

Chapter 3

Random Process

&

Partial Differential Equations

Deterministic model (repeatable results)

Consider N particles with coordinates $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N$

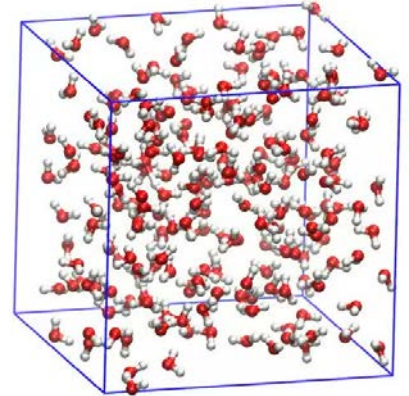
- the interactions between particles modeled by potential

$$V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$$

- the dynamics of the system represented by ordinary differential equations

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{f}_i, \quad i = 1, 2, 3 \dots N$$

$$\mathbf{f}_i = -\nabla_{\mathbf{r}_i} V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \left(-\frac{\partial V}{\partial x_i}, -\frac{\partial V}{\partial y_i}, -\frac{\partial V}{\partial z_i} \right)$$



These coupled equations can be solved using *numerical method*

Verlet algorithm

Taylor expansion

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 + (1/6)\mathbf{b}(t)\Delta t^3 + \underline{O(\Delta t^4)}$$

$$\mathbf{r}(t - \Delta t) = \mathbf{r}(t) - \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 - (1/6)\mathbf{b}(t)\Delta t^3 + \underline{O(\Delta t^4)}$$



相加 $\mathbf{r}(t + \Delta t) = 2\mathbf{r}(t) - \mathbf{r}(t - \Delta t) + \mathbf{a}(t)\Delta t^2 + \underline{O(\Delta t^4)}$

相減 $\mathbf{v}(t) = \frac{\mathbf{r}(t + \Delta t) - \mathbf{r}(t - \Delta t)}{2\Delta t} + \underline{O(\Delta t^2)}$

Verlet integrator is an order more accurate than integration by simple Taylor expansion alone, with the same term Δt^2

velocity Verlet algorithm

Verlet algorithm is not self-starting, we will use velocity Verlet algorithm in molecular dynamics simulations.

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 + O(\Delta t^3)$$

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \frac{\mathbf{a}(t) + \mathbf{a}(t + \Delta t)}{2} \Delta t + O(\Delta t^2)$$



Probabilistic model (unrepeatable results)

Consider the same system of N particles as before

- when there is uncertainty, say *random force* \mathbf{R}_i , which has a Gaussian probability distribution with correlation function

$$\langle \mathbf{R}_i(t) \cdot \mathbf{R}_i(t') \rangle = 6\gamma k_B T \delta(t - t') \quad \gamma: \text{friction coefficient}$$

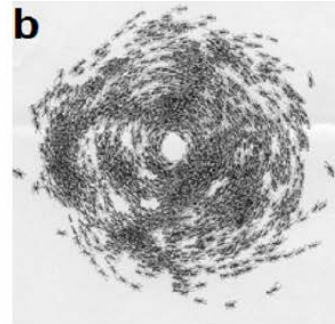
Langevin Equation:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} + \gamma \frac{d\mathbf{r}_i}{dt} = \mathbf{f}_i + \mathbf{R}_i(t), \quad i = 1, 2, 3 \dots N$$

$$\mathbf{f}_i = -\nabla_{\mathbf{r}_i} V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \left(-\frac{\partial V}{\partial x_i}, -\frac{\partial V}{\partial y_i}, -\frac{\partial V}{\partial z_i} \right)$$

Each particle's motion can be described by certain **probabilities**, derived from *Fokker-Planck Equation*.

