PHY566 Group Assignment

Group A
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April 2, 2015

1 2D random walk

In this part, we would do a problem about random walk in 2 dimensions, taking steps of unit length in ±x or ±y direction on a discrete square lattice.

1.1 Part(a)

In this part,we plot $\langle x_n \rangle$ and $\langle {x_n}^2 \rangle$ up to n=100 by averaging over at least 104 different walks. The result are shown in Fig.2.

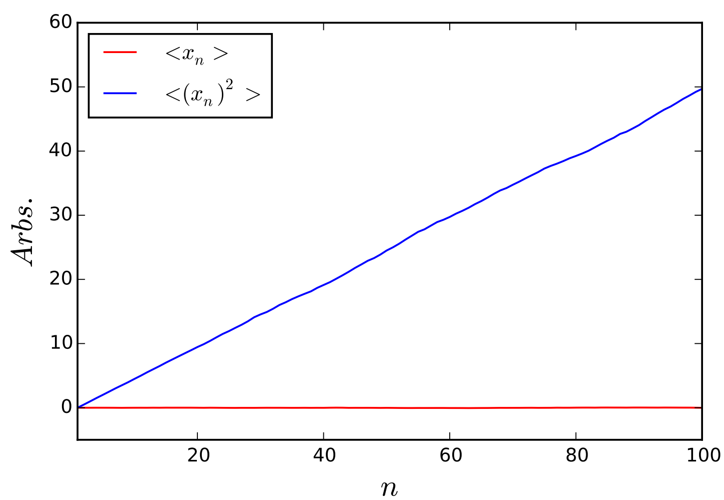

Figure 1: $\langle x_n \rangle$ **and** $\langle {x_n}^2 \rangle$ **up to n=100 by averaging over at least 104 different walks.**

You can see that the $\langle x_n \rangle$ is always zero which is agree with our expectation. For the random walk is walking randomly along +x direction and -x direction, so the average of that would be zero after many times of random walks. As you can see that correlation between $\langle {x_n}^2 \rangle$ and n is linearly, and the ratio is like 0.5. The reason for that is that the random walks in two axis, neither ±x direction or ±y direction, so the probability of walking in ±x direction is almost 0.5 which is also agree with our results.

1.2 Part(b)

By seeing the mean square distance from the starting point ¡ r2 ¿ up to 100 times by averaging over at least 104 different walks, shown in Fig.**??**, we can see that the motion is diffusive and the value of the diffusion constant after an curve fit is like 0.99995 which is very close to 1. The reason for that the mean square distance from the starting point stands for the walk of two axis (x and y), so the probability of that is equal to 1 which is agree with our plot.

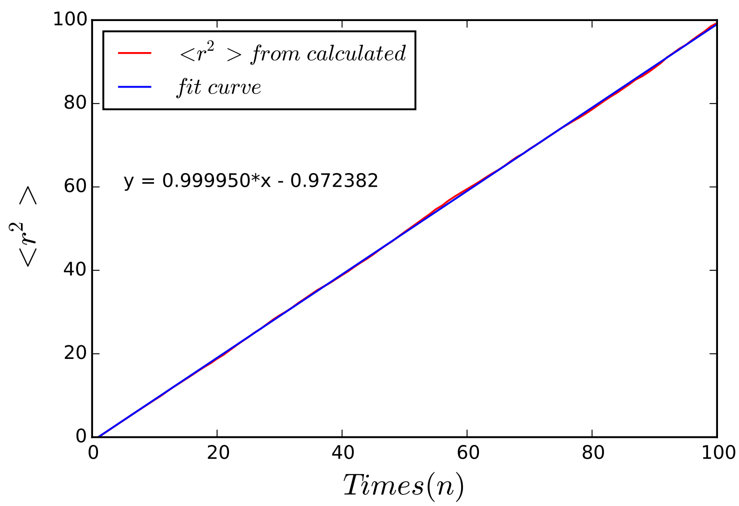

Figure 2: $\langle r^2 \rangle$ **up to n=100 by averaging over at least 104 different walks.**

2 Diffusion Equation

In this section, we will solve the diffusion problem both analytically and numerically given the initial density distribution.

2.1 Part(a)

In this section, the the spatial expectation value for $\left\langle x(t)^2 \right\rangle$ is determined analytically, given a 1D Normal Distribution$\rho(x,t)$.

