Modelling and Simulation
Lab Assignment - 5

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I. Abstract

Modeling 1-D Random Walk:
In this lab we will explore the variety of random walk problems in one dimension. The objective is to learn how to extract useful information from simulation-based study.

II. Symmetric Random Walk

In this first part we will simulate the symmetric random walk. Let the probability of a random walker going left or right be the same p = q = $\frac{1}{2}$. The walk starts from the site 0 and proceeds by successive steps of unit length. For direction we adopt the convention that right is positive and left is negative. Write a program to implement the random walk of n steps, using a uniform random number generator to choose the direction of each step. Run your code to calculate the mean and mean square displacement(msd). What is the size of the ensemble beyond which you observe Einstein's relationship (Show in a single figure by taking ensemble of different sizes.) What is the value of Diffusion constant? Make a histogram of the distribution of P_n(m) obtained from your data, where P_n(m) is the probability of being at the m^{th} site after n steps.

Here p = q = 0.5, so for higher number of time steps, the displacement is almost zero which can be seen from histogram plots of final position for different ensemble sizes (number of time steps n =100 in all cases). As the ensemble size increases the plot becomes normal.

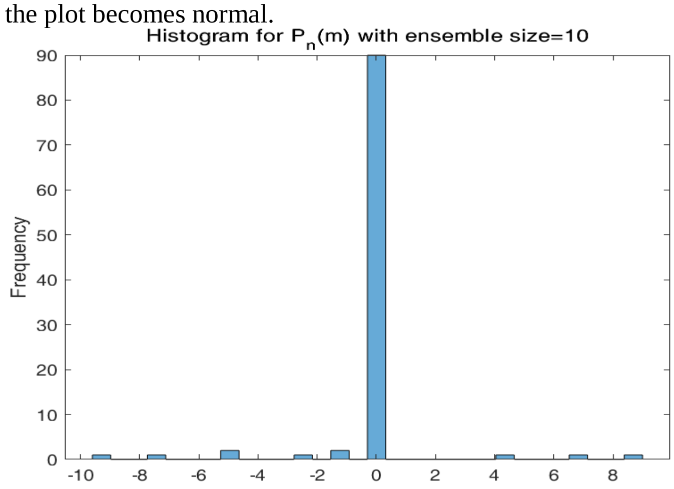

Figure 1.

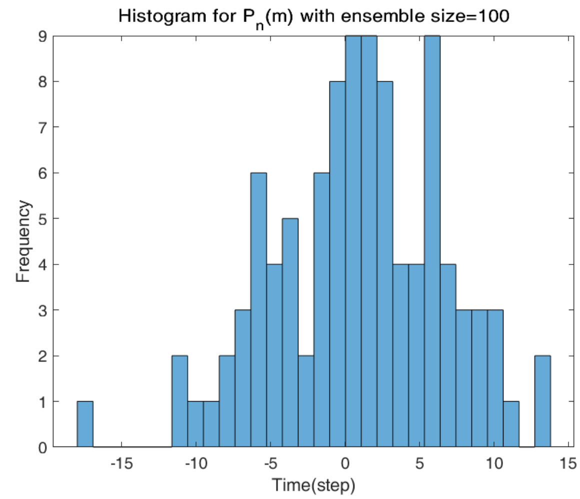

Figure 2.

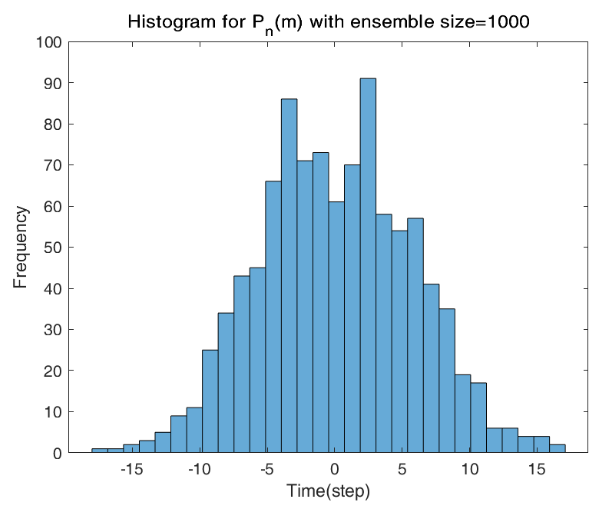

Figure 3.