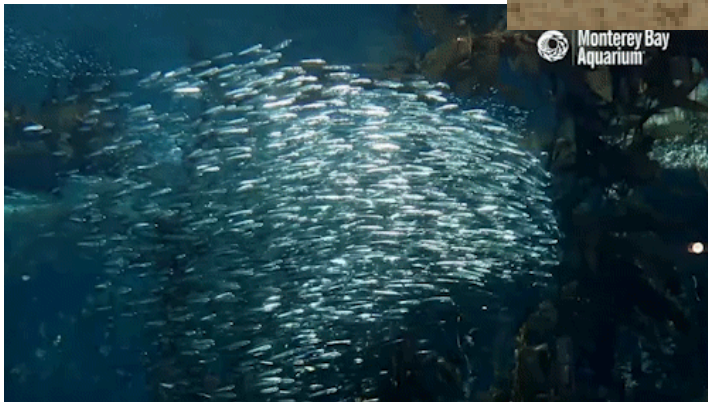
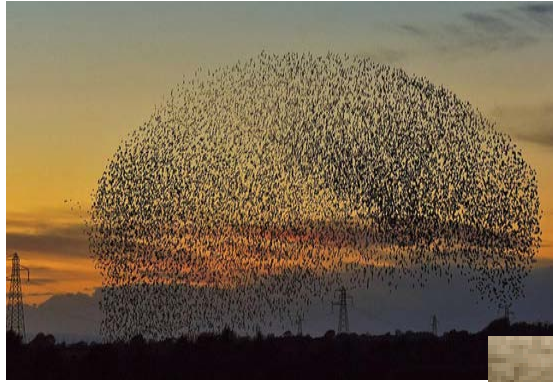
3.0 Introduction



- (a) Wingless Locusts marching in the field.
- (b) A rotating colony of army ants.
- (c) A three-dimensional array of golden rays.
- (d) Fish are known to produce such vortices.
- (e) Before roosting, thousands of starlings producing a fascinating aerial display.
- (f) A herd of zebra.
- (g) People spontaneously ordered into traffic lanes as they cross a pedestrian bridge in large numbers.
- (h) Although sheep are known to move very coherently, just as the corresponding theory predicts, when simply hanging around (no motion), well developed orientational patterns cannot emerge.

Tamás Vicsek, **Collective motion**,
Physics Reports, Vol 517, 2012, Pages 71-140

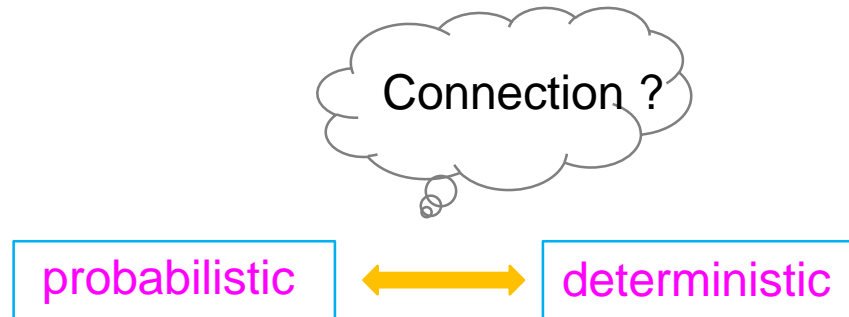
3.0 Introduction



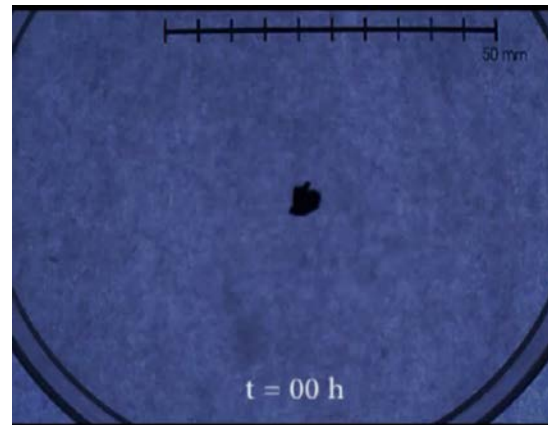
3.0 Introduction

our primary goal:

- to investigate the connection between **probabilistic** and **deterministic** models of the **same phenomenon**.



Micro view:
single random process



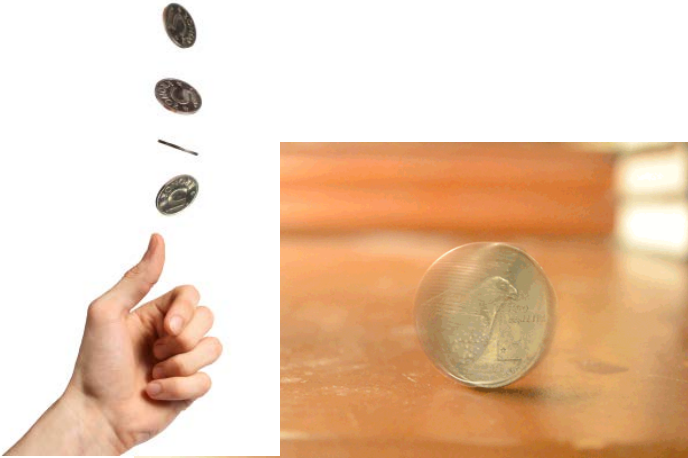
Macro view: **(ensemble average)**
definite distribution function

described by partial
differential equation

- Looks paradoxical that a random process can be characterized by a definite equation
- But we know it is true from a lot of daily experience, such as coin tossing.

3.0 Introduction

coin tossing



~50%

~50%

many parameters unknown

- the initial orientation, velocity, and spin;
 - the properties of the table surface;
 - Various atomic defects, dislocations, grains, voids...
-
- For single toss: no idea whether head or tail turns up.
 - After a large number of tosses, proportion of heads or tails is ~ 0.5 .
 - With this example, it is not so surprising that there is a determinable distribution of probabilities which characterizes a random process.

Probabilistic model originates from

- **Incompleteness of information**
e.g. coin tossing
- **Parameters sensitivity** --- tiny perturbation in input induces huge variation in output.
e.g. In kinetics of gases, a slight change in the initial conditions would result in a tremendous change after many collisions.

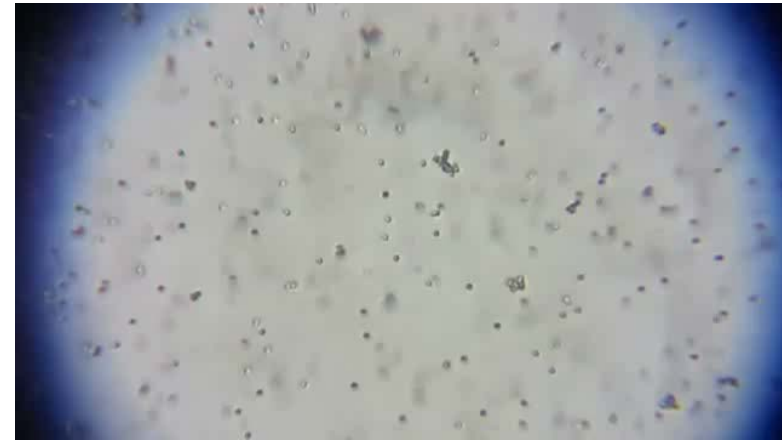
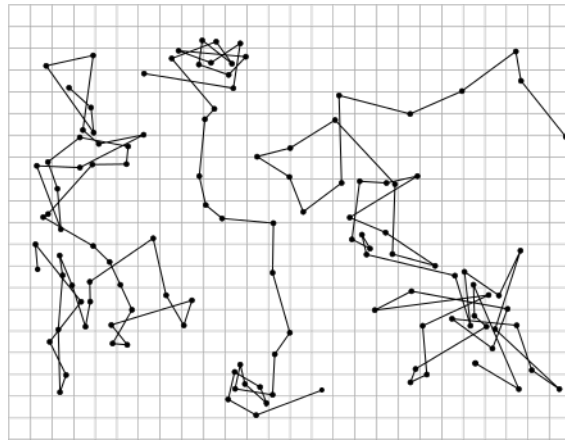
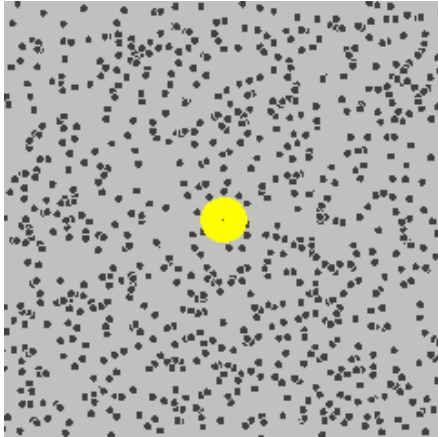
By an averaging of the solutions with varying initial conditions random processes can be modeled successfully.

in the following sections,

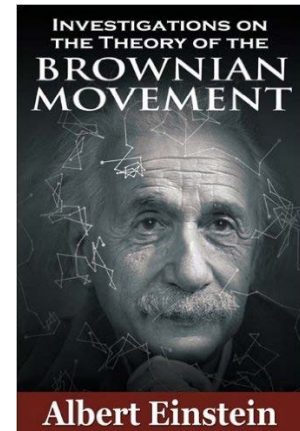
- Section 3.1
1-D Brownian motion. An explicit expression of the probability $w(m, N)$.
- Section 3.2
Simplified expression of $w(m, N)$. Asymptotic Series, Laplace's Method
- Section 3.3
a difference equation for $w(m, N)$ leads to a partial differential equation.
- Section 3.4
The connection between probability and differential equations.

