Diffusion excersise, FYS-PGP 4300

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(Dated: August 31, 2004)

These analytical excersises are intended to make you familiar with some solutions to the diffusion equation and to obtain valuable information from typical distributions.

DIFFUSION FROM A POINT SOURCE

Verify that

$$c(x,t) = \frac{A}{\sqrt{t}} e^{-x^2/4Dt} \tag{1}$$

is a solution to

$$\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial x^2} \tag{2}$$

DIFFUSION IN LIQUIDS

Figure 1 shows typical concentration curves, $c(x,t)$, for diffusion from a point source at the origin $x = 0$ at time $t = 0$. Measure the width of the curves to determine the diffusion constant.

RANDOM WALKER

Release n_p random walkers at the origin of the x-axis at time $t = 0$. The RW make steps of size d to the left or right at time steps τ. Assume that the random walk represents a diffusion process given by equation (1). Use the Einstein-Smoluchovski relation

$$D = \frac{d^2}{2\tau} \tag{3}$$

to calculate the distribution function $f(n_p, n_t)$ after $n_t = t/\tau$ timesteps. The Matlab m-file given below simulates $n_p = 10000$ random walkers performing $n_t = 100$ steps (of unit length, $d = 1$, $\tau = 1$) and plots the distribution histogram together with the theoretical curve.

DISTRIBUTED SOURCE, THE ERROR FUNCTION

When the concentration distribution at time 0 is a step function: $c(x \leq 0, t = 0) = c_0$, $c(x > 0, t = 0) = 0$ the solution to the diffusion equation is the integrated effect over point sources between $x = 0$ and $x = -\infty$:

$$c(x,t) = \int_x^{\infty} \frac{c_0}{2\sqrt{\pi D t}} e^{-\xi^2/4Dt} d\xi \tag{4}$$

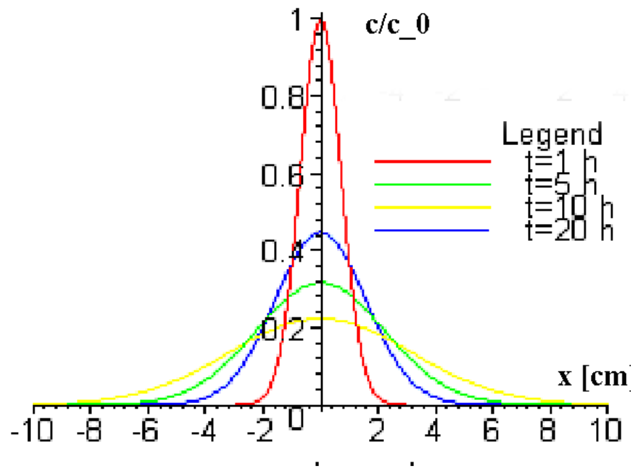

FIG. 1: Concentration curves $c(x,t)$ for diffusion from a point source at the origin at time $t = 0$.

Use the transformation

$$\eta = \frac{\xi}{2\sqrt{Dt}} \tag{5}$$

to express $c(x,t)$ in terms of the error function:

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\eta^2} d\eta \tag{6}$$

Use Matlab to plot the curves $c(x,t)$ and $c(\eta)/c_0$ at 1, 5, 10 and 20 hours for the diffusion coefficient you calculated in the first excersise. (The error function in Matlab is erf().)

APPENDIX

```
timesteps=100;
num_part=10000;
%Assume that no particle gets further in one
%direction than half the number of steps it does
xrange=timesteps/2;
%number of x positions is twice the range plus
%the origo
xnumbers=2*xrange+1;
%make a vector with all x positions from -xrange
%to xrange
x=linspace(-xrange,xrange,xnumbers);
%make an empty histogram
```

```
position_histogram=zeros(1,xnumbers);
%repeat this for every particle
for i=1:num_part;
    %create an array (of length timesteps) of
    %random numbers with equal probability of
    %being positive and negative.
    dummy=rand(1,timesteps)-1/2;
    %round negative numbers to -1 and positive
    %numbers to +1
    random_jumps=floor(dummy)+ceil(dummy);
    %the final position is the sum of individual
    %jumps. Add (xrange+1) which is the position
    %of the origo in the histogram array
    final_position=sum(random_jumps)+xrange+1;
    %increment with one the bin in the histogram
    %array where the particle ended up
    position_histogram(final_position)=...
        position_histogram(final_position)+1;
end
%Figure 1 shows that the odd x positions are
%unobtainable for an even number of moves.
%This is in fact unimportant, it only means
% we have data for intervals of 2 instead of 1.
%figure(1)
%plot(x,position_histogram,'o')
%Interpolate for odd x-positions to get a nice plot
position_histogram(2:xnumbers-1)=...
    position_histogram(2:xnumbers-1)+...
    position_histogram(1:xnumbers-2)/2+...
    position_histogram(3:xnumbers)/2;
figure(2)
plot(x,position_histogram)
hold on
%calculate and plot the Maxwell distribution
%corresponding to this many particles and timesteps
halfwidth=sqrt(2*timesteps);
plot(x,2*num_part/(halfwidth*sqrt(pi))*...
     exp(-(x/halfwidth).^2),'r')
```