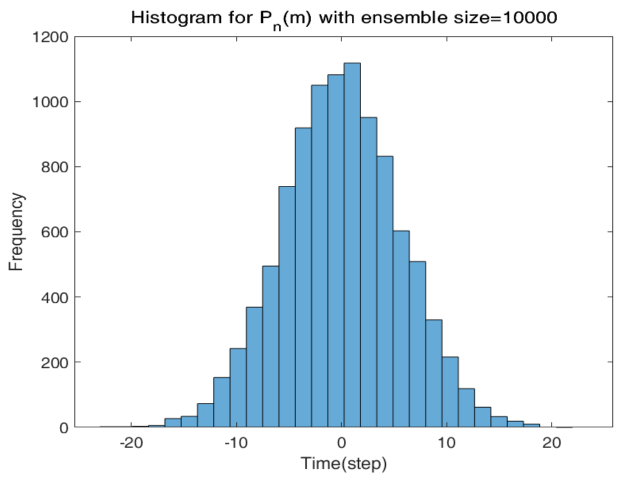

Figure 4.

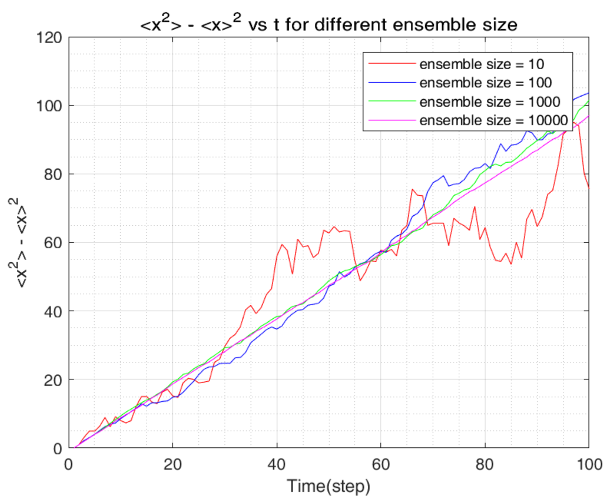

Figure 5.

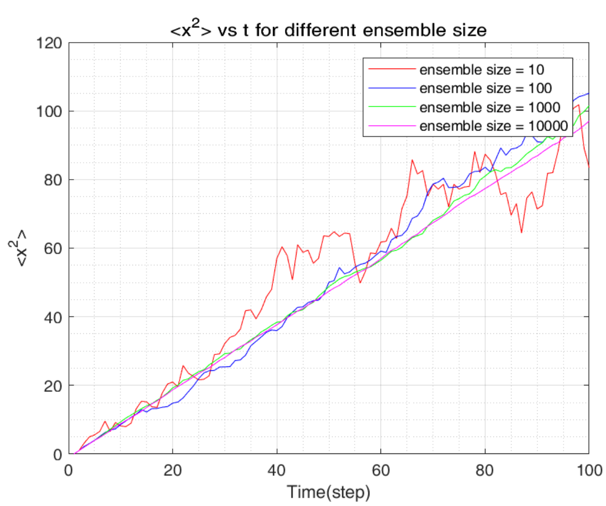

Figure 6.

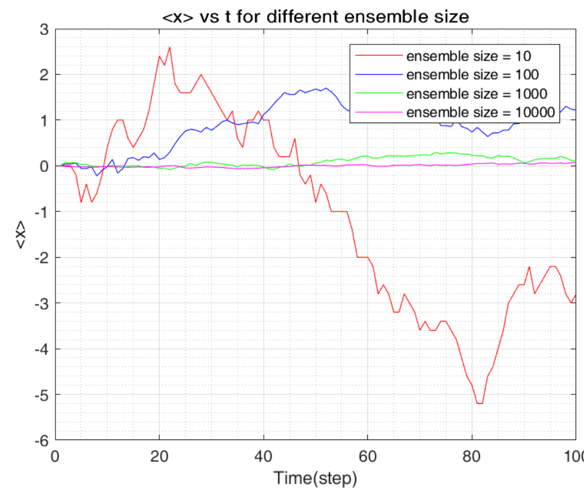

Figure 7.

- For ensemble size of 10000, the curve of $< x^2 > - < x >^2 \;\; vs\; t$ is almost linear with non-zero slope.
- The curve of $< x^2 > vs\; t$ is also linear with non-zero slope for large ensemble size.
- The curve of $< x > vs\; t$ is fitting x-axis i.e. $< x > = 0$ for large ensemble size.
- Diffusion constant
  D = Slope of $< x^2 > - < x >^2 \;\; vs\; t$
  $D = \frac{97.72}{100} = 0.977 \approx 1.$

It is clear that Einstein relationship is observed after ensemble size of 1000.

III. Asymmetric Random Walk

Let us now consider the case of unequal probabilities of going left or right. Such a situation arises quite often when we force the random walker to prefer one of the directions. Think of the motion of an electron inside the metal in the presence of electric field. Let p be the probability of going right and q = 1- p be the probability of going left. Assuming that the random walker takes unit steps at each step what is the mean distance and mean squared displacement. Compare with the previous case.

Here p = 0.7 and q = 0.3. Hence after n = 100 steps there are almost 70 right steps and 30 left steps leading to final position of 40 which can be seen from following histogram plots. As the ensemble size increases the plot becomes normal.

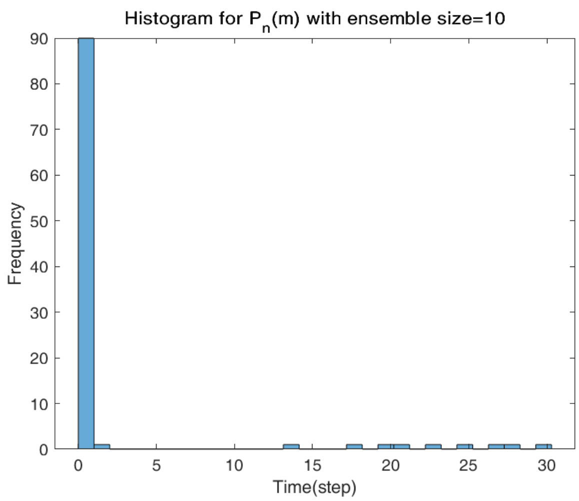

Figure 8.

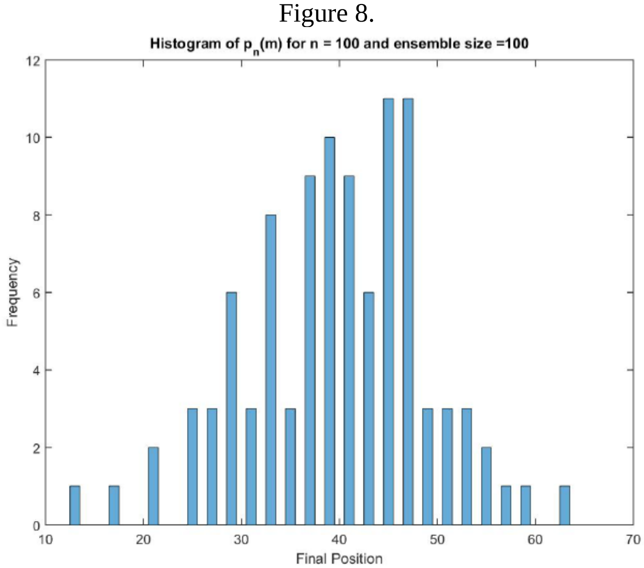

Figure 9.

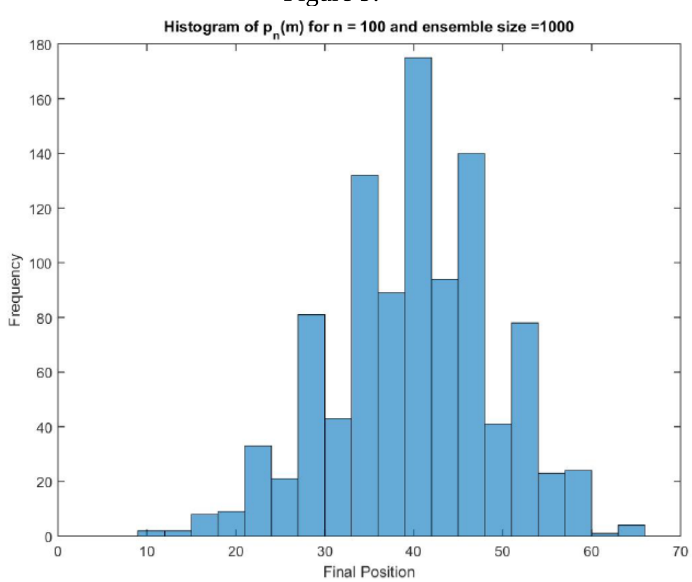

Figure 10.

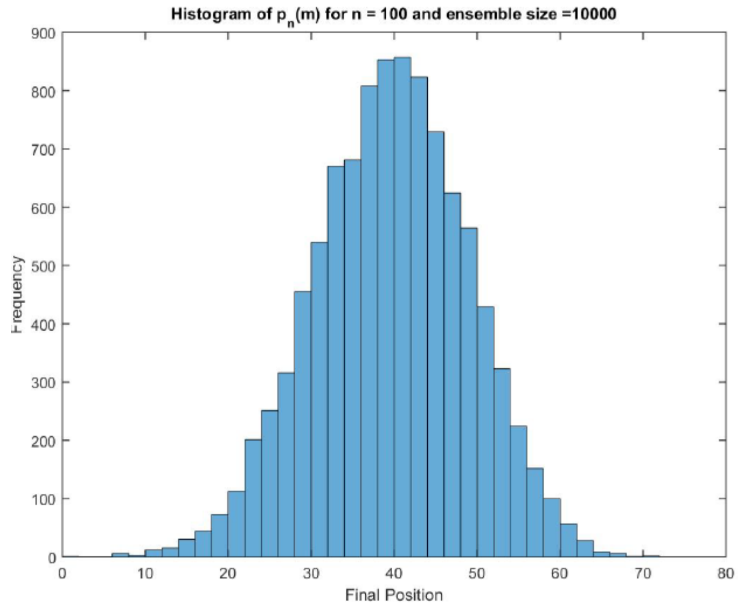

Figure 11.

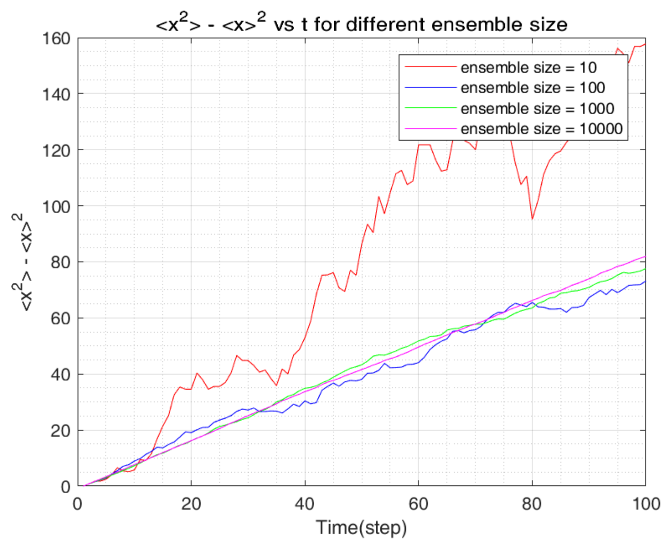

Figure 12.

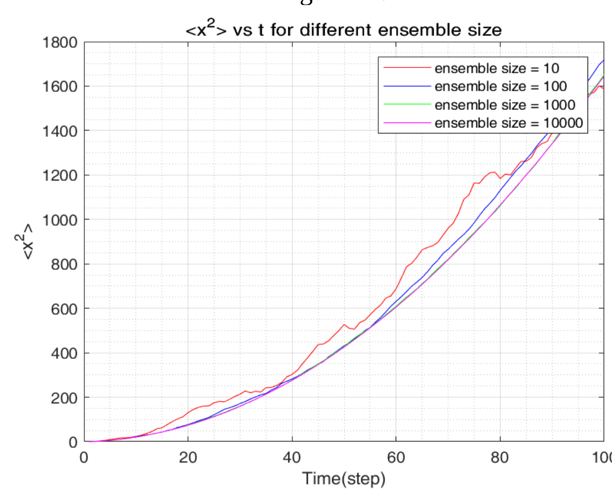

Figure 13.

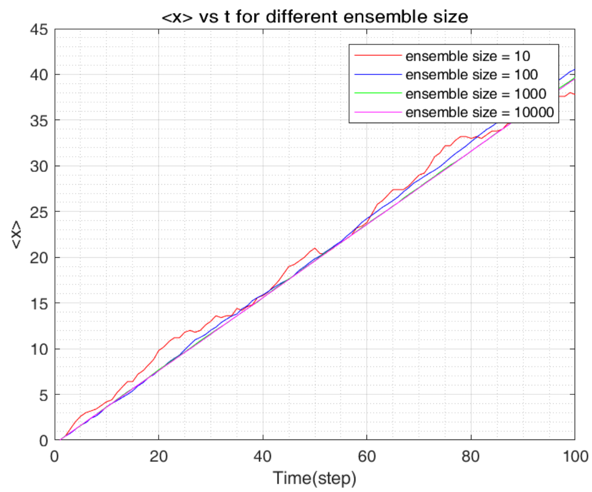

Figure 14.

- For ensemble size of 10000, the curve of $< x^2 > - < x >^2 \ \ vs\ t$ is almost linear with non-zero slope.
- The curve of $< x^2 > vs\ t$ is parabolic for large ensemble size.
- The curve of $< x > vs\ t$ is not fitting x-axis t i.e. $< x > \neq 0$ for large ensemble size.
- Diffusion constant
  D = Slope of $< x^2 > - < x >^2 \ \ vs\ t$
  D = $\frac{84.12}{100}$ = 0.8412 < 1.

It is clear that Einstein relationship is observed after ensemble size of 1000.

IV. Symmetric Random Walk Variant

Let us consider the random walk of part (a) but with another state added. The random walker moves to the left or right with probability p, however, now it can decide not to move with probability r = 1 - 2p. If p = 1/2 then it is the exact same problem of part (a). Analyse this random walk problem as we take different values of r.

Here the random walker choses not to move based on the value of r. First, we generate a random value of r. If the value of r $< r_0$ (r_0 = threshold for making the decision for moving or not), then the walker choses not to move. So, the position of the walker remains constant.

Now if the value of r >= r_0, then the walker moves. Now we have to decide in which direction he moves.
For that, we are given that r = 1 - 2p. So, $p = \frac{1-r}{2}$.
Now here the value of p ranges from 0 to $\frac{1-r_0}{2}$.
We call the value $\frac{1-r_0}{2} = p_0$ which is threshold of p.

So, now if the value of p < p_0, the random walker moves to left else it moves to right.
The following figure shows the random walk generated based on the above properties:

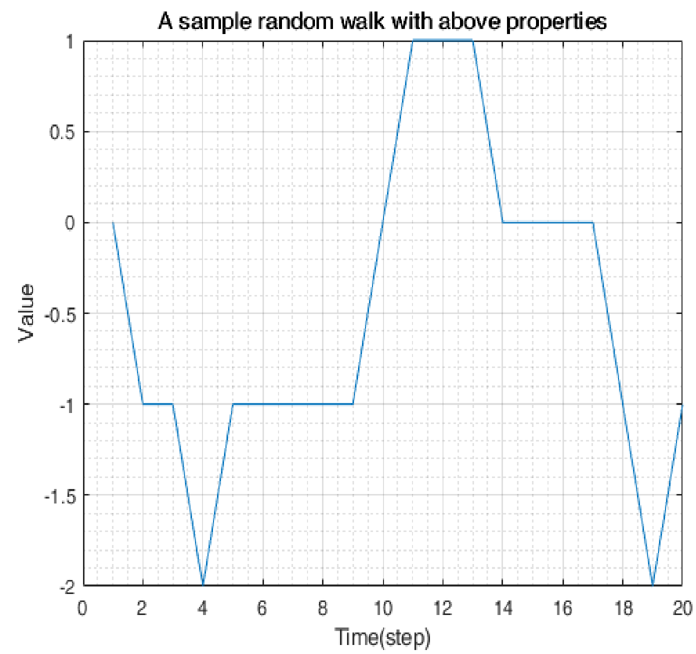

Figure 15.

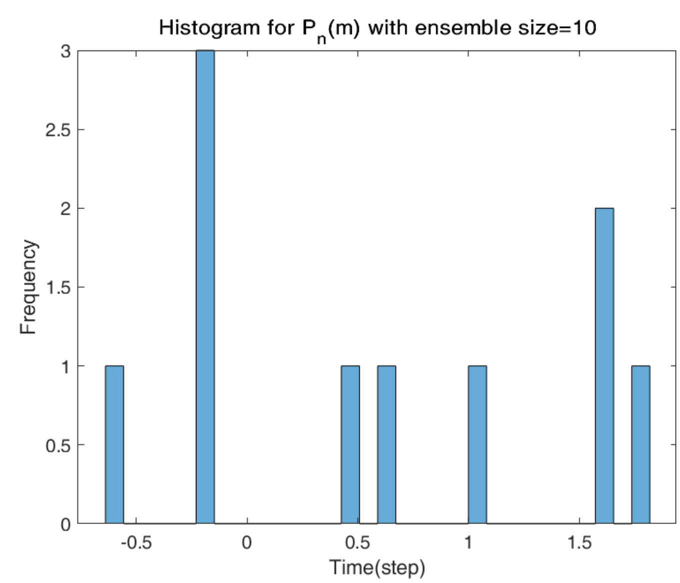

Figure 16.

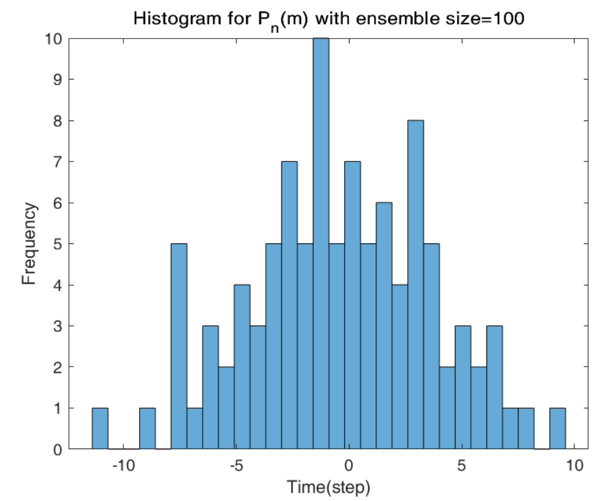

Figure 17.

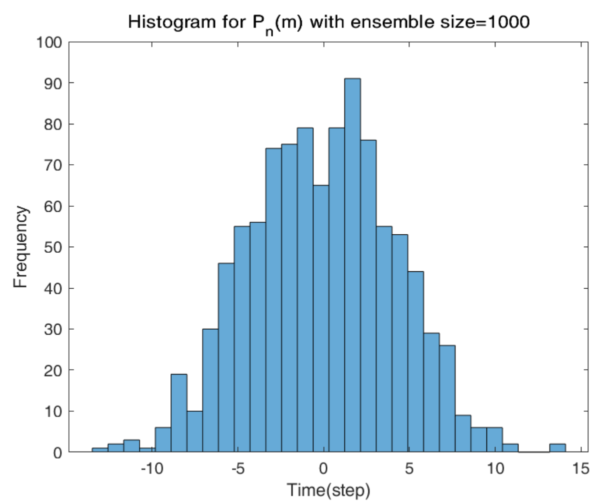

Figure 18.

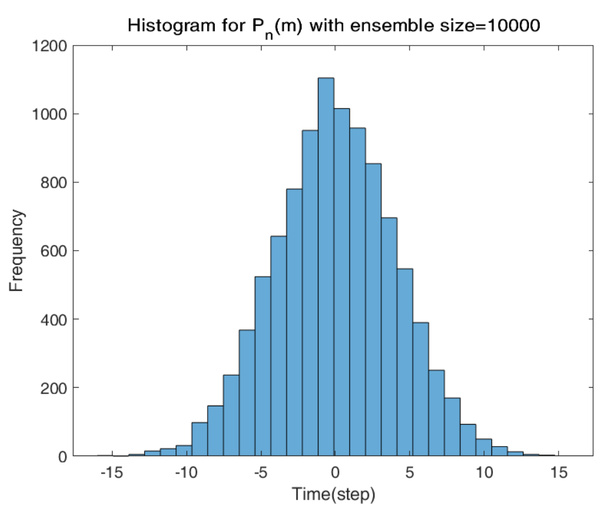

Figure 19.

