Tutorial Two Solutions

Exercise 1:

[1] Why are only six values listed? Aren't there 16 possible separations?
On a 4x4 lattice with periodic boundary conditions, there are only six inequivalent lattice separations. The separations (0,1) and (1,0) are obviously equal by the x/y symmetry of the lattice. The separations (0,3) and (0,1) are equivalent through use of the periodic boundary conditions. We thus have to report correlation functions only for a small "wedge" of possible separations. The same is true in momentum space. The code automatically averages over the equivalent separations, just as it averages over the initial point j in any correlation function $\langle A(j+l)A(j)\rangle$.
[2] Is the pattern of signs in your low T data consistent with antiferromagnetism?
You should find the spin correlations are negative for separations (0,1), (2,1) and positive for separations (0,0), (0,2), (1,1), and (2,2). It is easy to see that in the former case the spins are on different sublattices, while in the latter case they are on the same sublattice. Thus the signs are indeed consistent with AF order.
[3] Why is the $(0,0)$ correlation function enhanced over its $T=\infty$ value of 0.500 even at the highest temperatures, $T=2$ $(\beta=0.5)$ while the other separations only start to build up at much lower T?
The (0,0) correlation function is the local moment, the correlation of a spin with itself. The energy scale of moment formation is the repulsion U, which suppresses double occupancy. On the other hand, the energy scale for spin order is $J=4t^2/U$, a factor of four smaller.
[4] It looks like the correlation functions for (0,2) and (1,1) separations are the same to within error bars. Yet these are not the same separation in space. Or are they?!
This is not a coincidence. If you draw the lattice connections of a 4x4 square lattice with periodic boundary conditions, and those of a 2x2x2x2 (four dimensional hypercube of linear dimension 2 sites), you can see that all the lattice connections are equivalent. On the 2x2x2x2 hypercube you can see that the (0,2) and (1,1) separations on the 4x4 lattice are identical.

Exercise 2:

[1] If you compare spin correlations at the same separation and same temperature for different lattice sizes, what happens? Why?
The spin correlations on the smaller lattice are larger, when all other parameters are held fixed. The reason is that on small lattices the periodic boundary conditions provide additional paths connecting sites, enhancing their correlations. I am not sure of this, but perhaps in a frustrated system things could be different. For example if you ran the code on a 3x3 lattice with periodic boundary conditions, spin correlations might be reduced over those of larger lattices.

Exercise 3:

[1] Why don't you need to get data at $\mu>0$? Did you really need to run $\mu=0$?
We know from particle-hole symmetry that $\langle n\rangle(\mu)=2-\langle n\rangle(-\mu)$. This immediately also tells us that $\langle n\rangle(\mu=0)=1$, so it is not necessary to run that value.
[2] Make a plot of density versus μ for each β. Do you see a Mott plateau?
[3] Make a plot of the error bars in the density as a function of the density. Also make a plot of the average sign versus density. Do these help you understand my claim that $\beta\approx 6$

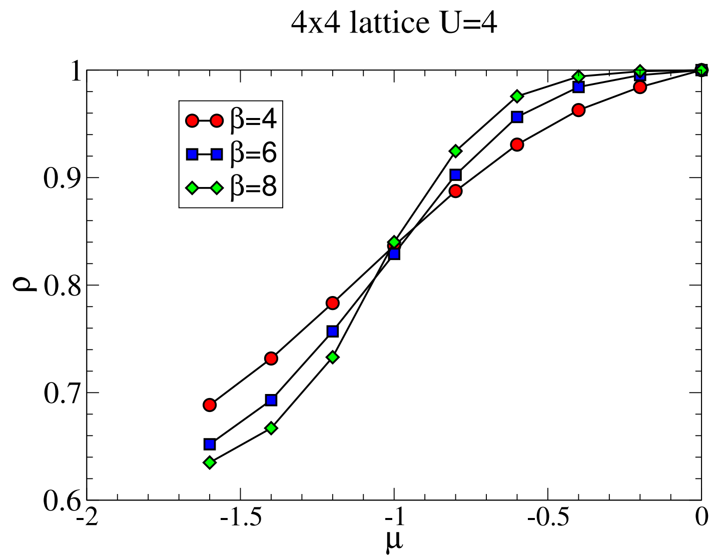

FIG. 1: Density ρ vs chemical potential μ. As the temperature is lowered, the curve becomes increasingly flat near $\mu = 0, \rho = 1$.

is the temperature limit in these simulations?
[4] It looks like some sort of plateau might also be developing around $\rho = 0.6$. Do you have any idea where that might come from?
This is a finite size effect. $\rho = 0.625$ is a special 'shell' filling. As the $U = 0$ Fermi surface expands from the origin, it encounters four new k points at $(\pm\pi/2, 0)$ and $(0, \pm\pi/2)$, and the filling jumps from $2/16$ (just the $k = (0, 0)$ point occupied by the two spin species) to $10/16 = 0.625$. $U = 4$ is not sufficiently strong coupling to wipe out this vestige of the discrete k points. Obviously as the lattice size increases, such effects become less evident. However, there is an important lesson here: weak couplings are often more subject to finite size effects that stronger ones.

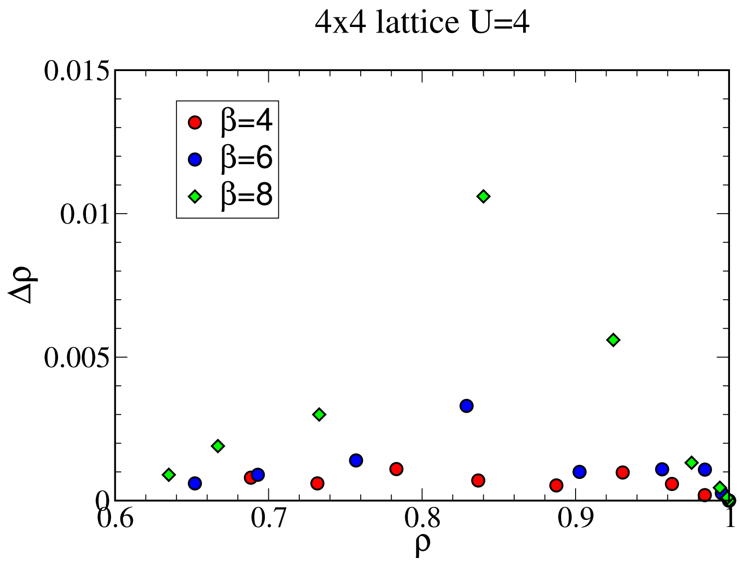

FIG. 2: Error bars in the density as a function of the density for different temperatures. For $\beta = 8$ the error bar in the density is almost 2 percent of the density. While we can reduce the error bars by running longer (four times as long for a factor of two reduction in error bars), we also find the error bars at fixed run length gro exponentially with β. The origin is the sign problem. (See next plot.)

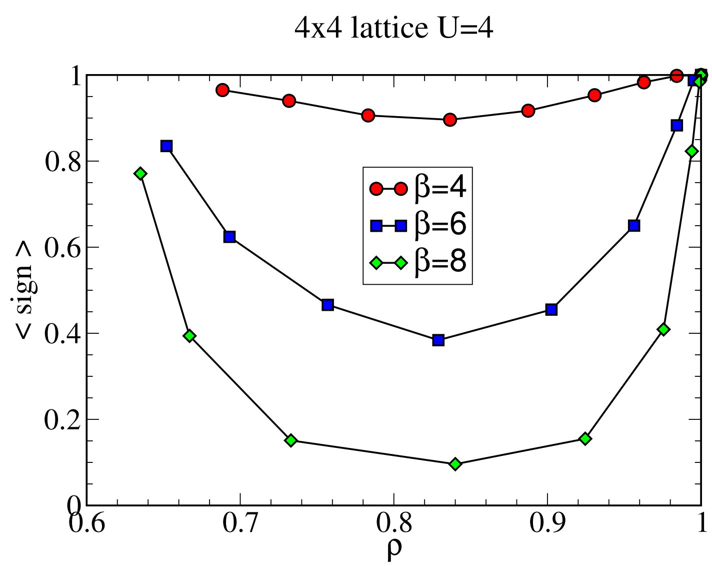

FIG. 3: