

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;  
deltat=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.

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.

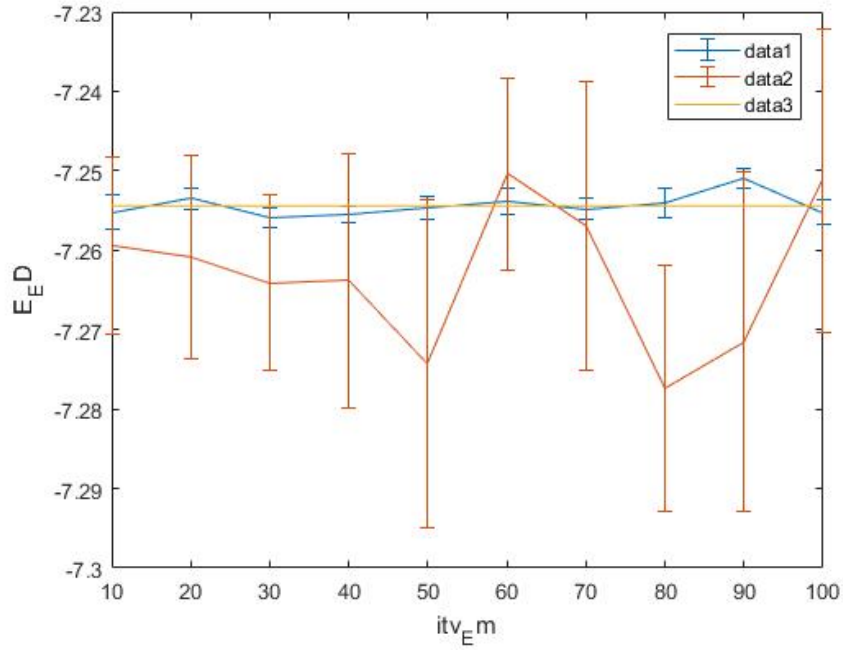


Figure 1: Data 1 is mixed Groundstate Energy, Data 2 is Back Propagation Ground State Energy, Data 3 is Exact Diagonalization Back Propagation Energy. $itv_{Em} \cdot \delta\tau$ is the length of back propagation and the length of detect distance.

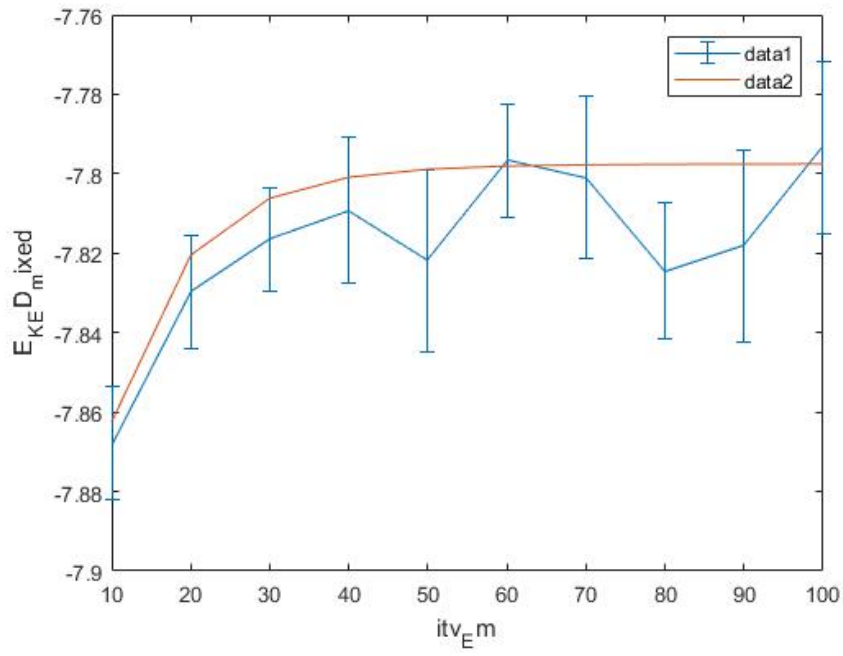


Figure 2: Data 1 is Back Propagation Kinetic Energy, Data 2 is Exact Diagonalization Back Propagation Kinetic Energy. $itv_{Em} \cdot \delta\tau$ is the length of back propagation and the length of detect distance.

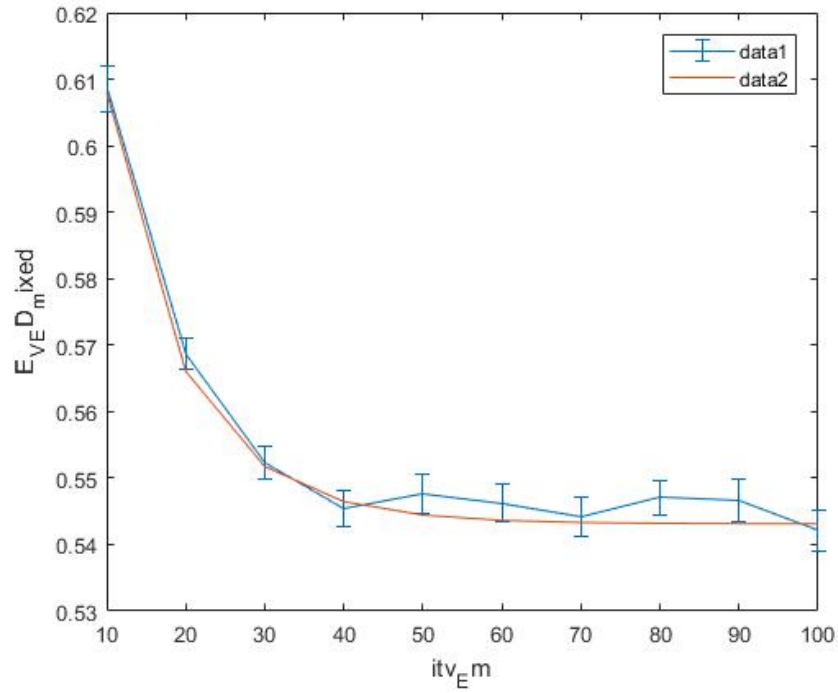


Figure 3: Data 1 is Back Propagation Potential Energy, Data 2 is Exact Diagonalization Back Propagation Potential Energy. $itv_Em \cdot \delta\tau$ is the length of back propagation and the length of detect distance.