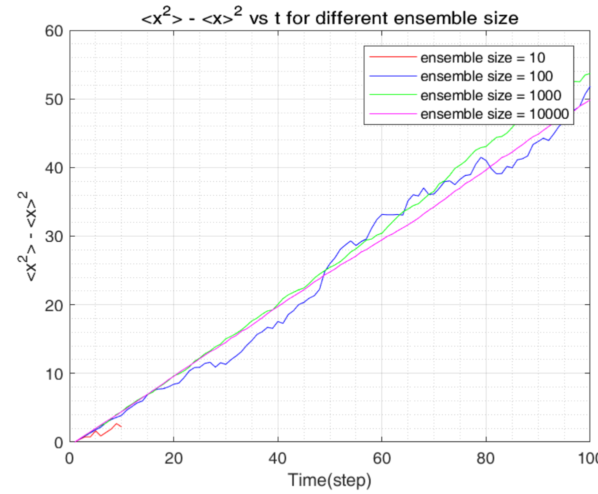

Figure 20.

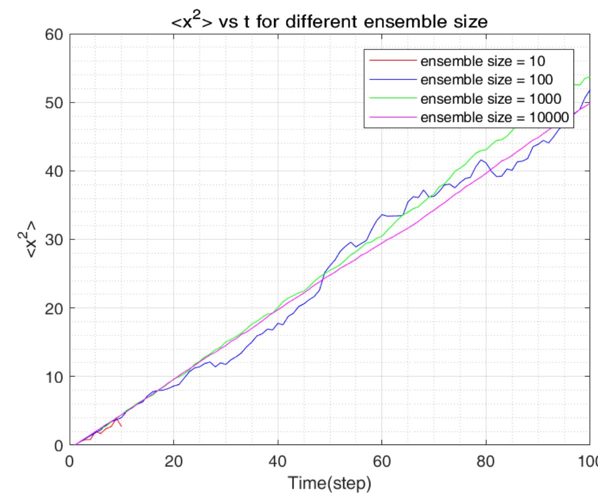

Figure 21.

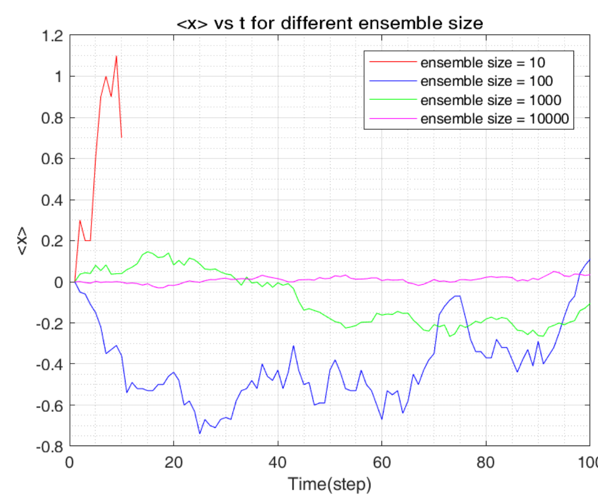

Figure 22.

- For ensemble size of 10000, the curve of $< x^2 > - < x >^2 \ vs\ t$ is almost linear with non-zero slope.
- The curve of $< x^2 > vs\ t$ is also linear with non-zero slope for large ensemble size.
- The curve of $< x > vs\ t$ is almost fitting x-axis t i.e. $< x > \approx 0$ for large ensemble size.
- Diffusion constant
  D = Slope of $< x^2 > - < x >^2 \ vs\ t$
  D = $\frac{49.85}{100}$ = 0.4985 < 1.

It is clear that Einstein relationship is observed after ensemble size of 1000.