

# ChE-402

## Solution to exercise problems



Prof. Kumar Varoon Agrawal

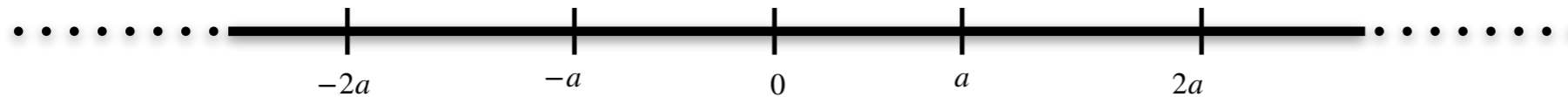
# Exercise problem 1

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.



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

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

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

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

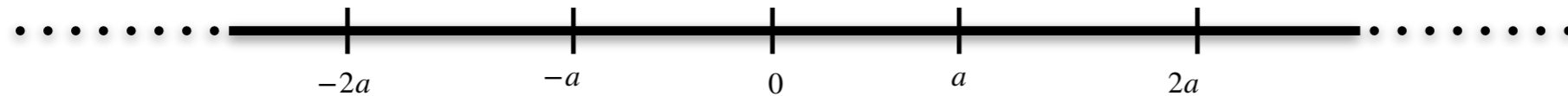
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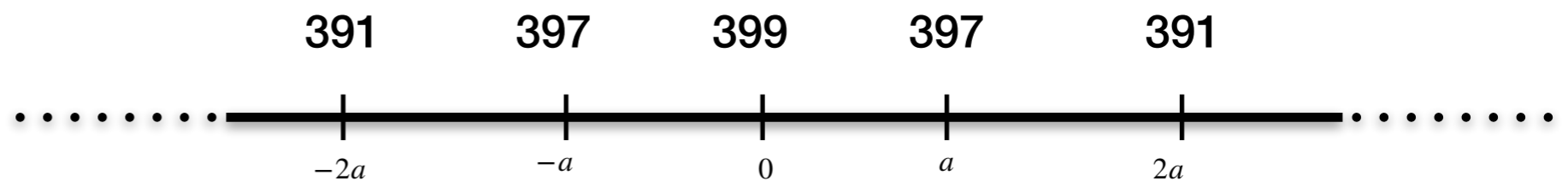
$$N(z, t) = \frac{N_o(t = 0, z_0)}{\sqrt{4\pi D_o t}} \exp\left(\frac{-z^2}{4D_o t}\right)$$

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

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

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

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



(Numbers are rounded off)

# Exercise problem 2

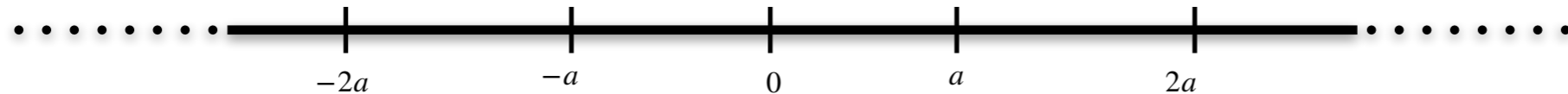
Continuation of previous problem:

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 1 s.



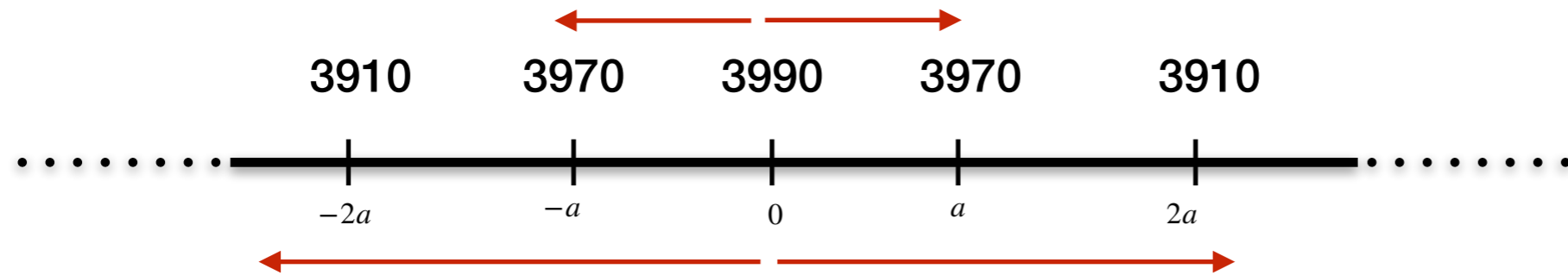
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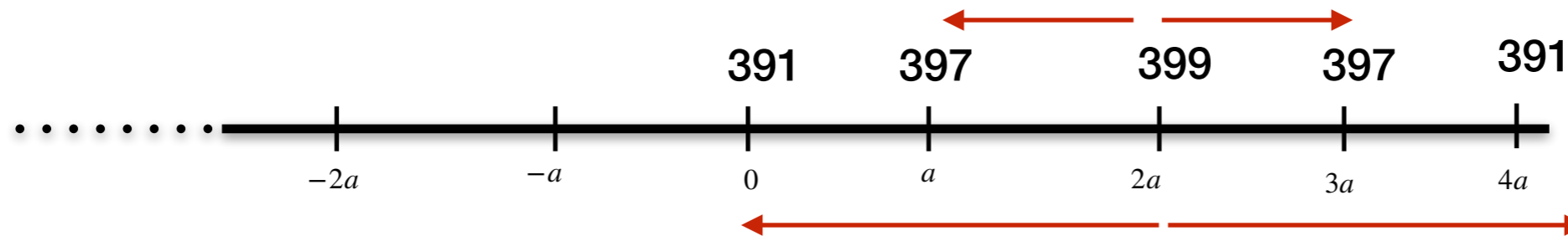
# Exercise problem 2

We can solve just like previous case:



Profile at 1s  
originating from  
10000 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  $a$

$$\text{Net directional flow at } a = 3970 - 397 = 3573$$

# Exercise problem 3

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

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

For 1D diffusion

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

For 1D diffusion

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

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

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

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