Back Propagation and Exact Diagonalization

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1 Back Propagation and Exact Diagonalization

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=2;
Ly=2;
Lz=1;
N_up=1;
N_dn=1;
kx=0;
ky=0;
kz=0;
U=4;
tx=1;
ty=1;
tz=1;
deltau=0.01;
N_wlk=100;
N_blksteps=[100:100:1000];
N_eqblk=5;
N_blk=10;
itv_modsvd=5;
itv_pc=5;
itv_Em=[10:10:100].

1.1 Pre-analysis

N_up=1 and N_dn=1 is used because in this situation commutation relation of Fermions can be ignored and it is easier to programming.

1.2 Matlab Program Modification

batchsample_itv_Em_BP_ED.m;
CPMC_Lab_ED.m;
initialization_ED.m.

1.3 Input/Output

3.1.mat; 3_1.jpg; 3_2.jpg; 3_3.jpg; 3.2.mat; 3_4.jpg; 3_5.jpg; 3_6.jpg;

1.4 Discussion

The error of back propagation method is from the difference between $e^{itv\_Em*deltau*H}$ and $\sum W_i * B_i$ which is the QMC estimation of $e^{itv\_Em*deltau*H}$ and is hard to corrected by increasing itv_Em*deltau.

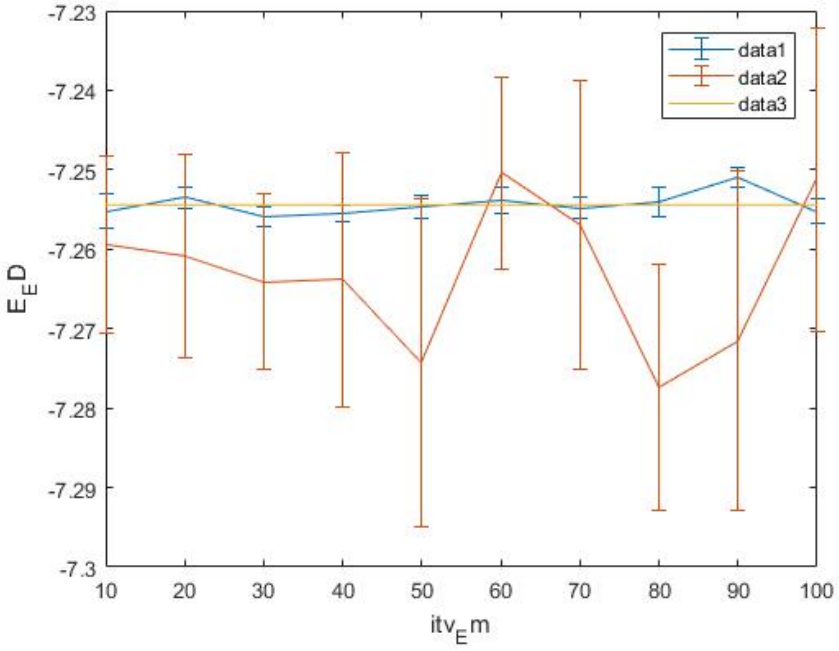


Figure 1: Data 1 is mixed Groundstate Energy, Data 2 is Back Propagation Ground State Energy, Data 3 is Exact Diagonalization Back Propagation Energy. itv_Em*deltau is the length of back propagation and the length of detect distance.

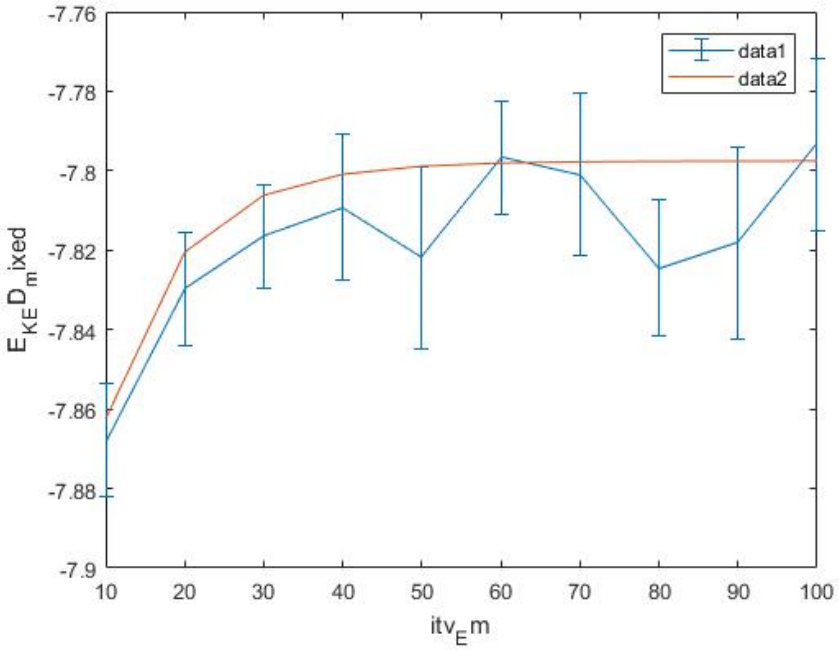


Figure 2: Data 1 is Back Propagation Kinetic Energy, Data 2 is Exact Diagonalization Back Propagation Kinetic Energy. itv_Em*deltau is the length of back propagation and the length of detect distance.

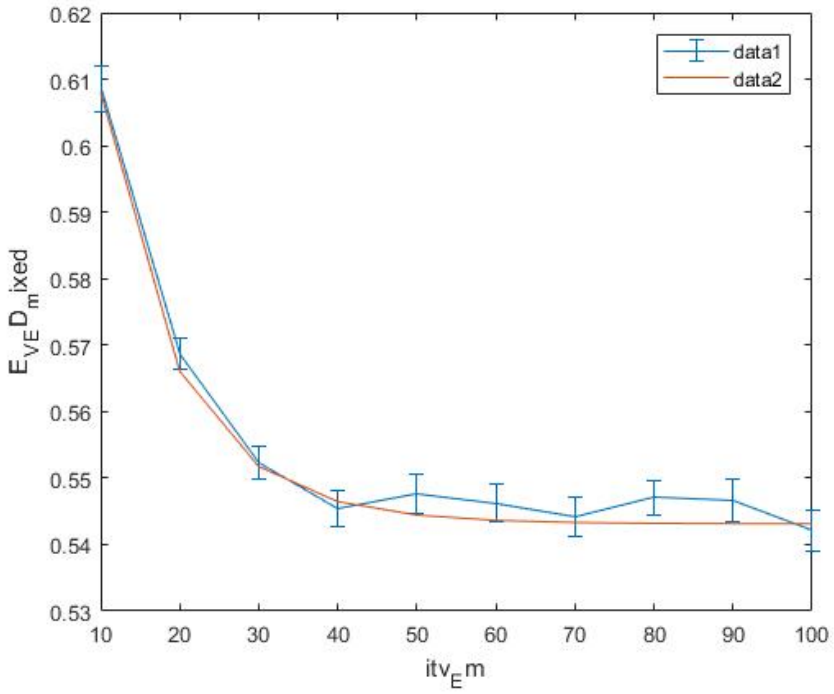
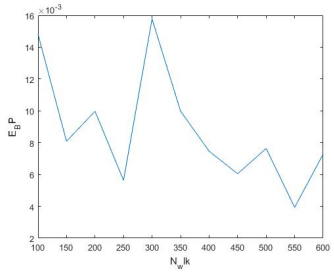
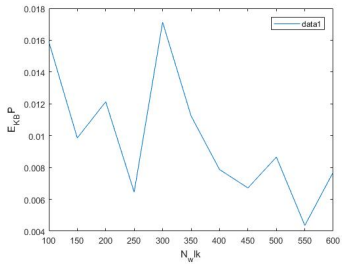


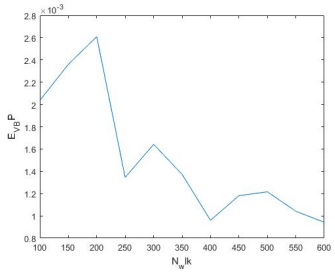
Figure 3: Data 1 is Back Propagation Potential Energy, Data 2 is Exact Diagonalization Back Propagation Potential Energy. itv_Em*deltau is the length of back propagation and the length of detect distance.



(a) The Y axis is the error bar of Back Propagation Groundstate Energy and the X axis is the number of walker.

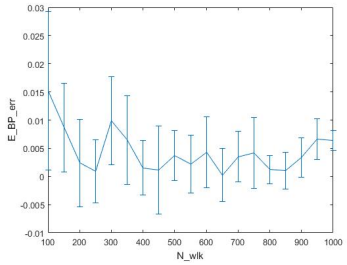


(b) The Y axis is the error bar of Back Propagation Kinetic Energy and the X axis is the number of walker.

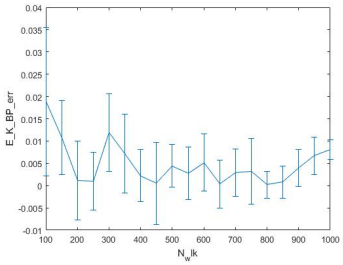


(c) The Y axis is the error bar of Back Propagation Potential Energy and the X axis is the number of walker.

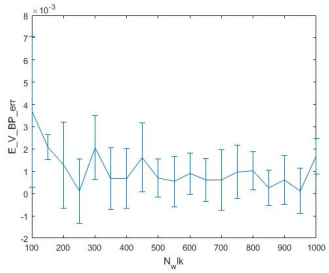
Figure 4:



(a) The Y axis is the error of Back Propagation Groundstate Energy ("E_BP-E_ED") and the X axis is the number of walker.



(b) The Y axis is the error of Back Propagation Kinetic Energy ("E_K_BP-E_K_ED") and the X axis is the number of walker.



(c) The Y axis is the error of Back Propagation Potential Energy ("E_V_BP-E_V_ED") and the X axis is the number of walker.

Figure 5: