**Physics 241– Quantum Magnetism**

**Comments on Problem Set 5, Problem 2**

Again, my apologies for not being able to cover this thoroughly in class. But Mean Field Theory for the Hubbard model is a problem well worth knowing how to do. Feel free to email me with any questions.

I also have a suggestion: First try writing a mean field code without considering the possibility of antiferromagnetism. This is a rather more simple code, and, also, is the case we discussed in class. My feeling is that if you can get such a mean field code going, then you 'have the idea' and the more complicated business of checking for antiferromagnetic solutions is 'straightforward'. That is, you would know how to do it if you ever need to. For those of you with the time and inclination, the argument for pressing forward with the antiferromagnetic solution is the connections to other solid state physics problems mentioned at the end of these notes.

First I will review the ferromagnetic case. Here is what you do:

(1) Fix the lattice size, $N$ to some fairly large value, say $N = 128$ or greater.

(2) Choose a total particle number $N_{\rm tot}$ and on-site repulsion $U$.

(3) Loop over $N_\uparrow = 0, 1, 2, \ldots . N_{\rm tot}$. For each choice, set $N_\downarrow = N_{\rm tot} - N_\uparrow$. (Actually, your answers should be symmetric on interchange of $N_\uparrow$ and $N_\downarrow$, so you really only need do half the values $N_\uparrow = 0, 1, 2, \ldots . N_{\rm tot}/2$.) Define the densities, $n_\uparrow = N_\uparrow/N$ and $n_\downarrow = N_\downarrow/N$.

(4) Loop over the $N$ allowed momentum values $k = 2\pi/N\{-N/2+1, -N/2+2, \ldots N/2\}$. Fill up the lowest $N_\uparrow$ and $N_\downarrow$ of the energy levels. That is, add the associated energy values to some accumulator which stores the total energy. Recall that the levels are given by $E(k,\uparrow) = -2\,t\,{\rm cos}k + Un_\downarrow$ and $E(k,\downarrow) = -2\,t\,{\rm cos}k + Un_\uparrow$.

(5) Finally, normalize your energy accumulator to the number of sites (divide by $N$) and add in the term $-Un_\uparrow n_\downarrow$. This gives the energy for the given $N_\uparrow$ and $N_\downarrow = N_{\rm tot} - N_\uparrow$. Make a list of them and see which is lowest.

(6) Repeat the calculation for different $U$ and $N_{\rm tot}$ to get the phase diagram.

The basic idea is identical for antiferromagnetism. The thing we need to do is figure out the energy levels for an antiferromagnetic configuration. First, I better tell you what an antiferromagnetic configuration is! A paramagnetic configuration has the same exact density $n_{l\sigma} = n$ regardless of site $l$ or spin $\sigma$. A ferromagnetic configuration allows the density to depend on $\sigma$ but not $l$: $n_{l\uparrow} = n_\uparrow$, and $n_{l\downarrow} = n_\downarrow$ (see above). An antiferromagnetic configuration allows a simple *spatial* dependence in which the densities alternate: $n_{l\uparrow} =$

$n + (-1)^l m$, $n_{l\downarrow} = n - (-1)^l m$. That is, the even sites have a surplus of up spin electron density: $n_{\mathrm{even}\uparrow} = n + m$, $n_{\mathrm{even}\downarrow} = n - m$. The odd sites have a surplus of down spin electron density: $n_{\mathrm{odd}\uparrow} = n - m$, $n_{\mathrm{odd}\downarrow} = n + m$. Note that the total number of up and down electrons in the whole system is the same, $nN$, and that each site has the same density $2n$, once the densities of the individual spin species are summed. More generally one might have some sort of mixed ferromagnetic and antiferromagnetic configuration.

The form of the Hamiltonian in mean field theory is, $H = \sum_{j,l} c^\dagger_{j\sigma} M_\sigma(j,l) c_{l\sigma}$, where $M_\sigma(j,l)$ has $-t$ just above and below the main diagonal, with $M_\uparrow(l,l) = U(n-(-1)^l m)$, or $M_\downarrow(l,l) = U(n+(-1)^l m)$ along the diagonal. We discussed the form of the eigenvalues for this sort of tridiagonal matrix when the diagonal is constant ($m = 0$). When $m$ is nonzero, the eigenvectors of momentum $k$ and $k+\pi$ are mixed (see below for further discussion) and the eigenvalues become: $E(k) = \pm\sqrt{(-2\,t\,\cos k)^2 + (Um)^2} + Un$. Here $k$ is now defined in a 'reduced zone', $k = 2\pi/N\{-N/4+1, -N/4+2, \ldots, +N/4\}$, so that there are still $N$ eigenvalues as there should be for this $N$ dimensional matrix (two eigenvalues for each $k$, but only half as many $k$. The eigenvalues are the same for $\sigma =\uparrow$ and $\sigma =\uparrow$.) You might want to check that these eigenvalues reduce to the old ones when $m = 0$. Can you also check the eigenvalues make sense when $t = 0$? (Check that all the counting (degeneracies) are correct!)

The process for computing the energy of an antiferromagnetis configuration is the same as the steps (1–5) above, with the replacement of the ferromagnetic eigenvalues by the antiferromagnetic ones. Since we are assuming the total up and down densities over the whole lattice are identical, one no longer loops over different $N_\uparrow$. However, one does have to loop over different $m$. More precisely, one fixes $n = N_{\mathrm{tot}}/2$ and then tries $m = 1/N, 2/N \ldots,$.

One reason this problem is worth doing is because of its formal connections to so many other problems in solid state physics. The most obvious is the opening of a gap in an energy band by a periodic potential $V(G)$ with wavevector $G$ (e.g. see Ashcroft and Mermin). In our problem we can think of the up spin electrons as moving in a periodic potential which has period $\pi$ resulting from the oscillating down spin density (and vice-versa). A gap is opened at $k = \pm\pi/2$. There is also a connection to simple phonon problems where one makes the masses or spring constants vary: $m_1, m_2, m_1, m_2, \ldots$ or $k_1, k_2, k_1, k_2, \ldots$. Again, the single phonon dispersion curve for uniform masses and springs breaks into two branches, optic and acoustic. Some of you are presently doing this problem in Physics 240B. There are many other examples.

Let me conclude this discussion by mentioning an alternate procedure. The way I described writing the mean field code (for ferromagnetism) is to fix the total particle number $N_{\mathrm{tot}}$ and and loop through the different choices of the number of up particles, $N_\uparrow = 0, 1, 2, \ldots N_{\mathrm{tot}}$, choosing always $N_\downarrow = N_{\mathrm{tot}} - N_\uparrow$. I suggested computing the energy

$E$ for each choice, by filling up the lowest energy levels for each spin type, and then seeing which choice of $N_\uparrow$ minimizes $E$. If the minimum is at $N_\downarrow = N_\uparrow = N_{\rm tot}/2$ then the state is paramagnetic.

There is another way to write the code, which you might find easier. Work in the grand-canonical ensemble. That is, provide a chemical potential $\mu$ and then *compute* $N_\downarrow$ and $N_\uparrow$ by filling those levels which are below $\mu$. The density then comes out of the choice of $\mu$, and, indeed, you will need to tune $\mu$ to get the density you desire. (This process is a bit annoying.)

One advantage of this method is that one can let the code find the lowest energy configuration, instead of searching through all the possible choices of magnetization. This is done in the usual way: Start at some densities $n_\uparrow, n_\downarrow$, compute $E(n_\uparrow, n_\downarrow)$, and then alter $n_\uparrow, n_\downarrow$, to reduce $E$ (using your favorite gradient descent algorithm or whatever). Continue iterating until you reach the minimum.

Another reason this second, 'grand canonical', approach is more convenient is that it is easy to do things at finite temperature. One simply replaces the process where one accumulates the energies of all levels $E(k,\sigma) < \mu$ with accumulating $E(k,\sigma)$ times the Fermi function $1/[1 + e^{\beta(E(k,\sigma)-\mu)}]$. (Likewise, one puts this Fermi function in the computation of the density). Another reason the grand canonical approach is sometimes preferable is that it also generalizes better to states where the lowest energy is more complex, 'striped phases' etc, where the density of electrons is allowed to depend in a completely general way on the lattice site and spin species. In that situation, though, there is usually no longer an analytic form for the energy levels and one has to diagonalize a matrix to get them.