ChE-402

Solution to exercise problems

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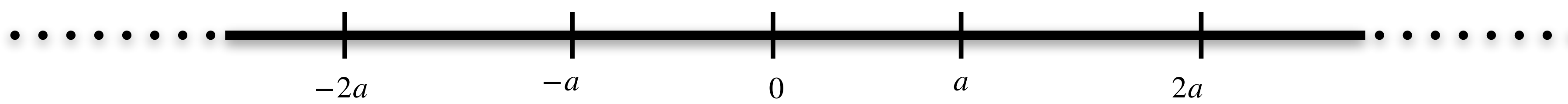
In class exercise 1

Let's look at one-dimensional space divided across several hopping sites.
Initially there are no particles.
At time t = 0, you place 10000 particles at 0.
Calculate number of particles at 0, -a and a, -2a and 2a after 1 s.



$$\Gamma = 100 \ \ \text{hop/s}$$
$$a = 1 \text{ length unit}$$

$$D = \frac{\Gamma a^2}{2}$$

$$P(z,t) = \frac{1}{\sqrt{4\pi D_o t}} \exp\left(\frac{-z^2}{4D_o t}\right)$$

$$N(z,t) = \frac{N_o(t=0, z_0)}{\sqrt{4\pi D_o t}} \exp\left(\frac{-z^2}{4D_o t}\right)$$

In class exercise 1: solution

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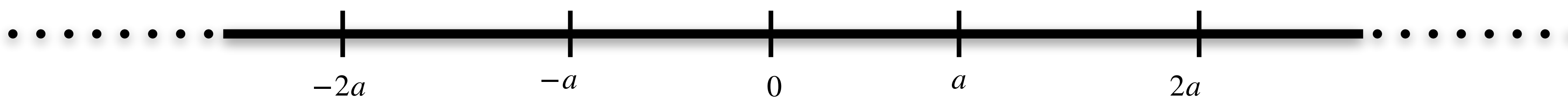

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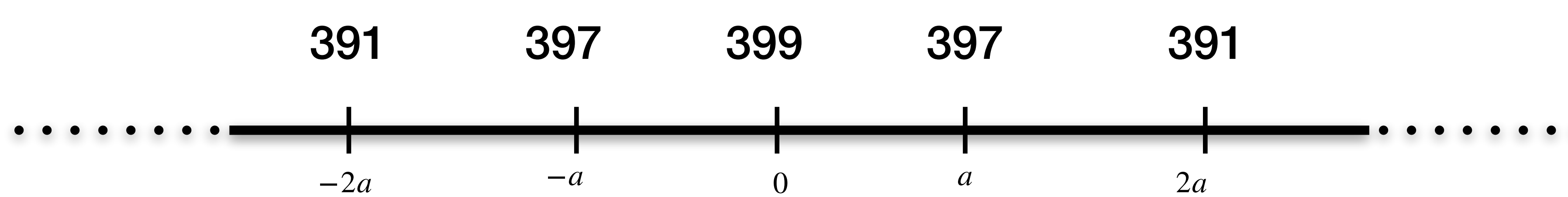
$$D = 50 \text{ length}^2/\text{s}$$



(Numbers are rounded off)

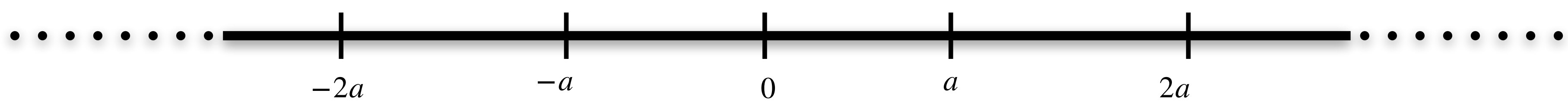
$$N(0,1s) = 399$$

$$N(a,1s) = N(-a,1s) = 397$$

$$N(2a,1s) = N(-2a,1s) = 391$$

In class exercise #2

Continuation of previous problem:
Initially there are no particles.
At time t = 0, you place 100000 particles at 0 and 10000 particles at 2a to make a negative concentration gradient along the x-direction.
Calculate the direction of particle flow at the position a (midway between 0 and 2a) after 1 s.
Calculate the net directional flow of particle (from left to right) at the position a after 1s.



$$\Gamma = 100 \ \text{hop/s}$$
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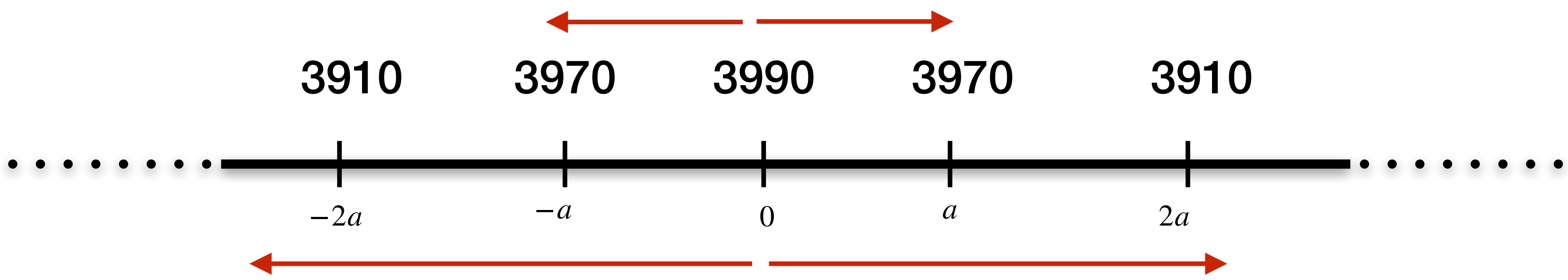
$$N(z,t) = \frac{N_o(t=0, z_0)}{\sqrt{4\pi D_o t}} \exp\left(\frac{-z^2}{4D_o t}\right)$$

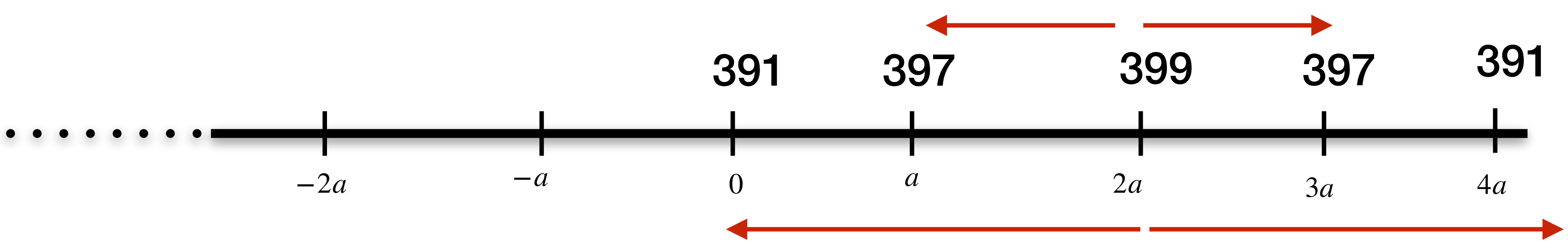
In class exercise #2

We can solve just like previous case:



Profile at 1s originating from 100000 particles at 0 at t =0.

(Numbers are rounded off)



Profile at 1s originating from 10000 particles at 2a at t=0.

(Numbers are rounded off)

Net direction at position a $=$ towards right

Superimpose to get the net directional flow at position a

Net directional flow at a $= 3970 - 397 = 3573$

In class exercise #3: self-diffusion

A gas molecule, He, is diffusing in a one dimensional channel, 1 μm away from the end of channel. Assuming the diffusion coefficient, D_o, to be 10^{-8} cm^2 s^{-1}, calculate the time that it take He to reach the end of channel.

$$\langle r^2(t) \rangle = 2D_o t$$

For 1D diffusion

In class exercise #3: self-diffusion

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For 1D diffusion

$$t = \frac{\langle r^2(t) \rangle}{2D_o}$$

$$r = 1\ \mu m = 10^{-6}\ m$$

$$D_o = 10^{-8}\ cm^2 s^{-1} = 10^{-12}\ m^2 s^{-1}$$

$$t = \frac{\langle 10^{-12} \rangle}{2 * 10^{-12}} = 0.5\ s$$