Mean Field Theory for d=1 Hubbard Model: Ferromagnetism

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Here I show some results for Mean Field Theory for the energy of the one–dimensional Hubbard model as a function of the magnetization m. This tells us the values of U/t and ρ for which the system is unstable to ferromagnetism. I will deal with antiferromagnetism in a later note.

I. THE CODE

```
implicit none
integer i,N,Nup,Ndn,Ntot
real*8 t,U,tpin,k,ekup,ekdn,denup,dendn
real*8 efup,efdn,eftot

write (6,*) 'N,Ntot,t,U'
read  (5,*)  N,Ntot,t,U
tpin=8.d0*datan(1.d0)/dfloat(N)
do 1000 Nup=0,Ntot,2

Ndn=Ntot-Nup
denup=dfloat(Nup)/dfloat(N)
dendn=dfloat(Ndn)/dfloat(N)

efup=0.d0
efdn=0.d0
do 200 i=-N/2+1,N/2
    k=tpin*dfloat(i)
    if (i.ge.-Nup/2+1.and.i.le.Nup/2) then
       ekup=-2.d0*t*dcos(k)+U*dendn
       efup=efup+ekup
    endif
    if (i.ge.-Ndn/2+1.and.i.le.Ndn/2) then
       ekdn=-2.d0*t*dcos(k)+U*denup
       efdn=efdn+ekdn
    endif
200 continue
eftot=(efup+efdn)/dfloat(N)-U*denup*dendn

write (36,990) Nup,Ndn,eftot
990 format(2i6,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 magnetization m is defined such that $m = (\rho_\uparrow - \rho_\downarrow)/(\rho_\uparrow + \rho_\downarrow)$.

You see that at $U/t = 2$ the optimal energy is paramagnetic: the energy E is minimized at $m = 0$. This is still the case at $U/t = 4$ (see next page), but the energy of the spin polarized solutions (m nonzero) are getting much closer to $m = 0$. (Note the energy scale.) When $U/t = 4.2$ the energies for large $|m|$ have started to turn down and are lower than intermediate m, though $E(m = 0)$ is still lowest. $U/t = 4.4$ has just gone ferromagnetic.

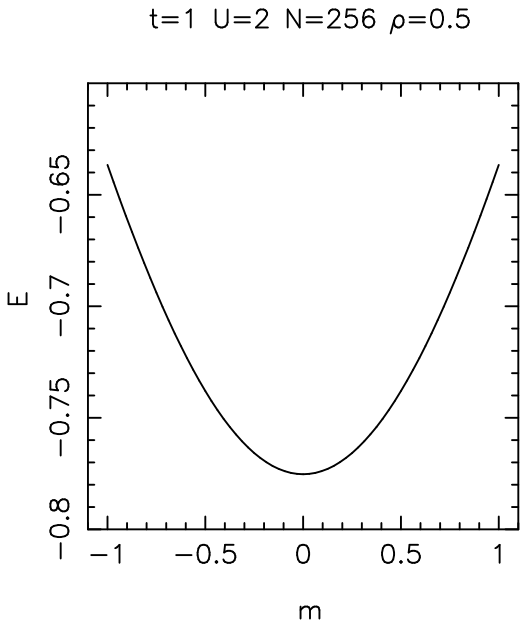

FIG. 1: Energy versus magnetization of $d = 1$ Hubbard model at $U/t = 2$ and $\rho = \frac{1}{2}$ (128 electrons on an $N = 256$ site lattice).

Notice that the transition is *first order*. That is, as U/t increases we jump suddenly from a minimum at $m = 0$ to a minimum at $m = \pm 1$. Another possibility would have been a second order transition in which the minimum at $m = 0$ gradually shifts to larger m and partially polarized solutions are best for a range of U/t. Without examining other MF solutions (like antiferromagnetic ones) we cannot tell if this first order transition is 'real' or simply occurs because we have restricted to ferromagnetic solutions and something even lower in energy is actually winning.

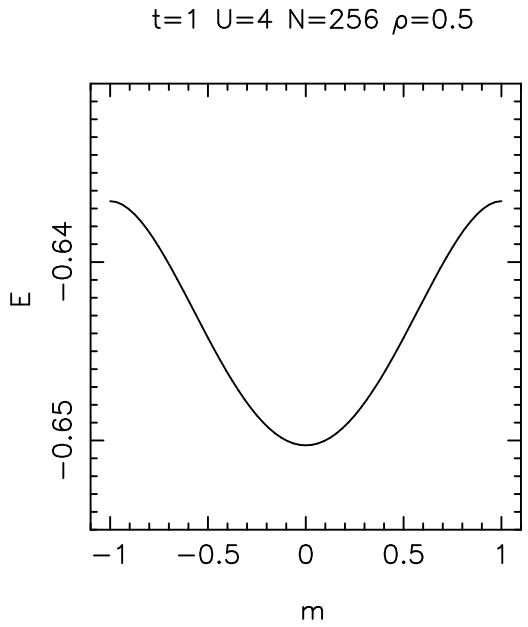

FIG. 2: Same as Fig. 1 except $U/t = 4$.

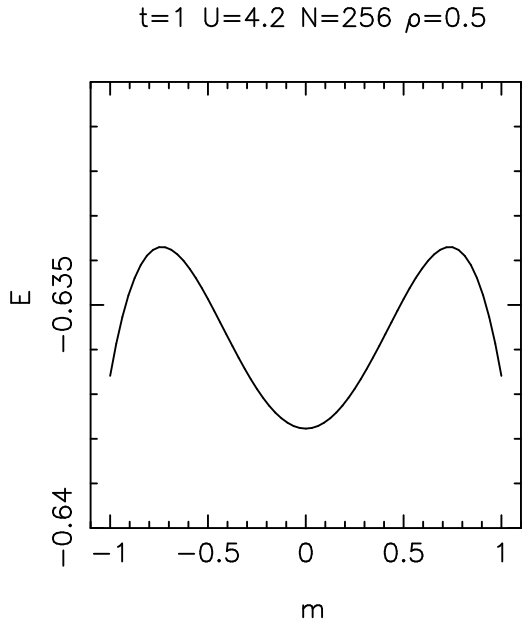

FIG. 3: Same as Fig. 1 except $U/t = 4.2$.

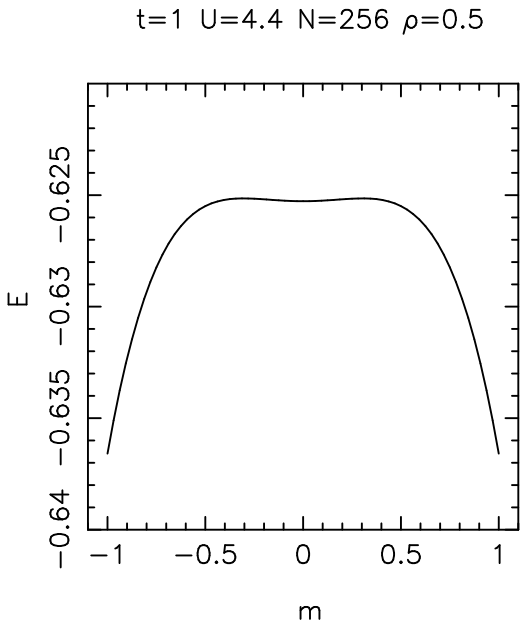

FIG. 4: Same as Fig. 1 except $U/t = 4.4$.

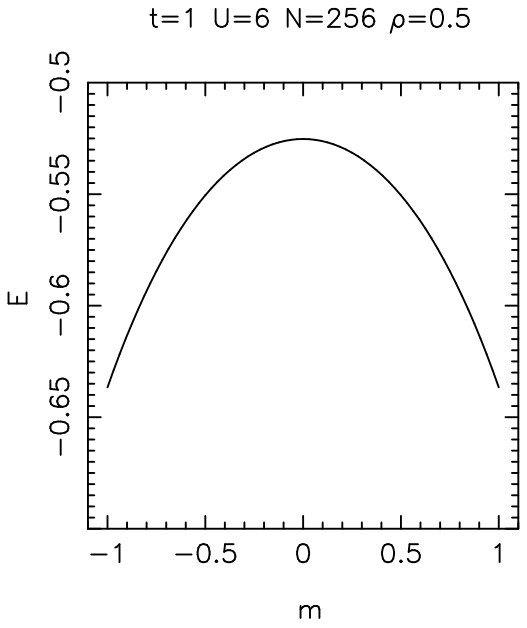

FIG. 5: Same as Fig. 1 except $U/t = 6$.

III. CONSISTENCY WITH STONER CRITERION

In class we derived the Stoner Criterion for Ferromagnetism $UN(E_{\rm F}) > 1$. For the d=1 Hubbard model we can compute,

$$N(E) = 2\sum_k \delta(E - \epsilon_k) = 2\int \frac{dk}{2\pi}\delta(E - \epsilon_k) \qquad (1)$$

with $\epsilon_k = -2t\cos(k)$. A simple calculation gives

$$N(E) = \frac{1}{\pi\sqrt{4t^2 - E^2}}. \qquad (2)$$

This is the density of states for a single spin species, which is what was used in the Stoner criterion.

