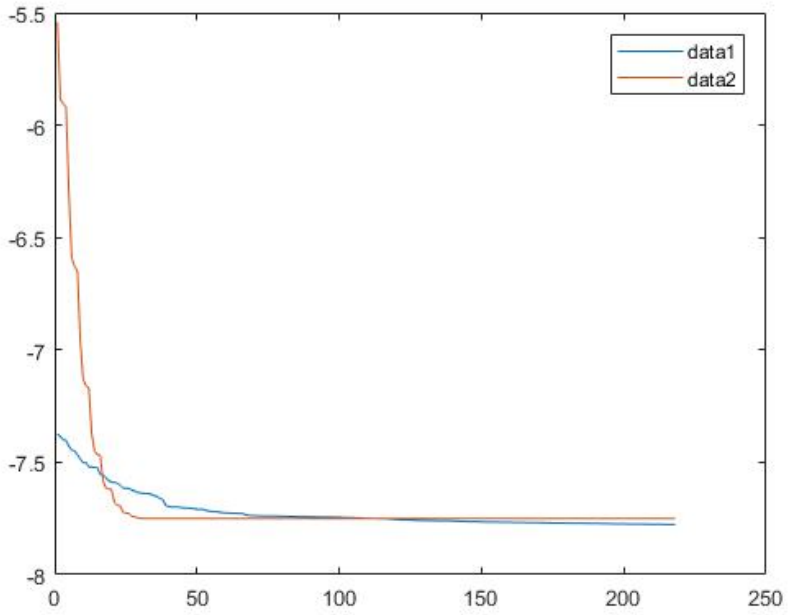


Figure 1: 21.fig; L_x=4,L_y=4,N_up=1,N_dn=1,N_y=4; data1 are X-Method results and data2 are Normal Variational Function results.

1.4 Discussion

1. The Number of walkers is N_y, which can be chosen as an arbitrary integer. According to the calculation, larger N_y leads to more exact result and is better than Normal Variational Method.

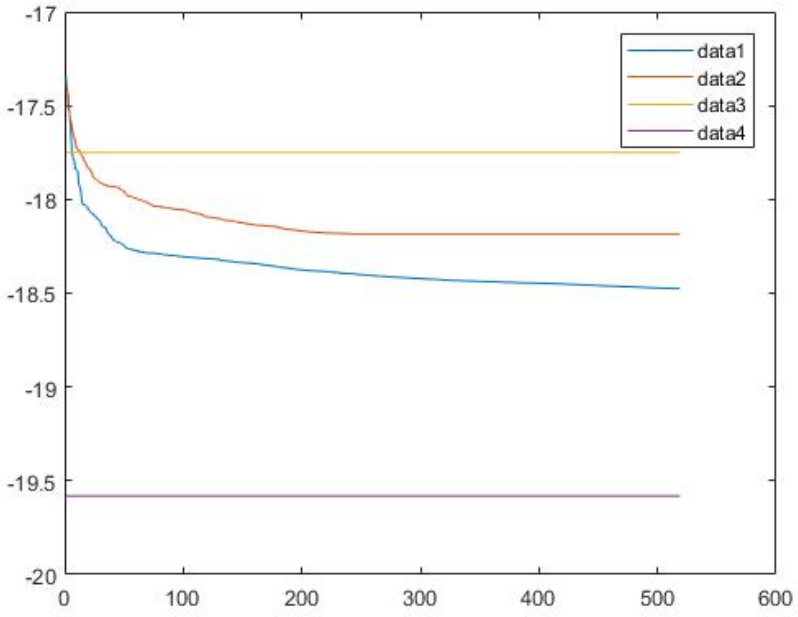
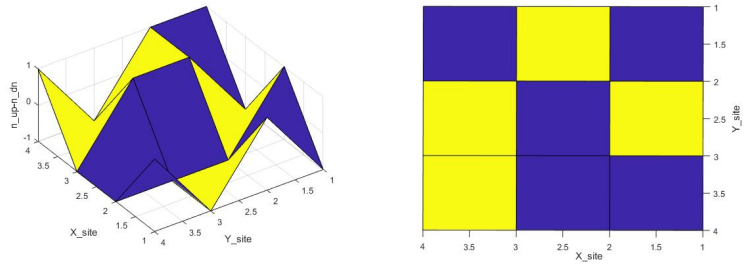


Figure 2: 22.fig; L_x=4,L_y=4,N_up=5,N_dn=5; data1 are X-Method results with N_y=8, data2 are X-Method results with N_y=4, data3 are Normal Variational Function, and data4 is exact result.



(a) (b)

Figure 3: 23.jpg, 24.jpg; L_x=4,L_y=4,N_up=8,N_dn=8,N_y=4,U=99; Spin Density of X-Method Variational Function results: can somehow capture the structure of Ground-State.

2. This Method is less depend on initial state which can get much better result in large U system with Trivial K States than Normal Variational Method.

3. This method can somehow capture the structure of Ground-State which is important to be used as Initial Wave Function in CPMC.

4. However, the variational field is not such smooth which means a clever Variational Method is needed.