Tutorial Three

Computational:

In Tutorial 2 we saw evidence for AF spin correlations in the half-filled Hubbard model. Here we ask whether we can convince ourselves, using simple finite size scaling, that there is in fact *long range* AF order. [WARNING: Trying to get this data in just a one hour training section doesn't enable us to do a very good job. The error bars on the data will be a bit too big, and the largest lattice size will be 8x8. However, if you are willing to run for a couple of days (eg after you return home), you can both beat the error bars down and also do 10x10 and even 12x12 lattices.]

Run hubvietri.f for $t = 1, U = 4, \mu = 0, \beta = 8$, using ($L = 64$ and $\Delta\tau = 0.125$. Run length should be nwarm=500 and npass=5000. Do $n = 4, 6, 8$ (lattices 4x4, 6x6, and 8x8). The 8x8 lattice took 45 minutes on my laptop to complete. Record the spin-spin correlations at maximal separation, ie the last value $(n/2, n/2)$ listed in
zz Spin correlation function
xx Spin correlation function

Average these two values. Also get the AF structure factors. They are called 'AF correlation function(xx)' and 'AF correlation function(zz)'. (These are not good names! We should label them the 'structure factor'!) Average them, and also divide by the volume n^2. Plot these two averaged quantities versus $1/n$.
[1] Are the extrapolations to $1/n = 0$ (that is, $n = \infty$) nonzero?
[2] Do the extrapolations agree?
[3] Again, the data will not be so great. I suggest if you are serious, try running the code with npass=20000 and also do 10x10 and 12x12 lattices. Actually, because the code can get stuck with the spin order in a particular direction, it is best to run npass=5000 with ten or so random number seeds and average the results.

Analytic:

Try some of the analytic exercises in the notes and the morning meetings. E.g.
[1] Get the dispersion relation $E(k)$ for the triangular lattice Hubbard model at $U = 0$. Does it have a van-Hove singularity? Is it symmetric about $E = 0$?
[2] Compute $A(\omega)$ for the $t = 0$ Hubbard model $H = U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2}) + \epsilon(n_\uparrow + n_\downarrow)$
[3] Get the density of states for the honeycomb lattice and show it is a semi-metal.
[4] Solve the four site $J_1 - J_2$ Heisenberg Hamiltonian. Show you get a level crossing.
[5] Work out the Hubbard-Stratonovich transformation for the $U < 0$ Hubbard model. Why is there no sign problem in determinant QMC simulations?
...etc...