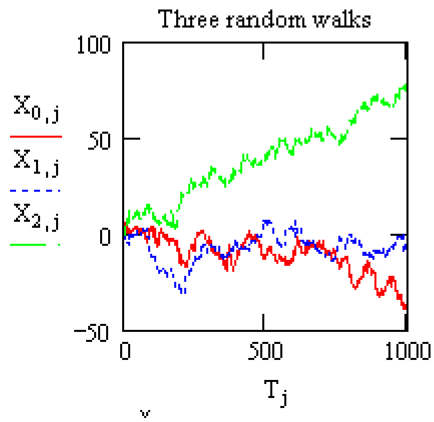
Random walks and diffusion

Two dimensional random walk with mean free time τ:



First we will look at a two dimensional random walk. We will assume that an electron is moving through a plasma and has elastic collisions with neutral atoms that randomize the direction of travel. The length of the velocity vector remains the same in the collision but the angle θ of the vector is given a new value between zero and 2π. We will follow 251 particles (subscript i) for 1001 time steps (subscript j). The particles' position on the x axis will be calculated and recorded and the y position will not be. During each time interval, the particle moves an additional distance v cos (θ) Δt. The distances will be added in a program loop.

In the random numbers exercise, we learned that if the mean time between random events is τ, the random intervals between events can be chosen using $-\tau$ { ln [rnd(1)] }.

Define some variables:

$v := 1$ $imax := 250$ particle number $jmax := 1000$ time step number

$j := 0 .. jmax$ $i := 0 .. imax$ $\tau := 1$

We find the location of the particle by adding up the distances travelled in a program loop. Within each step, the particle moves at an angle in the x,y plane that is selected randomly.

```
X := | X[imax, jmax] ← 0
     | for  i ∈ 0 .. imax
     |   for  j ∈ 1 .. jmax
     |     | Δt ← −τ·ln(rnd(1))
     |     | θ ← 2·π rnd(1)
     |     | X[i,j] ← X[i,j−1] + v cos(θ)·Δt
     | X
```

i is the row number
j is the column number, for the matrix
Initialize all X to zero by initializing the last element of the array.

Δt is selected so that the probability of a time t between collision is proportionals to exp(-t/τ)

θ is selected randomly on the interval (0,2π). The distance along the x axis increases by v cos(θ) Δt at each time step.

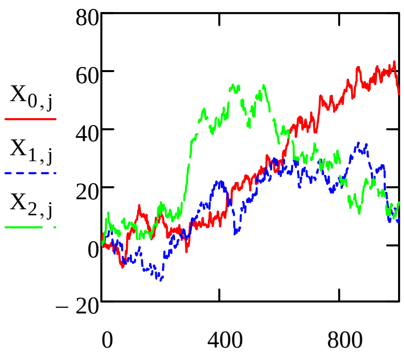
Calculate the mean square distance from the origin after collision j:

$$MSX_j := \sum_{i=0}^{imax} \frac{\left(X_{i,j}\right)^2}{imax + 1}$$

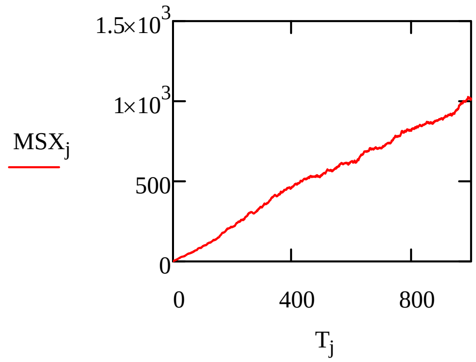
MSX stands for mean square X value. The sum over i above is a sum over particles.

$T_j := j \cdot \tau$ mean time after the jth collision.

Three of the random walks look like:



The mean square distance for the group as a function of time:



The slope of the graph of the mean square distance MSX is: $\text{slope}(T, MSX) = 0.995$

This slope is related to the diffusion coefficient.

How are the final locations distributed in x?
We can look at this by making a histogram of the final locations.
These are in the last column of the matrix X.
First we put the last column of X into a vector S using the submatrix command.

$S := \text{submatrix}(X, 0, imax, jmax, jmax)$

For a histogram plot, we need to sort the values into bins. We will make 20 bins 10 units wide going from -100 to +100. The hist function sorts the values of S into the bins.

$k := 0 .. 20$

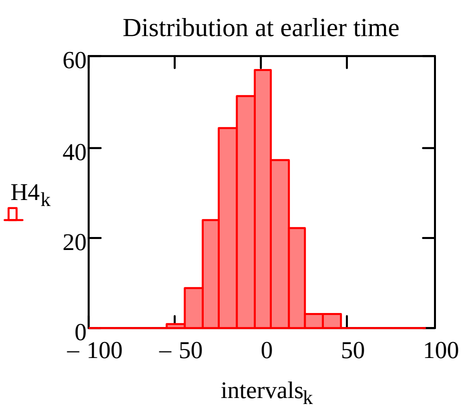
$intervals_k := 10 \cdot (k - 10)$

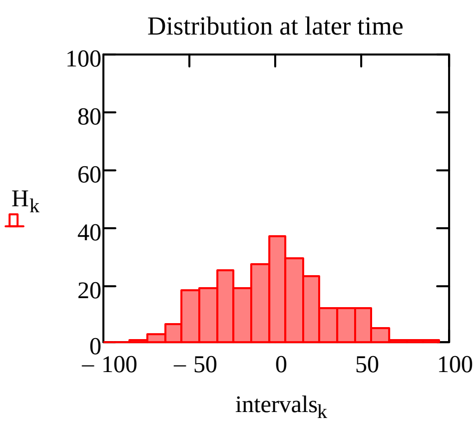
Make a histogram $H := \text{hist}(intervals, S)$

Make another histogram after 1/4 of the collisions: $j4 := \text{ceil}\left(\frac{jmax}{4}\right)$ $S4 := \text{submatrix}(X, 0, imax, j4, j4)$

$H4 := \text{hist}(intervals, S4)$

At earlier times, the distribution is narrower and higher:





Are these distributions what we expect?

$N := imax$ is the number of particles in our sample $N = 250$

What is D, the diffusivity?
For a 2-d random walk characterized by a mean free time τ, the diffusivity is $D = \frac{1}{2}\langle v^2 \rangle \tau$

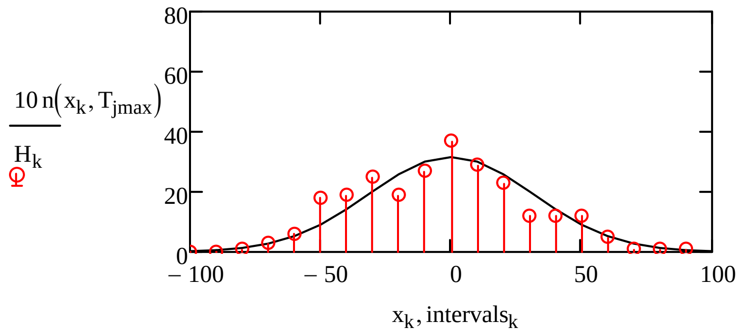
where $\langle v^2 \rangle$ is the mean squared velocity, which is unity for our case with v = 1. In 3-d, the 1/2 is replaced by 1/3. For $\tau = 1$ we have that:

$D := \frac{1}{2}$ When all particles begin at the origin, the solution to the diffusion equation is

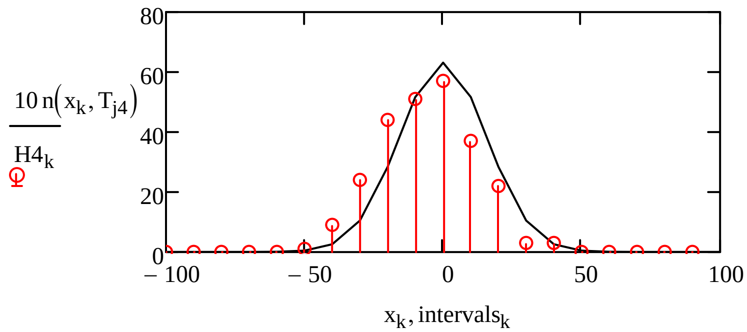
$x_k := intervals_k$

$$n(x,t) := \frac{N}{\sqrt{4 \cdot \pi \cdot D \cdot t}} \cdot e^{\frac{-x^2}{4 \cdot D \cdot t}}$$

Now compare the "simulation" with the expected Gaussian curve.



Distribution after jmax collisions.



Distribution after 1/4 of the collisions.

This shows that the distributions that we get from the random walk above is reasonably well represented by a Gaussian. We have multiplied n(x,t) by 10 because our histogram bars are calculated for a bin width of 10 and n(x,t) is defined for a bin width dx of one.

Try it:
1. If you select "calculate worksheet" from the Math menu the answers will change because a different set of random numbers is used. How much is the change?

2. Does the histogram become closer to the Gaussian if the number of particles imax is increased from 250 to 1000?

Random walk in 3 dimensions with mean free time τ

$imax := 250$ particle number $jmax := 1000$ time step number

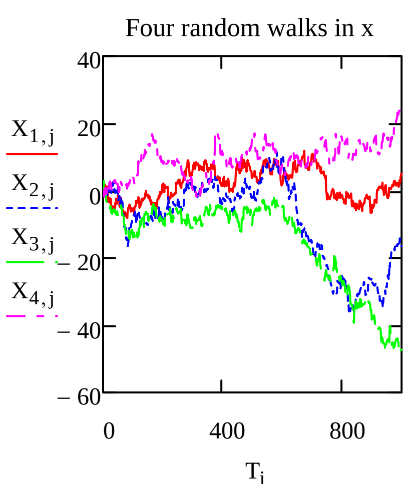
```
X := | X[imax, jmax] ← 0
     | for i ∈ 0 .. imax
     |   for j ∈ 1 .. jmax
     |     | s ← rnd(2) − 1
     |     | v_z ← v·s
     |     | v_xy ← v·√(1 − s²)
     |     | θ ← 2·π rnd(1)
     |     | Δt ← −τ·ln(rnd(1))
     |     | X[i,j] ← X[i,j−1] + v_xy cos(θ)·Δt
     | X
```

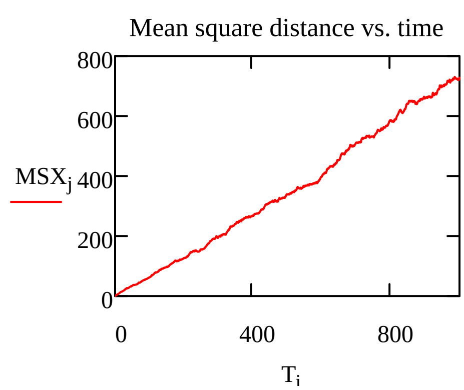
This program loop stores the X values for a random walk in three dimensions. How do I project the velocity vector randomly onto the polar and azimuthal angles? It is not correct to choose a polar angle randomly on the interval $-\pi/2$ to $+\pi/2$. On a globe, there is more land within a degree of the equator than within a degree of the poles. All areas on the spherical surface must be equally represented. We have to use a different weighting that makes angles near the equator more common. It can be shown that if v is the length of the vector, the random projection onto the z direction is simply $v_z = v$ [rnd(2)-1], in other words, v_z is uniformly distributed between -v and +v. The part of v that is left for the x,y plane is the square root of $v^2 - v_z^2$. We then take this remainder and use a random azimuthal angle between 0 and 2π to project it onto v_x and v_y.

Find the mean square distance of all particles (sum over i) at each time j:

$$MSX_j := \frac{1}{imax+1} \cdot \sum_{i=0}^{imax} \left(X_{i,j}\right)^2$$

$T_j := j$ The time at the jth time step





$slope(T, MSX) = 0.745$

From the characteristics of the Gaussian n(x,t) on p.3, we can find that the mean square value of x is $\langle x^2\rangle = 2\,D\,t$. We also have found that $D = 1/3$ for our 3-d problem, so the slope of the plot of $\langle x^2\rangle$ versus t should be 2/3.

Try it: How does the slope of MSX versus t (for constant τ) compare with the expected 2/3? Does the agreement improve if imax (the number of particles -1) is increased from 250 to 1000?

Random walk in 3 dimensions with mean free path λ

$imax := 250$ particle number $jmax := 1000$ time step number

Supppose our collisions are characterized by a constant mean free path. Constant, in this case, means that the mean free path does not vary with velocity. Then the distance traveled, Δs, must be chosen randomly, not the time interval Δt. The distance s is the distance in all three dimensions. We have been plotting only the distance in the x direction. Our program loop will find the path length between collisions, Δs, then project this onto x using the ratio of v_x to total v.

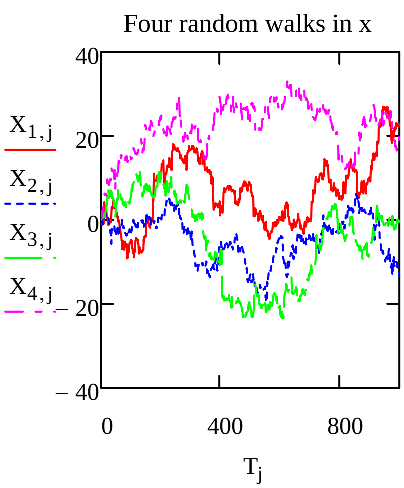
If λ is the mean free path, the distance between collisions can be chosen using Δs = -λ ln (rnd(1)).

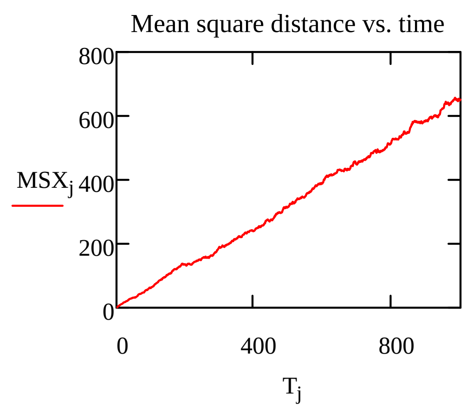
the mean free path $\lambda := 1$

```
X := | X[imax,jmax] ← 0
     | for i ∈ 0 .. imax
     |   for j ∈ 1 .. jmax
     |     | s ← rnd(2) − 1
     |     | v_z ← v·s
     |     | v_xy ← v·√(1 − s²)
     |     | θ ← 2·π rnd(1)
     |     | v_x ← v_xy·cos(θ)
     |     | Δs ← −λ·ln(rnd(1))
     |     | X[i,j] ← X[i,j−1] + Δs·(v_x / v)
     | X
```

Find the mean squared distance at time step j:

$$MSX_j := \sum_{i=0}^{imax} \frac{(X_{i,j})^2}{imax + 1}$$





$slope(T, MSX) = 0.657$

For a random walk with a constant mean free path, the diffusivity is:

$$D = \frac{1}{3}\langle \mathrm{v} \rangle \lambda$$

where <v> is the mean value of the speed and λ, the mean free path, is the mean distance between collisions.

If the cross section for collisions is σ, and if the field particles (those we are colliding with) are at rest, the mean free path is:

$$\lambda = \frac{1}{n\sigma}$$

where n is the number density of field particles. If the field particles are moving, the mean free path is reduced.

Try it: If 1000 time intervals are chosen using - τ ln[rnd(1)], what is the mean value of the interval?

Notes

1. Selection of the time between collisions or the distance travelled between collisions using the -ln[rnd(1)] function is covered in the first random numbers exercise.

2. There is a nice elementary discussion of random walks and diffusion in P. W. Atkins, *Physical Chemistry* (Oxford University Press, Oxford, 1994), Fifth Edition, Chapter 24 and the Appendix on random walks.