UHF iteration method

icf

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1 HF iteration method

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:
kx=2*rand(1)-1;
ky=kx;
kz=0;
U=4.0;
tx=1;
ty=1;
tz=1;
N_it=500;
a=0.75;

1.1 Pre-analysis

Model:

$$H = -t \sum_{\{ij\},\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_{i} n_{i,\sigma} < n_{i,\bar{\sigma}} > - \frac{1}{2} U \sum_{i} < n_{i,up} >< n_{i,dn} >$$

Only calculate once to get the results and without nealing, since the results have Translation symmetry and Particle-Hole Symmetry, it is hard to summarize in the same frame.

The error: $err = \sum((n\_old\_out - n\_old\_in)^2)$ at each iteration step can be used to describe the convergency of Charge Density.

1.2 Matlab Program Modification

HFsample.m; HF_n.m; HF_H.m; HF.m.

1.3 Input/Output

1) Pattern and doping:
   like 4.1.mat;
   4.1.fig;4.3.fig;4.5.fig;4.7.fig;
   4.9.fig;4.11.fig;4.13.fig;4.15.fig.

2) Wave Length and Lattice Period Length:
   ky=kx*Ly/Lx.
   4.28.fig;4.29.fig;4.30.fig.

3) Wave Length and doping:
   Kx=Ky=0;
   4.17.fig;4.17.mat;
   4.20.fig;4.20.mat;
   4.22.fig;4.22.mat;

4) Pattern and U:
   4.24.mat;
   4.24.fig;4.25.fig.
   4.26.mat;
   4.26.fig;4.27.fig.

1.4 Discussion

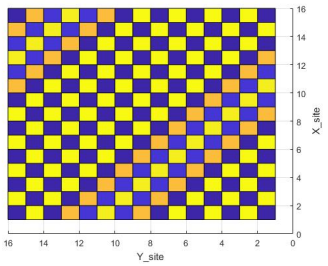
There are three difference between my results and those results in the paper:

1) Figure 1 (a), maybe agree with the paper result after summarizing of kx and ky or by adding nealing.

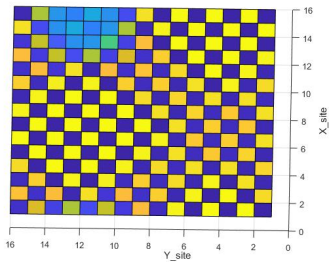
2) Figure 3 (c), maybe agree with the paper result after summarizing of kx and ky or by adding nealing.

3) Figure 5, maybe agree with the paper result after more iteration or by adding nealing.

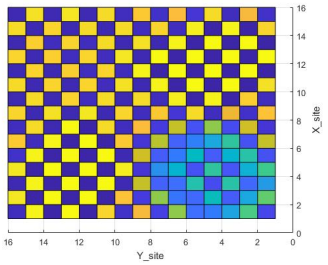
Without nealing,kx and ky sometimes affect the convergency and accuracy and in UHF, the difference between N_up and N_dn also affect the convergency and accuracy.



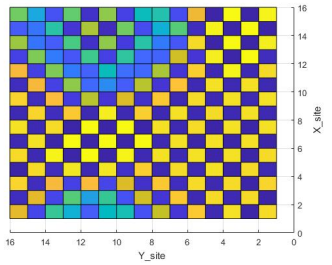
(a) Pattern and doping, Charge Density vs. Position, $N_{hole} = 4$.



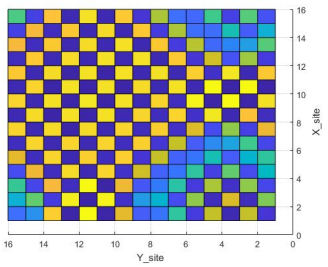
(b) Pattern and doping, Charge Density vs. Position, $N_{hole} = 8$.



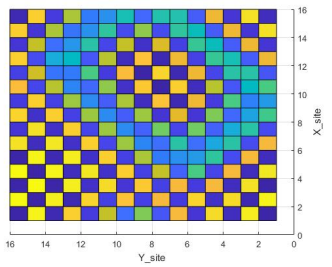
(c) Pattern and doping, Charge Density vs. Position, $N_{hole} = 12$.



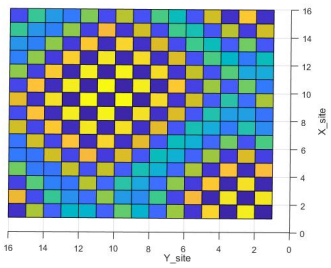
(d) Pattern and doping, Charge Density vs. Position, $N_{hole} = 16$.



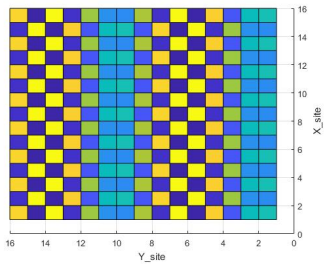
(e) Pattern and doping, Charge Density vs. Position, $N_{hole} = 20$.



(f) Pattern and doping, Charge Density vs. Position, $N_{hole} = 24$.

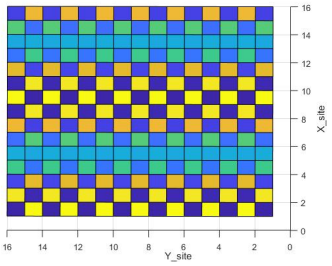


(g) Pattern and doping, Charge Density vs. Position, $N_{hole} = 28$.

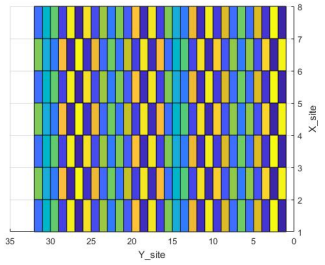


(h) Pattern and doping, Charge Density vs. Position, $N_{hole} = 32$.

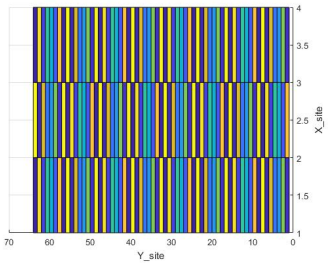
Figure 1:



(a) Wave Length and Lattice Period Length, Charge Density vs. Position, $Lx = 16$,$Ly = 16$.

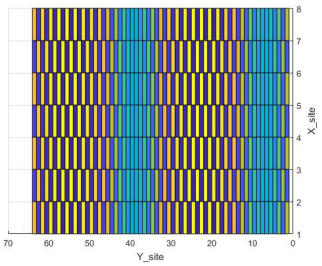


(b) Wave Length and Lattice Period Length, Charge Density vs. Position, $Lx = 8$,$Ly = 32$.

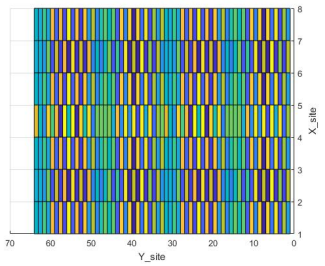


(c) Wave Length and Lattice Period Length, Charge Density vs. Position, $Lx = 4$,$Ly = 64$.

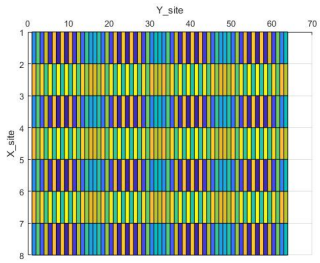
Figure 2:



(a) Wave Length and doping, Charge Density vs. Position, $N_{hole} = 16$.

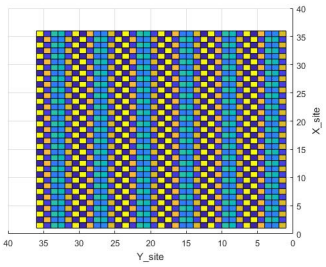


(b) Wave Length and doping, Charge Density vs. Position, $N_{hole} = 32$.

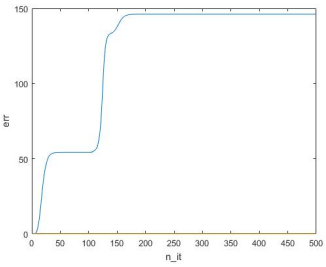


(c) Wave Length and doping, Charge Density vs. Position, $N_{hole} = 48$.

Figure 3:

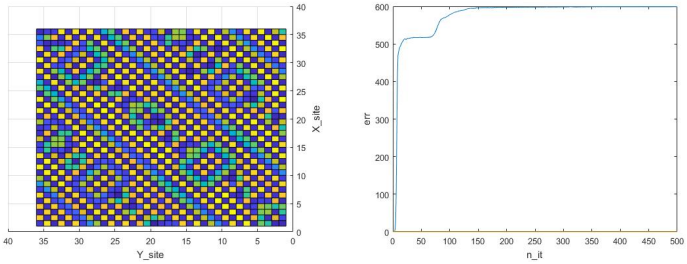


(a) Pattern and U, Charge Density vs. Position, $U = 5.0$.



(b) Error vs. Iteration Times.

Figure 4:



(a) Pattern and U, Charge Density vs. Position, $U = 9.0$.

(b) Error vs. Iteration Times.

Figure 5: