PHYS580 Lab 9, Oct 17, 2019

Assignment:

1. The first starter program provided for this lab, *montecarlo.m* , performs Monte Carlo integration of a simple function, $f(x)=\sqrt{4-x^2}$ (by default). Use the code (or your own equivalent one) to integrate this $f(x)$ from x = 0 to 2, and thus compute π numerically, to 3, 4, and 5 significant digits. Observe how the average error (standard error of the mean) decreases as a function of the total number N of random numbers used (N = numbers generated per trial × the number of trials). Then, try to compute via Monte Carlo the following two integrals: i) $\int_{-2}^{2} \frac{dx}{\sqrt{4-x^2}}$ and ii) $\int_{0}^{\infty} e^{-x} \ln x \, dx$. Take care to handle any divergences in the integrand as well as the range of integration extending to infinity.

2. Second, use the two starter programs (*rw2d.m/generate_rw.m*) to generate random walks on the square lattice in two dimensions (the same programs and their outputs have been discussed in class already). For this lab, modify the programs (or write your own equivalent ones) to walks of <u>random</u> step length $0 < d < 1$ in (continuously) random directions (i.e., the walk is still in two dimensions, but no longer on a lattice). Analyze the mean square displacement $\langle r_n^2 \rangle$ for n-step continuous random walks, and calculate the mean fluctuation (standard deviation) of r_n^2 (i.e., the square root of the variance of r_n^2 defined by $\sqrt{\langle (r_n^2)^2 \rangle - \langle r_n^2 \rangle^2}$). Is the latter of the same order as $\langle r_n^2 \rangle$ itself? If that is true, then the fluctuation is just as large as the mean, and thus you cannot tell its statistical properties by generating just a few random walks, however long (i.e., many steps) they may be.

3. Finally, use the starter programs *saw2d.m/generate_saw.m* (or your own equivalent codes) to simulate self-avoiding walks (SAW) on the square lattice. Obtain an estimate of the Flory exponent ν, defined in terms of the relation $\langle r_n^2 \rangle = const \times n^{2\nu}$ between the mean squared displacement and the length n of the SAW. Also study the fluctuations of $\langle r_n^2 \rangle$ as you did for the random walks. Make sure that you understand the algorithm that implements self-avoidance, i.e., how the algorithm keeps the desired properties of the ensemble (namely, equal probability for each SAW of equal number of steps).