

Section 3.3

A Difference Equation and Its Limit

An essential practice of approaching the same problem in different ways, enabling a deeper understanding.

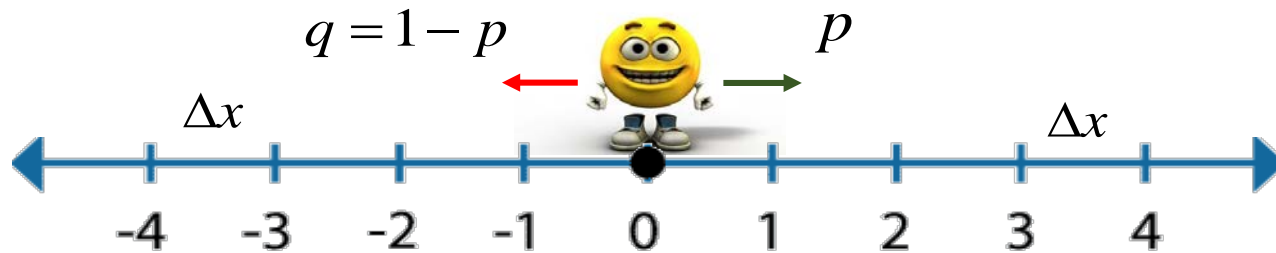
Here is a new way to study random walk:

- Start with a difference equation
- Reach to a PDE solution.

$$w(m, N) = \frac{N!}{2^N p!(N-p)!} \approx \sqrt{\frac{2}{\pi N}} \exp\left(-\frac{m^2}{2N}\right)$$

3.3.1 Difference equation for the probability function

$\bar{w}(x, t)$: the probability that the particle is found at point x at time t .



$$x = m\Delta x \quad t = N\Delta t$$

$$\Delta m = 2$$

N is even $\rightarrow m$ is even. N is odd $\rightarrow m$ is odd

$$\begin{aligned} w(m, N) &= \frac{N!}{2^N p!(N-p)!} = w\left(\frac{x}{\Delta x}, \frac{t}{\Delta t}\right) \\ &= \frac{(t/\Delta t)!}{2^{t/\Delta t} \left(\frac{t/\Delta t + x/\Delta x}{2}\right)! \left(\frac{t/\Delta t - x/\Delta x}{2}\right)!} = \bar{w}(x, t) \end{aligned}$$

3.1.2 Explicit solution

To find $w(m, N)$, the probability that a particle at a point $m \in [-N, N]$ steps to the right of its origin after total N steps.

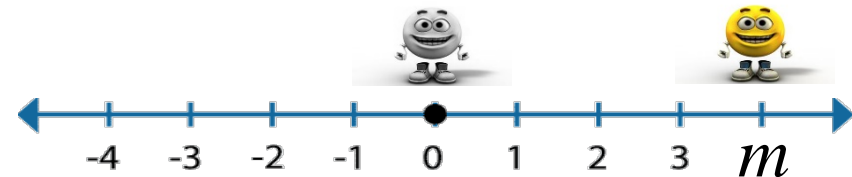
Suppose that the particle

- p steps to the right, $p > 0$
- $N - p$ steps to the left

Displacement m

$$m = p - (N - p) = 2p - N$$

$$p = (N + m)/2$$



e.g. $N=12$ $N-p=5$ $p=7$ $m=2$

N is even $\rightarrow m$ is even. N is odd $\rightarrow m$ is odd

For example,

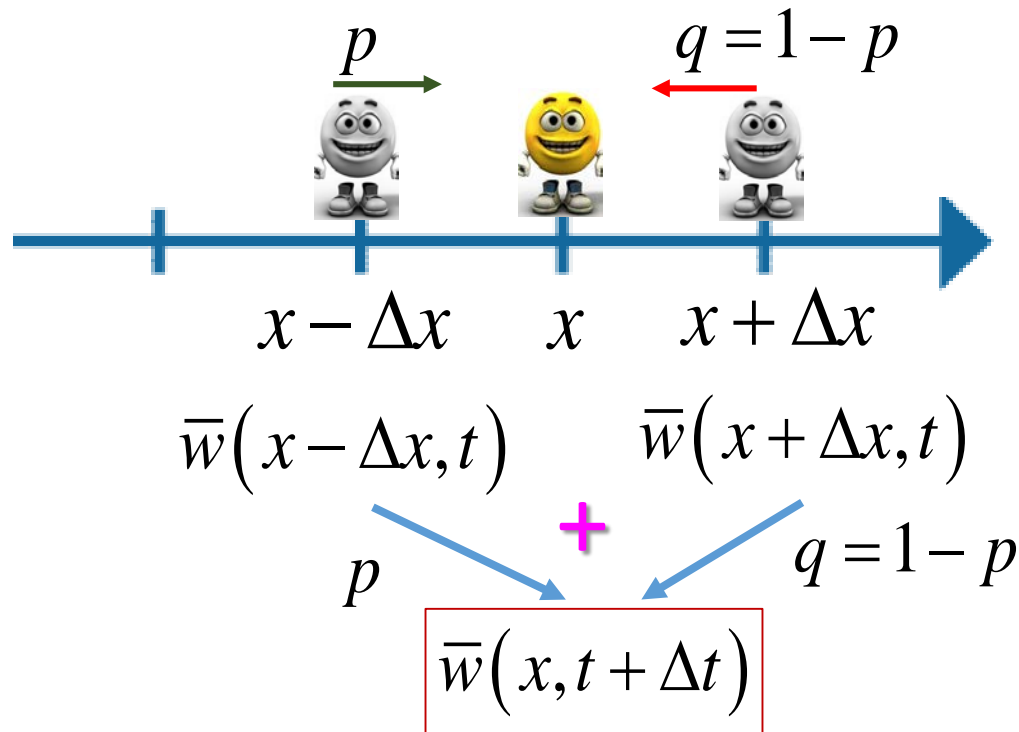
if $N=3$, the possible values of $m = -3, -1, 1, 3$.

if $N=4$, the possible values of $m = -4, -2, 0, 2, 4$.

3.3.1 Difference equation for the probability function

the probability of the particle at point x at $t + \Delta t$

$$\bar{w}(x, t + \Delta t) = p \bar{w}(x - \Delta x, t) + q \bar{w}(x + \Delta x, t)$$



as $p = q = 1/2$

$$\bar{w}(x, t + \Delta t) = \frac{1}{2} \bar{w}(x - \Delta x, t) + \frac{1}{2} \bar{w}(x + \Delta x, t)$$

3.1.2 Explicit solution

General random walk model

- Consider a continuous 1-D random walk process of n steps
- we have recursion relation:

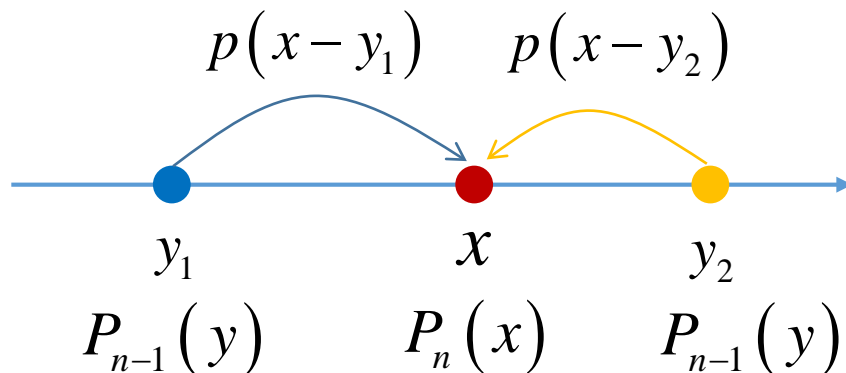
$$P_n(x) = \int_{-\infty}^{\infty} P_{n-1}(y) p(x-y) dy$$
$$= P_{n-1}(x) * p(x)$$

convolution

$$f(x) * g(x) = \int_{-\infty}^{\infty} f(y) g(x-y) dy$$

This means that the probability $P_n(x)$ of a particle at x after n steps is

- $P_{n-1}(y)$ the probability of arriving at y in $n-1$ steps
- $p(x-y)$ the probability of displacements $x-y$ in one step.



