Tutorial One

You will find three fortran codes:

hubvietri.f (determinant QMC code for $d = 2$ square lattice Hubbard model)

ueq0vietri.f (analytic solution of $U = 0$ Hubbard model, $d = 2$ square lattice)

teq0vietri.f (analytic solution of $t = 0$ Hubbard model)

I apologize that the codes are not very user-friendly and readable (eg well commented). You will also find one input file:

hubvietri.in (input for determinant QMC code)

The inputs for the other codes are simple enough just to enter while you run. The input file hubvietri.in contains comments explaining what all the parameters that you need to know about are. There are other parameters having to do with numerical stability that you should just leave alone. Two important notes: First, the name of the file which holds the output is specified as a character string in the input file (as is explained there). Second, the lattice sizes, both the linear spatial size n and the number of imaginary time slices l which determines β via $\beta = l\Delta\tau$ are set in parameter statements in the fortran code hubvietri.f. That is, they are *not* inputs. Note that when you change the settings for n and l you must change them globally. (They appear 31 times in the code!) An editor with a global replace feature is useful here. (This is one of the ways the code is not use friendly. At some point I will rewrite it so n and l are set globally at one location only.)

To compile the code

ifort hubvietri.f

(You might want to explore if ifort has any optimization swtiches.)

To run the code

a.out < hubvietri.in

Some information on the progress of the run will come to the screen. Specifically, every 10 sweeps through the lattice you will be told the accpetance rate for the Monte Carlo moves (should be around 0.5) and the "redo ratio" (should be small, like 0.0001). If you don't want this on your screen, use

a.out < hubvietri.in > outjunk

TO DO:

Your job is to verify the QMC code and the analytic codes agree.

For example, setting $n = 6, t = 0, U = 4, \mu = 1$ and $\Delta\tau = 0.125, l = 4$ so that $\beta = l\Delta\tau = 0.5$, I found that the QMC code run with nwarm=500 and npass=5000 gave: $\langle n_\uparrow \rangle = 0.5695 \pm 0.0009$ and $\langle n_\downarrow \rangle = 0.5659 \pm 0.0008$. The analytic answer is 0.56775. Likewise, for the QMC, $\langle n_\uparrow n_\downarrow \rangle = 0.2143 \pm 0.0002$, with an analytic answer 0.21435. Of course, since $t = 0$, the code should give the same answer (to within error bars) for all n. When $n = 6$ it was just running 36 single site simulations in parallel.

Similarly, setting $n = 6, t = 1, U = 0, \mu = -1$ and $\Delta\tau = 0.125, l = 4$ so that $\beta = l\Delta\tau = 0.5$, I found that the QMC code run with nwarm=10 and npass=100 gave: $\langle n_\uparrow \rangle = \langle n_\downarrow \rangle = 0.39906 \pm 0.00000$. The analytic answer is $\langle n_\downarrow \rangle = 0.39903$. Comments: (1) The QMC code should give the *exact* answers whenever $U = 0$ since it traces over the fermions analytically and there is no coupling to the Hubbard-Stratonovich field. That's why one could do such a short run (nwarm=10, npass=100.) The reason one does not just set npass=1, which should work in principle, is the way the code generates error bars. It assumes a certain minimal number of samples are taken. (2) The small disagreement between the codes is due to the Trotter error in the checkerboard breakup of the kinetic energy. (3) You will need to multiply the energy written by ueq0vietri.f by two, because it is does a single spin species.