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)^2}} e^{-\frac{x^2}{2\sigma(t)^2}}$$

In general, the expected value of a measurable function of x, $g(x)$, given that x has a probability density function $f(x)$, is given by the inner product of f and g.

$$\langle g(x) \rangle = \int_{-\infty}^{\infty} g(x) f(x)\, \mathrm{d}x$$

In this case, we substitute $g(x)$, and$f(x)$ with $x(t)^2$ and $\rho(x,t)$ receptively. For every instant, t can be regarded as a constant in the integrand, hence the expected value for x^2 is a function of t.

$$\left\langle x^2 \right\rangle = \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2\pi\sigma(t)^2}} e^{-\frac{x^2}{2\sigma(t)^2}}\, \mathrm{d}x = \sigma(t)^2$$

2.2 Part(b)

In this subsection a program to solve the 1D diffusion equation using the finite difference form with a diffusion constant D = 2, with an initial density profile that is sharply peaked around x = 0, but extends over a few grid sites (box profile). To avoid the determination of the number of particles that are involved in this diffusion system, we use the notion of probability to study such system. Fig.3 illustrates the initial probability density.

Then we apply the finite difference form of the diffusion equation to solve the problem numerically.

$$\rho(t+dt,x) = \rho(t,x) + D\frac{\Delta t}{\Delta x^2}[\rho(t,x+dx) + \rho(t,x-dx) - 2\rho(t,x)]$$

After that, we fit the calculated densities at later time equal to 50s, 100s, 300s, 500s and 900s corresponding to a Normal Distribution with $\sigma(t) = \sqrt{2Dt}$. Fig.4 shows the results.

As it can be seen from raw eyes that all the numerically calculated densities can be fitted well by the the normal distribution with $\sigma(t) = \sqrt{2Dt}$.

We could also compare the fitting parameter with the idea Normal Distribution with $\sigma(t) = \sqrt{2Dt}$. Table.1 contains these values. By comparing the analytical and fit results we can verified that the numerically calculated density profile corresponds to a Normal Distribution with $\sigma(t) = \sqrt{2Dt}$ at later times.

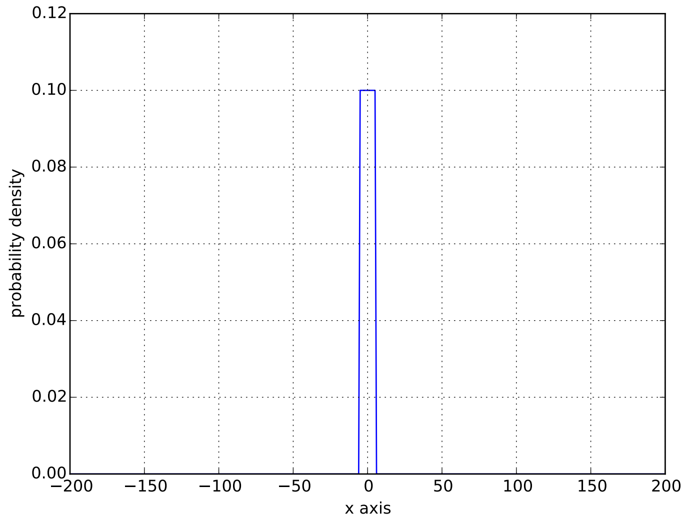

Figure 3: **Initial probability density that is sharply peaked around x = 0, but extends over a few grid sites (box profile)**

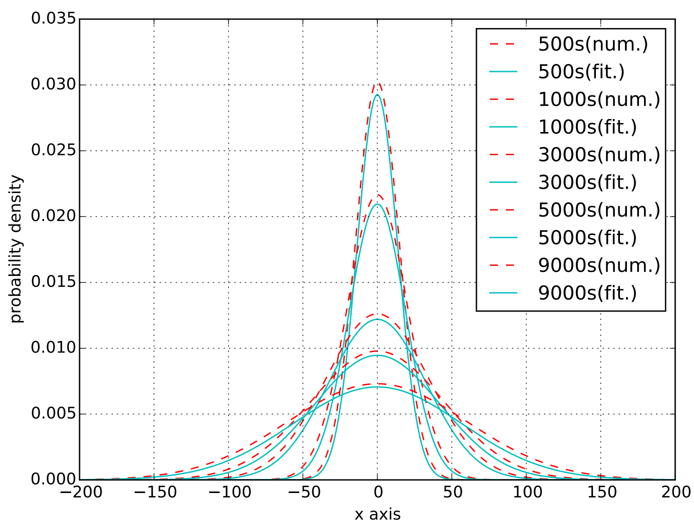

Figure 4: **Numerically calculated probability densities with the fitting line at different times**

Table 1: Analytical and fit parameters for density distribution

Time[s]	μ(analytical)	μ(numerical)	σ(analytical)	σ(numerical)
500	0	-1.74$\times 10^{-8}$	14.14	13.63
1000	0	-1.21$\times 10^{-8}$	20.00	19.04
3000	0	-2.01$\times 10^{-8}$	34.64	32.71
5000	0	1.19$\times 10^{-8}$	44.72	42.15
9000	0	-2.74$\times 10^{-8}$	60.00	56.49