We also need the relation between the density ρ and

the Fermi energy $E_{\rm F}$:

$$\rho = 2\int_{-2t}^{E_{\rm F}} dE\ N(E). \tag{3}$$

I put in the factor of two for spin here, so that when I plug in ρ I use the total density (including both spin species). This yields,

$$\rho = \frac{2}{\pi}\cos^{-1}(\frac{-E}{2t}). \tag{4}$$

You can check this latter relation obeys the expected limits: $\rho = 0$ when $E_{\rm F} = -2t$, $\rho = 1$ when $E_{\rm F} = 0$, and $\rho = 2$ when $E_{\rm F} = +2t$.

Putting these equations together, we can get the density of states at $E_{\rm F}$ for a given filling:

$$N(\rho) = \frac{1}{2\pi t}\frac{1}{\sin(\pi\rho/2)} \tag{5}$$

For half-filling, $\rho = 1$ we see that $N(\rho = 1) = \frac{1}{2\pi t}$ and hence $U_{\rm crit} = 2\pi t$. For quarter-filling, $\rho = \frac{1}{2}$ we see that $N(\rho = 1) = \frac{1}{\sqrt{2}\pi t}$ and hence $U_{\rm crit} = \sqrt{2}\pi t = 4.44t$. This is in pretty good agreement with Figures 1–5 which showed us that $U_{\rm crit}$ was around $4.4t$. I suspect that the slight disagreement (Figure 4 suggests $U_{\rm crit}$ a bit less than $4.4t$ while Stoner gives $U_{\rm crit}$ a bit more than $4.4t$) is due to the fact that Figures 1-5 were run on $N = 256$ site lattices. That is, I believe the small difference is likely a finite size effect.

IV. PARTICLE-HOLE SYMMETRY

A lattice which can be divided into two distinct sublattices A and B such that the only neighbors of sites in A are sites in B and *vice-versa* are referred to as bipartite lattices. A two-dimensional square lattice is bipartite, but not a two-dimensional triangular lattice. A one-dimensional linear chain is bipartite. I did not discuss this in class, but the Hubbard model on a a bipartite lattice exhibits 'particle-hole' symmetry. This means all physical properties at fillings $\rho = 1+x$ and $\rho = 1-x$ are identical. We saw an example of this in all the preceding figures where $E(\rho = 1-x) = E(\rho = 1+x)$. The phase diagram would then be symmetric about $\rho = 1$ as well.

The proof of particle-hole symmetry is simple. Do the change of variables $c_{\mathbf{i},\sigma} \rightarrow (-1)^{\mathbf{i}} c^\dagger_{\mathbf{i},\sigma}$. This interchanges creation and destruction operators, hence the name particle-hole transformation. Here $(-1)^{\mathbf{i}} = 1$ on sites $\mathbf{i}$ in sublattice A $(-1)^{\mathbf{i}} = -1$ on sites $\mathbf{i}$ in sublattice B. Check that the kinetic energy is unchanged by this transformation. What is the role of the $(-1)^{\mathbf{i}}$ factor? How does the bipartite lattice enter? How do the anticommutation relations of fermion operators enter?

The potential energy is slightly more tricky. First note how the number operator changes: $n_{\mathbf{i},\sigma} \rightarrow (1 - n_{\mathbf{i},\sigma})$. In other words, empty sites and filled sites are exchanged $n_{\mathbf{i},\sigma} = 0 \leftrightarrow n_{\mathbf{i},\sigma} = 1$. This of course also motivates the name 'particle-hole' transformation. Second, notice that one can rewrite the interaction and chemical potential terms in the Hubbard model (to within an irrelevant overall constant) as:

$$\begin{aligned} & U\sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} - \mu\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow}) \\ & = U\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow} - \frac{1}{2})(n_{\mathbf{i}\downarrow} - \frac{1}{2}) \\ & -(\mu - U/2)\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow}). \end{aligned} \tag{6}$$

We call this way of expressing the interaction the 'particle-hole symmetric' form. It is easy to see that when the $\frac{1}{2}$ factors are subtracted from the density, the expression which U multiplies does not change under the particle-hole transformation.

The other term with the shifted chemical potential *does* change under the particle-hole transformation, but if its coefficient is zero ($\mu = U/2$) then the whole Hamiltonian H is invariant. This has many consequences for expectation values of operators. The most simple one is $\langle n_{\mathbf{i}\,\sigma}\rangle = \langle 1 - n_{\mathbf{i}\,\sigma}\rangle$ and hence $\langle n_{\mathbf{i}\,\sigma}\rangle = \frac{1}{2}$ (as expected!)

It is also fairly easy to see finally that all physical properties at fillings $\rho = 1 + x$ and $\rho = 1 - x$ are identical, our original claim.

There are many other beautiful symmetries which can be uncovered by similar particle-hole transformations. For example one can map the repulsive ($U > 0$) Hubbard model onto the attractive ($U < 0$) Hubbard model. This allows one to develop insight into charge density wave and superconductivity in the attractive Hubbard model from your knowledge of the behavior of magnetism in the repulsive Hubbard model.