$$P_n(x) = \sum_i P_{n-1}(y_i) p(x-y_i)$$
$$\rightarrow P_n(x) = \int_{-\infty}^{\infty} P_{n-1}(y) p(x-y) dy$$

Evolution equation of $\bar{w}(x, t)$:

$$\bar{w}(x, t + \Delta t) = \frac{1}{2} \bar{w}(x - \Delta x, t) + \frac{1}{2} \bar{w}(x + \Delta x, t)$$

Conditions in the beginning

$$\bar{w}(0, 0) = 1$$

$$\bar{w}(x, 0) = 0, \quad x \neq 0$$

It is easy to **verify** that the solution is

$$\bar{w}(x, t) = \frac{(t / \Delta t)!}{2^{t/\Delta t} \left(\frac{t / \Delta t + x / \Delta x}{2} \right)! \left(\frac{t / \Delta t - x / \Delta x}{2} \right)!}$$

3.3.2 Approximated by differential equation

Apply Taylor's formula about (x, t)

$$\bar{w}(x, t + \Delta t) = \bar{w}(x, t) + \frac{d\bar{w}}{dt} \Delta t + \frac{1}{2} \frac{d^2\bar{w}}{dt^2} (\Delta t)^2 + O((\Delta t)^3)$$

$$\bar{w}(x - \Delta x, t) = \bar{w}(x, t) - \frac{d\bar{w}}{dx} \Delta x + \frac{1}{2} \frac{d^2\bar{w}}{dx^2} (\Delta x)^2 + O((\Delta x)^3)$$

$$\bar{w}(x + \Delta x, t) = \bar{w}(x, t) + \frac{d\bar{w}}{dx} \Delta x + \frac{1}{2} \frac{d^2\bar{w}}{dx^2} (\Delta x)^2 + O((\Delta x)^3)$$

$$\bar{w}(x, t + \Delta t) = \frac{1}{2} \bar{w}(x - \Delta x, t) + \frac{1}{2} \bar{w}(x + \Delta x, t)$$



$$\bar{w}_t \Delta t + \frac{1}{2} \bar{w}_{tt} (\Delta t)^2 + O((\Delta t)^3) = \frac{1}{2} \bar{w}_{xx} (\Delta x)^2 + O((\Delta x)^3)$$



3.3.2 Approximated by differential equation



$$\bar{w}_t + \frac{1}{2} \bar{w}_{tt} \Delta t + O(\Delta t) = \bar{w}_{xx} \frac{(\Delta x)^2}{2\Delta t} + O\left(\frac{(\Delta x)^2}{\Delta t} (\Delta x)\right)$$

Consider two limits

$$N \rightarrow \infty, \quad N\Delta t = t \text{ fixed}, \quad \Rightarrow \Delta t \rightarrow 0$$

$$m \rightarrow \infty, \quad m\Delta x = x \text{ fixed}, \quad \Rightarrow \Delta x \rightarrow 0$$

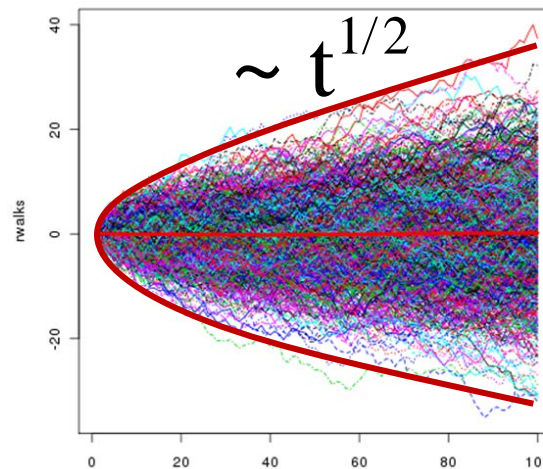
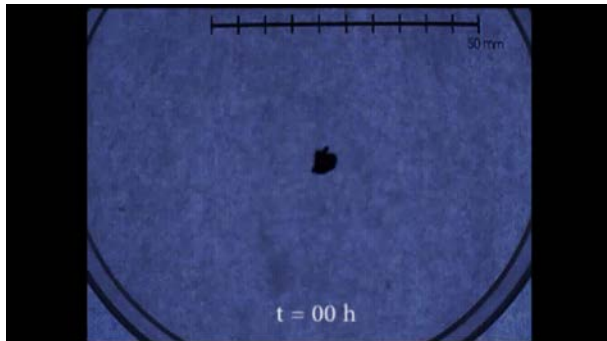
Recall diffusion coefficient D , we may assume

$$\lim_{\Delta x, \Delta t \rightarrow 0} \frac{(\Delta x)^2}{2\Delta t} = D \quad D \neq 0$$

Einstein (1905)

- assume that the macroscopic resistance on the particle is proportional to the velocity - using classical hydrodynamics
- predicated diffusion follows the statistical law

$$\langle x^2 \rangle = \frac{1}{3} [\langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle] = \frac{1}{3} \langle r^2 \rangle = 2Dt$$



$$\langle m^2 \rangle^{1/2} = N^{1/2}$$

Perrin:
 experiment in 1908.
 Nobel Prize in 1926

We obtain the differential equation of random walk

$$\bar{w}_t = D \bar{w}_{xx}$$

So far so good. But ... !

the probability density function u

$$u(x, t) = \frac{\bar{w}(x, t)}{2\Delta x}$$

$$m = \pm 1, \pm 3, \pm 5, \dots$$

$$\text{or } m = \pm 2, \pm 4, \pm 6, \dots$$

$$\Delta m = 2$$

The probability of finding a particle between $a=i\Delta x$ and $b=k\Delta x$ at time t can be expressed by

$$\sum_{m=i}^k \bar{w}(x, t) = \sum_{m=i}^k u(m\Delta x, t) \cdot 2\Delta x$$

Therefore, we get the PDE in terms of probability density u

$$\bar{w}_t = D\bar{w}_{xx} \quad \longrightarrow \quad u_t = Du_{xx}$$

The probability between a and b at time t

$$U(a, b; t) = \int_a^b u(x, t) dx$$

3.3.3 Solution of the PDE for the probability distribution function

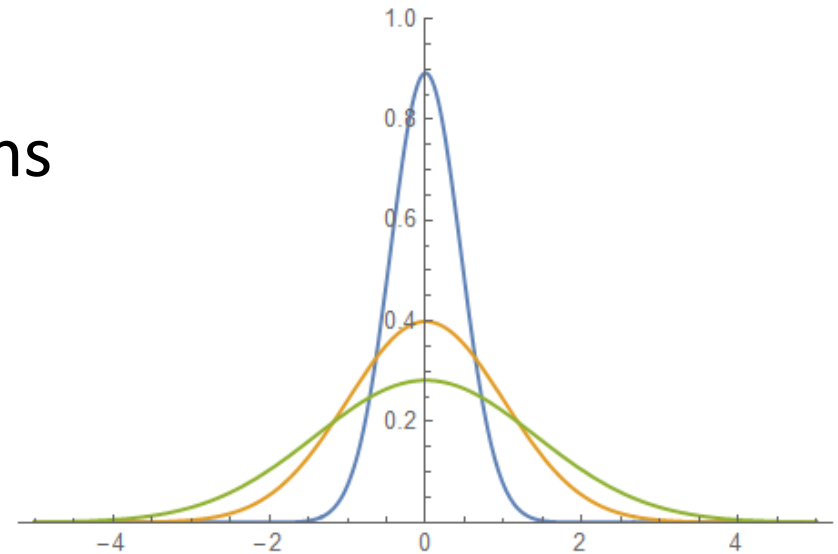
Partial differential equation for random walk

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$

Initial and normalized conditions

$$\int_{-\infty}^{\infty} u(x, t) dx = 1$$

$$\lim_{t \rightarrow 0^+} u(x, t) = 0, \quad x \neq 0$$



$Dt = 0.1, 0.5, 1.0$

Solution from self-similar form

$$u(x, t) \approx u_0(x, t) = \sqrt{\frac{1}{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

