# Mean Field Theory for d=1 Hubbard Model: AntiFerromagnetism

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Following up on the preceding note, here I show some results for MFT of the one–dimensional Hubbard model allowing for antiferromagnetism.

## I. THE CODE

```
      implicit none
      integer i,N,Ntot,istag
      real*8 t,U,tpin,k,ek,mstag
      real*8 rho,Umstag,Urho
      real*8 eaf,eaftot,lambdaminus

c       INPUTS

      write (6,*) 'N,Ntot,t,U'
      read  (5,*)  N,Ntot,t,U
      write (36,*) Ntot/2+1

      tpin=8.d0*datan(1.d0)/dfloat(N)
      rho=dfloat(Ntot)/dfloat(N)
      Urho=U*rho/2.d0

      do 1000 istag=0,Ntot,2

      mstag=dfloat(istag)/dfloat(N)
      Umstag=U*mstag/2.d0

      eaftot=0.d0
      do 200 i=-Ntot/4+1,Ntot/4
          k=tpin*dfloat(i)
          ek = -2.d0*t*dcos(k)
          lambdaminus=-dsqrt(ek*ek
     1          +Umstag*Umstag)
          lambdaminus=lambdaminus+Urho
          eaftot=eaftot+lambdaminus
200    continue
       eaftot=2.d0*eaftot/dfloat(N)
     1   -U*(rho*rho-mstag*mstag)/4.d0

      write (36,990) istag,eaftot
990   format(i6,f16.6)

1000  continue

      end
```

## II. RESULTS FOR $\rho = \frac{1}{2}$

Here are results for one quarter filling, that is, a density $\rho = \rho_\uparrow + \rho_\downarrow = \frac{1}{2}$ electrons per site. (This is one quarter of the maximal density of two electrons per site.) The staggered magnetization $m_s$ is defined such that the up and down spin densities are $\rho_\uparrow = \rho + (-1)^i m_s$ and $\rho_\downarrow = \rho - (-1)^i m_s$.

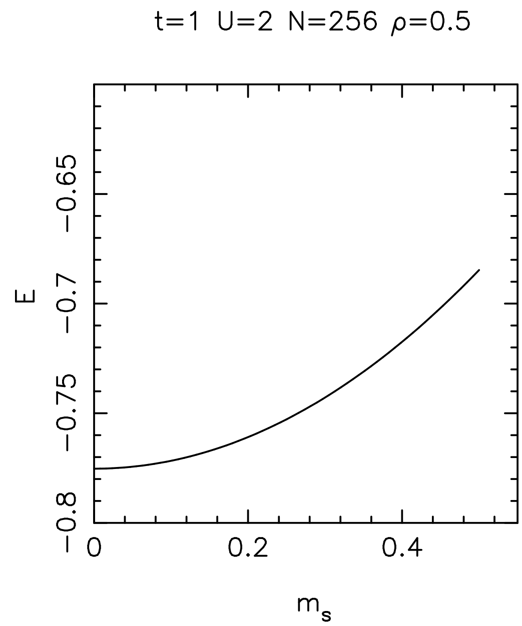


FIG. 1: Energy versus staggered magnetization of $d = 1$ Hubbard model at $U/t = 2$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

For $U = 2$ the paramagnetic solution $m_s$=0 has lowest energy. We know too from the preceding note that $m = 0$ is the lowest of the ferromagnetic energies. Notice as a check on the codes that one can compare Figure 1 here with the preceding Figure 1 and see that $E(m_s = 0) = E(m = 0)$.

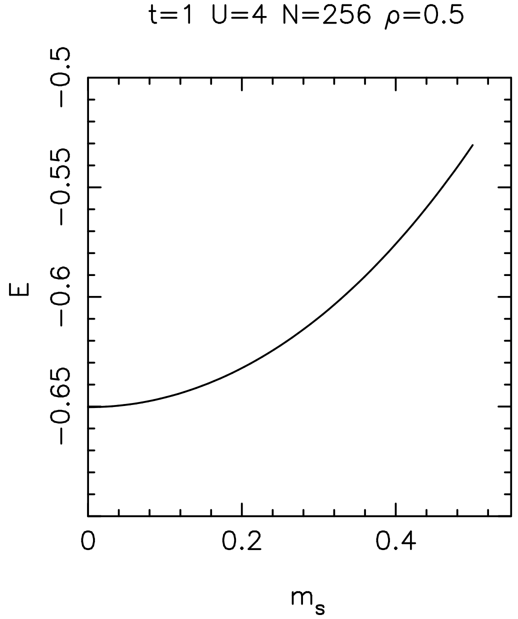


FIG. 2: Energy versus staggered magnetization of $d = 1$ Hubbard model at $U/t = 4$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

As before, we now start cranking up $U$. Figures 2 and 3 show the energy for $U = 4$ and $U = 8$ respectively. We see at $U = 8$ that a nonzero $m_s$ is better than zero $m_s$. However, the state is not actually antiferromagnetic because (Figure 4) the ferromagnetic energy is yet lower. (Again, check the fact that $E(m_s = 0) = E(m = 0)$. Really I should plot the ferromagnetic and antiferromagnetic data, Figures 3 and 4, on the same graph to make comparisons nicer.)

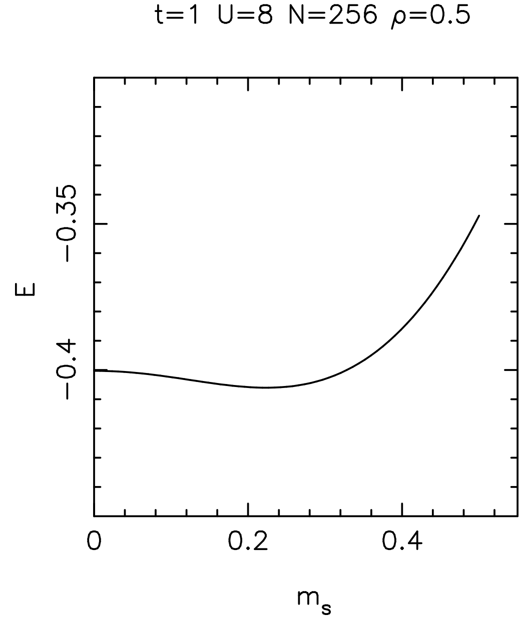


FIG. 3: Energy versus staggered magnetization of $d = 1$ Hubbard model at $U/t = 8$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

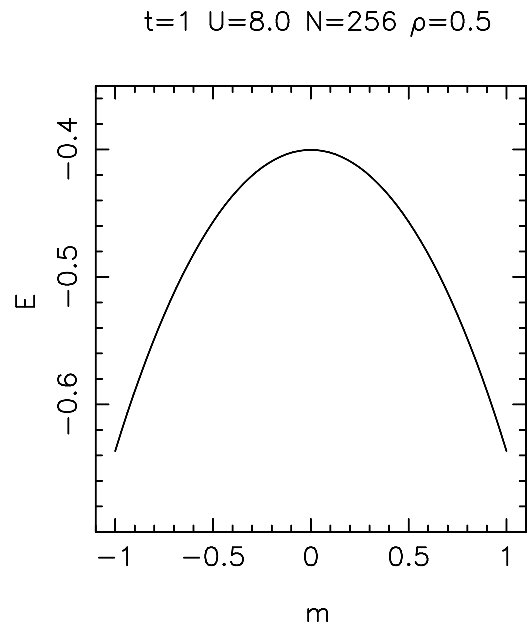


FIG. 4: Energy versus magnetization of $d = 1$ Hubbard model at $U/t = 8$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

## III. RESULTS FOR $\rho = 1$

The preceding results suggest that at quarter filling, $\rho = \frac{1}{2}$, the $d = 1$ Hubbard model is more prone to ferromagnetism than antiferromagnetism. Let's look at half-filling, $\rho = 1$, where antiferromagnetism tends to be most stable. Sure enough, Figures 5 and 6 show the antiferro-

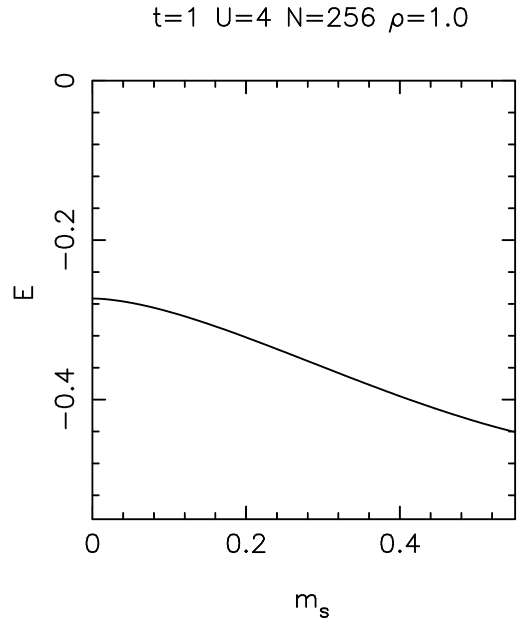


FIG. 5: Energy versus staggered magnetization of $d = 1$ Hubbard model at $U/t = 4$ and $\rho = 1$ (256 electrons on an $N = 256$ site lattice).

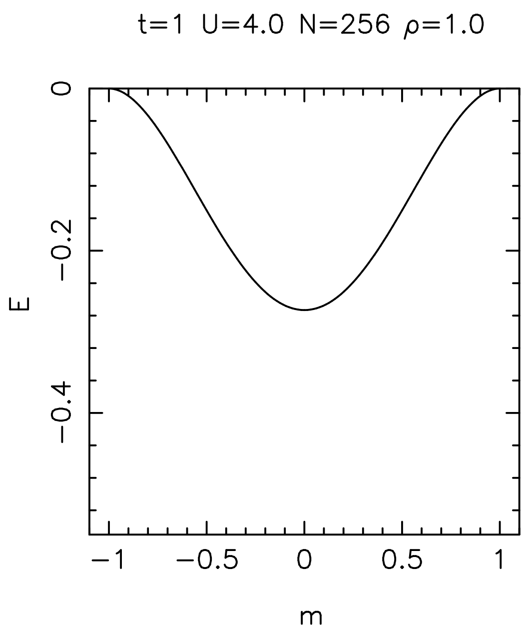


FIG. 6: Energy versus magnetization of $d = 1$ Hubbard model at $U/t = 4$ and $\rho = 1$ (256 electrons on an $N = 256$ site lattice).

magnetism is optimal (for $U = 4$). In fact, here, the best $m_s$ is the biggest it can be.

## IV. PHASE BOUNDARY

Our ultimate objective could be to analyze a bunch of energy curves, both ferro- and antiferromagnetic, for

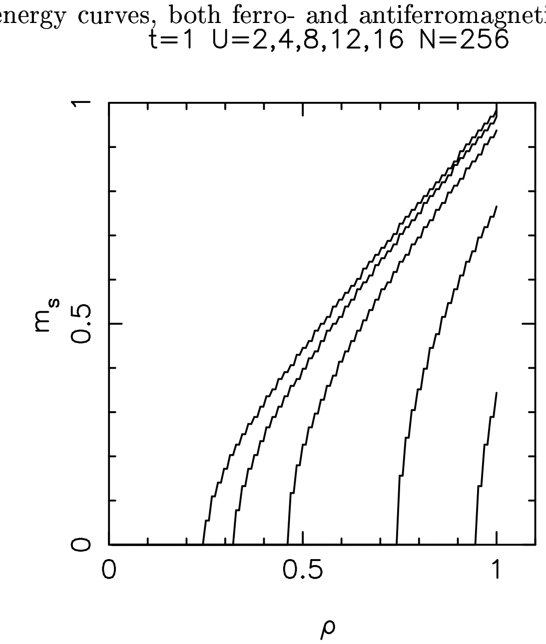


FIG. 7: Staggered magnetization $m_s$ which minimizes the energy, as a function of density $\rho$ for the $d = 1$ Hubbard model on a $N = 256$ site lattice. Curves are (left to right) $U = 16, 12, 8, 4, 2$.

different densities $\rho$ and couplings $U$ and figure out the whole phase diagram in the $\rho - U$ plane. As a first step in this direction, Figure 7 shows the value of the staggered magnetization which minimizes the energy, as a function of density for different values of $U$. For small $U = 2$, the energy is minimized in the paramagnetic phase $m_s = 0$ until close to half filling ($\rho = 1$). As $U$ increases, so does the regime of antiferromagnetism. For $U = 16$ the optimal staggered magnetization becomes nonzero around $\rho = 0.24$. So looking at the five points where $m_s$ becomes nonzero begins to give us a sense of the antiferromagnetic phase boundary. We have to do similar analysis for the ferromagnetic case (and compare energies) to complete the picture.