3.3.3 Solution of the PDE for the probability distribution function

$$u(x, t) \approx \sqrt{\frac{1}{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \longleftrightarrow w(m, N) \approx \sqrt{\frac{2}{\pi N}} \exp\left(-\frac{m^2}{2N}\right)$$

$$N\Delta t = t \quad m\Delta x = x \quad \lim_{\Delta x, \Delta t \rightarrow 0} \frac{(\Delta x)^2}{2\Delta t} = D \quad u = \frac{\bar{w}}{2\Delta x}$$

$$\sqrt{\frac{1}{4\pi Dt}} = \sqrt{\frac{1}{4\pi} \frac{2\Delta t}{(\Delta x)^2} \frac{1}{N\Delta t}} = \frac{1}{\Delta x} \sqrt{\frac{1}{2N\pi}}$$

$$\exp\left(-\frac{x^2}{4Dt}\right) = \exp\left(-\frac{(m\Delta x)^2}{4N\Delta t} \frac{2\Delta t}{(\Delta x)^2}\right) = \exp\left(-\frac{m^2}{2N}\right)$$

$$2\Delta x u(x, t) \approx \sqrt{\frac{2}{N\pi}} \exp\left(-\frac{m^2}{2N}\right) = w(m, N)$$

1. Dimensional analysis

$$\frac{\partial u}{\partial t} = D \frac{\partial u}{\partial^2 x}$$

$$1 = \int_{-\infty}^{\infty} u(x, t) dx$$

$$[x] = L, \quad [t] = T, \quad [u] = L^{-1}, \quad [D] = L^2 T^{-1}, \quad [Dt] = L^2$$

Two Dimensionless quantities

$$\Pi_1 = u(x, t) \sqrt{Dt} \quad \Pi_2 = \frac{x}{\sqrt{Dt}}$$

The solution must be of the form

$$\Pi_1 = f(\Pi_2)$$



$$u = \frac{f(s)}{\sqrt{Dt}}$$

define

$$s = \frac{x}{\sqrt{Dt}}$$

the number of independent variables reduced from 2 to 1.

2. From PDE to ODE

$$u = \frac{f(s)}{\sqrt{Dt}} \quad s = \frac{x}{\sqrt{Dt}}$$

The partial derivatives

$$\frac{\partial u}{\partial t} = \frac{f'}{\sqrt{Dt}} \frac{-x}{2\sqrt{Dt}^3} - \frac{f}{2\sqrt{Dt}^3} = -\frac{xf'}{2Dt^2} - \frac{f}{2t\sqrt{Dt}}$$

$$\frac{\partial u}{\partial x} = \frac{f'}{\sqrt{Dt}} \frac{1}{\sqrt{Dt}} = \frac{f'}{Dt}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x} \frac{f'}{Dt} = \frac{f''}{(Dt)^{3/2}}$$

inserting into the PDE, we get ODE

$$\frac{\partial u}{\partial t} = D \frac{\partial u}{\partial^2 x} \quad \rightarrow \quad f'' + \frac{s}{2} f' + \frac{1}{2} f = 0$$

the solution

$$f(s) = c_1 e^{-s^2/4} + c_2 e^{-s^2/4} \sqrt{\pi} \operatorname{Erfi}[s/2]$$

From initial and normalized conditions

$$\lim_{t \rightarrow 0^+} u(x, t) = 0, \quad x \neq 0 \quad \Rightarrow \quad c_2 = 0$$

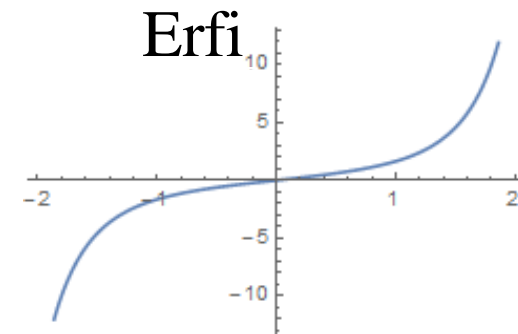
$$\int_{-\infty}^{\infty} u(x, t) dx = 1 \quad \Rightarrow \quad c_1 = \frac{1}{\sqrt{4\pi}}$$

Final solution

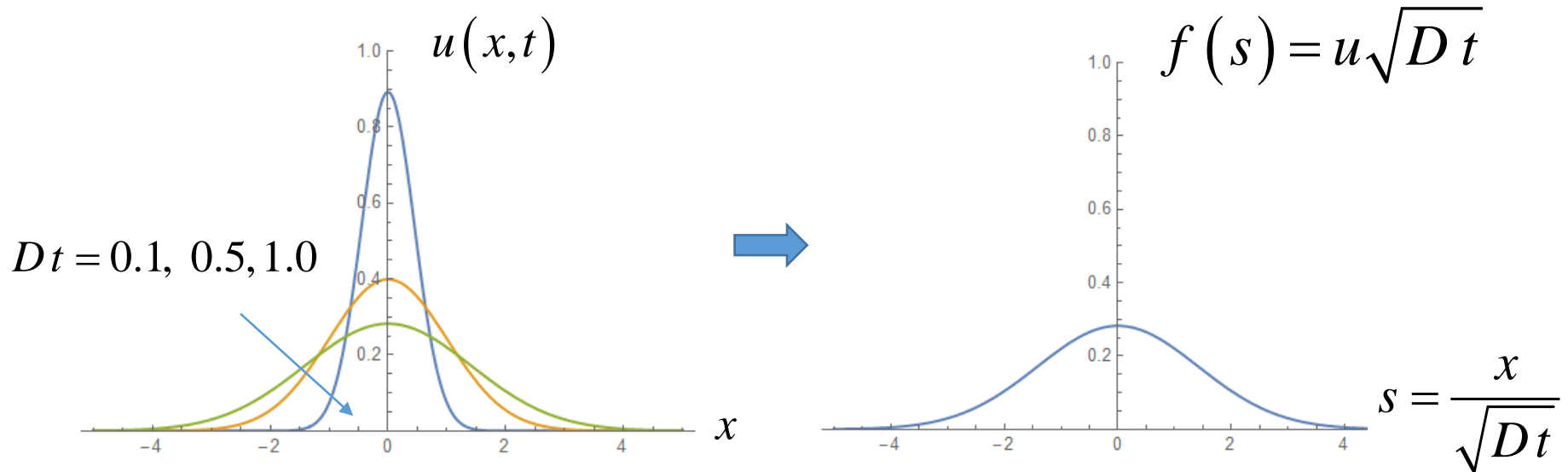
$$u(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

imaginary
error function

$$\operatorname{Erfi}[x] = \frac{2}{\sqrt{\pi}} \int_0^x e^{t^2} dt$$



why can we turn a PDE to an ODE ?



- All different curves **collapse onto one master curve** with the rescaling.
- called **self-similar solution**.
- x and t are not really 2 independent variables

- Self-similar solutions are **coincidences** in physical processes.
- We cannot always find self-similar solutions for a PDE.
- Self-similar solutions **exists only** when there is **no characteristic length scale** and **characteristic time scale** in the PDE problem. i.e.

~~$$\tilde{x} = \frac{x}{l}, \quad \tilde{t} = \frac{t}{\tau}$$~~

$$s = \frac{x}{\sqrt{Dt}}$$

Two ways to find the approximate solution

1. Stirling's formula applied to the exact solution

$$w(m, N) \sim \left(\frac{2}{\pi N} \right)^{1/2} \exp\left(\frac{-m^2}{2N} \right)$$

$$N \Delta t = t$$

$$m \Delta x = x$$

$$\bar{w}(x, t) \equiv w\left(\frac{x}{\Delta x}, \frac{t}{\Delta t} \right) \sim \left(\frac{2\Delta t}{\pi t} \right)^{1/2} \exp\left(\frac{-x^2 \Delta t}{2t(\Delta x)^2} \right)$$

$$u(x, t) = \frac{\bar{w}}{2\Delta x} = \lim_{\substack{\Delta t \rightarrow 0, \Delta x \rightarrow 0 \\ \frac{(\Delta x)^2}{2\Delta t} \rightarrow D}} \left(\frac{1}{4\pi t} \frac{2\Delta t}{(\Delta x)^2} \right)^{1/2} \exp\left(-\frac{x^2}{4t} \frac{2\Delta t}{(\Delta x)^2} \right) = \frac{\exp\left(-\frac{x^2}{4Dt} \right)}{\sqrt{4\pi Dt}}$$

2. by solving the partial differential equation

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \quad \rightarrow \quad u(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

3.3.4 Further examination of the limiting process

- Stirling's formula requires N , p and $N-p$ all large.
- Small p : most steps to the left, $m \sim -N$.
- Small $N-p$, most of the steps to the right, $m \sim +N$.
- Thus, those cases where $|m| \sim N$ is excluded.

$$m = p - (N - p) = 2p - N \sim \pm N$$

$$m \sim N^\alpha \quad \alpha = 1/2 \text{ or } 1/3 \text{ or } \dots?$$

$$\langle m^2 \rangle = N$$

3.1.2 Explicit solution

To find $w(m, N)$, the probability that a particle at a point $m \in [-N, N]$ steps to the right of its origin after total N steps.

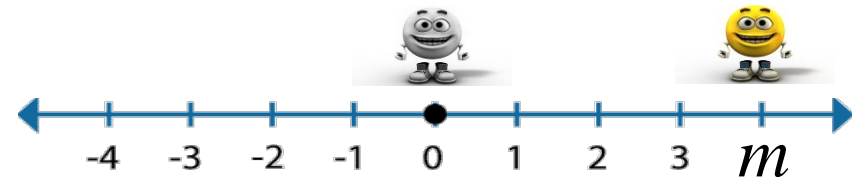
Suppose that the particle

- p steps to the right, $p > 0$
- $N - p$ steps to the left

Displacement m

$$m = p - (N - p) = 2p - N$$

$$p = (N + m)/2$$



e.g. $N=12$ $N-p=5$ $p=7$ $m=2$

N is even $\rightarrow m$ is even. N is odd $\rightarrow m$ is odd

For example,

if $N=3$, the possible values of $m = -3, -1, 1, 3$.

if $N=4$, the possible values of $m = -4, -2, 0, 2, 4$.

This requirement was not mentioned in the limiting differential equation. Why?

$$\Delta x \rightarrow 0, \quad \Delta t \rightarrow 0, \quad m \rightarrow \infty, \quad N \rightarrow \infty,$$

$$m\Delta x \rightarrow x, \quad N\Delta t \rightarrow t, \quad \frac{(\Delta x)^2}{2\Delta t} \rightarrow D$$

speed

$$\frac{\Delta x}{\Delta t} \sim \frac{2D}{\Delta x} \rightarrow \infty \quad \rightarrow \quad \Delta t = o(\Delta x) \quad \Delta t = (\Delta x)^2$$

$$\frac{m}{N} = \frac{m\Delta x}{N\Delta t} \frac{\Delta t}{\Delta x} = \frac{x}{t} \frac{\Delta t}{\Delta x} \rightarrow 0 \quad \rightarrow \quad |m| \ll N$$

$$x = m\Delta x \ll N\Delta x$$

try

$$\frac{m}{N^{1/2}} = \frac{x}{\Delta x} \left(\frac{\Delta t}{t} \right)^{1/2} = x \sqrt{\frac{2\Delta t}{2t(\Delta x)^2}} = \frac{x}{\sqrt{2Dt}} \sim 1 \quad \rightarrow \quad m \sim N^{1/2}$$

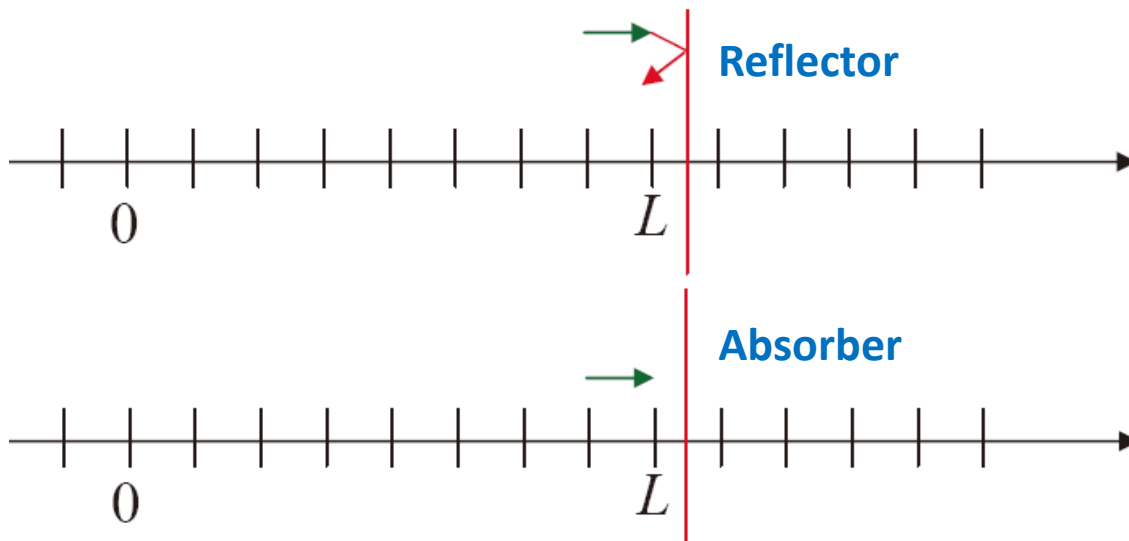
the probability of the particle reaching position L at $t + \Delta t$

Reflecting barrier

$$\bar{w}(L, t + \Delta t) = \frac{1}{2} \bar{w}(L - \Delta x, t) + \frac{1}{2} \bar{w}(L, t)$$

Absorbing barrier

$$\bar{w}(L, t + \Delta t) = \frac{1}{2} \bar{w}(L - \Delta x, t) + 0$$



Reflecting barrier

$$\bar{w}(L, t + \Delta t) = \frac{1}{2} \bar{w}(L - \Delta x, t) + \frac{1}{2} \bar{w}(L, t)$$

$$\bar{w}(L, t + \Delta t) = \bar{w}(L, t) + \bar{w}_t \Delta t + O(\Delta t^2)$$

$$\bar{w}(L - \Delta x, t) = \bar{w}(L, t) - \bar{w}_x \Delta x + O(\Delta x^2)$$



$$\bar{w}_t \Delta t + O(\Delta t^2) = -\frac{1}{2} \bar{w}_x \Delta x + O(\Delta x^2)$$



$$u_x(L, t) = 0$$

$$u = \frac{\bar{w}}{2\Delta x}$$

$$\frac{\Delta t}{\Delta x} \rightarrow 0$$

Absorbing barrier

$$\bar{w}(L, t + \Delta t) = \frac{1}{2} \bar{w}(L - \Delta x, t)$$

$$\bar{w}(L, t + \Delta t) = \bar{w}(L, t) + \bar{w}_t \Delta t + O(\Delta t^2)$$

$$\bar{w}(L - \Delta x, t) = \bar{w}(L, t) - \bar{w}_x \Delta x + O(\Delta x^2)$$



$$\bar{w}(L, t) + \bar{w}_t \Delta t + O(\Delta t^2) = \frac{1}{2} \bar{w}(L, t) - \frac{1}{4} \bar{w}_x \Delta x + O(\Delta x^2)$$



$$u(L, t) = 0$$

$$u = \frac{\bar{w}}{2\Delta x}$$

$$\frac{\Delta t}{\Delta x} \rightarrow 0$$

Reflecting barrier

$$\left\{ \begin{array}{l} \frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \\ \int_{-\infty}^L u(x, t) dx = 1 \\ \lim_{t \rightarrow 0^+} u(x, t) = 0, \quad x \neq 0 \\ u_x(L, t) = 0 \end{array} \right.$$

$$\begin{aligned} u &= u_R(x, t) \\ &= u_0(x, t) + u_0(x - 2L, t) \end{aligned}$$

Absorbing barrier

$$\left\{ \begin{array}{l} \frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \\ \int_{-\infty}^L u(x, t) dx = 1, \\ \lim_{t \rightarrow 0^+} u(x, t) = 0, \quad x \neq 0 \\ u(L, t) = 0 \end{array} \right.$$

$$\begin{aligned} u &= u_A(x, t) \\ &= u_0(x, t) - u_0(x - 2L, t) \end{aligned}$$