3.1 Random Walk in One Dimension; Langevin's Equation

In Brownian motion, small particles move about in liquid or gas.

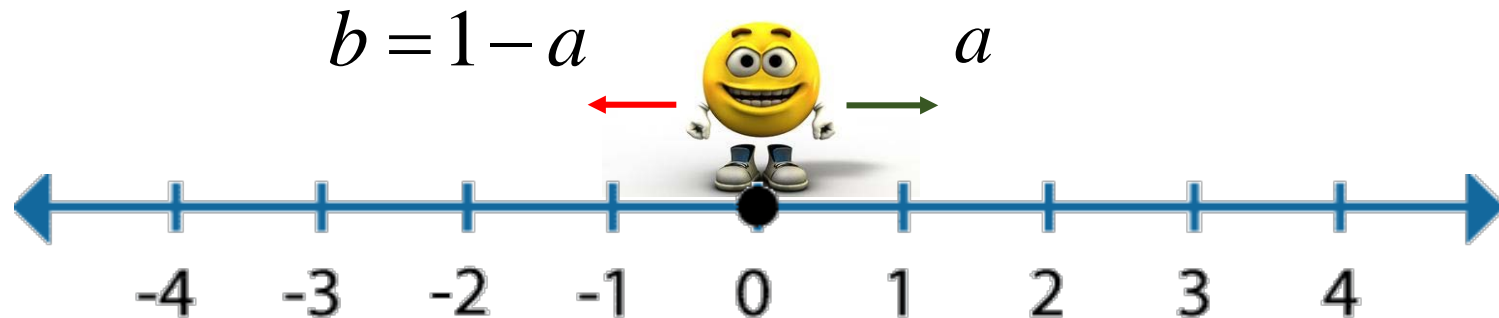


- **no possibility** and **no interest** of computing the trajectory of each molecule.
- one wishes to have an average understanding of the phenomenon.
- The Roman Lucretius's (卢克莱修) described Brownian motion of dust in his scientific poem "On the Nature of Things" (60 BC)
- Botanist [Robert Brown](#) in 1827 studied pollen grains suspended in water.
- Albert Einstein in 1905 solved this problem.



3.1.1 An one dimension random walk model

The minimum model of random walk: 1-D lattice model



Particle moves according to the following rules:

- Move in steps of a fixed length dx in a fixed time interval dt .
- The probability to the right p and to the left $q=1-p$.

Goal: to obtain the probability $w(m, N)$

- m steps to the right of the origin
- N the total steps

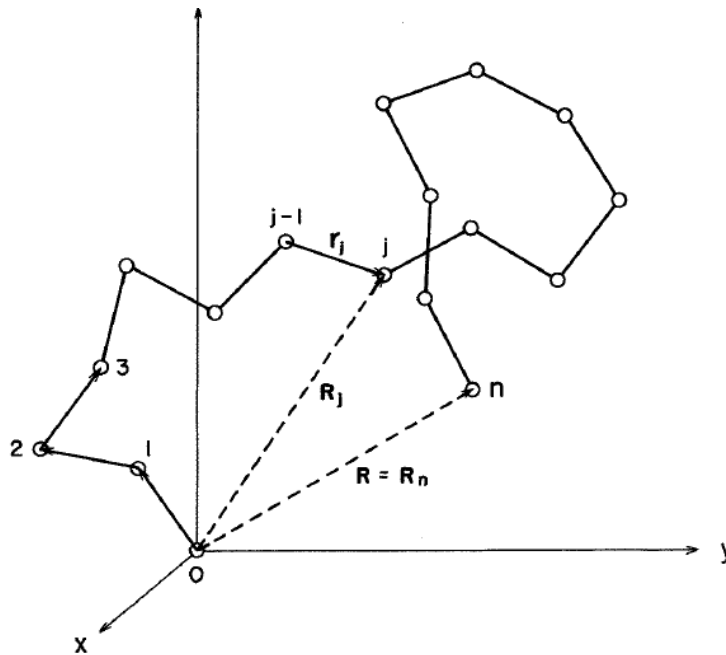
$$\text{Probability} = \frac{\text{number of observed events}}{\text{total number of events}}$$

3.1.1 An one dimension random walk model

random walk model can be found in various situations

- ✓ a drunk staggering down a street
- ✓ a gambling game in which a coin is tossed
- ✓ Polymer Physics: Freely jointed chain model

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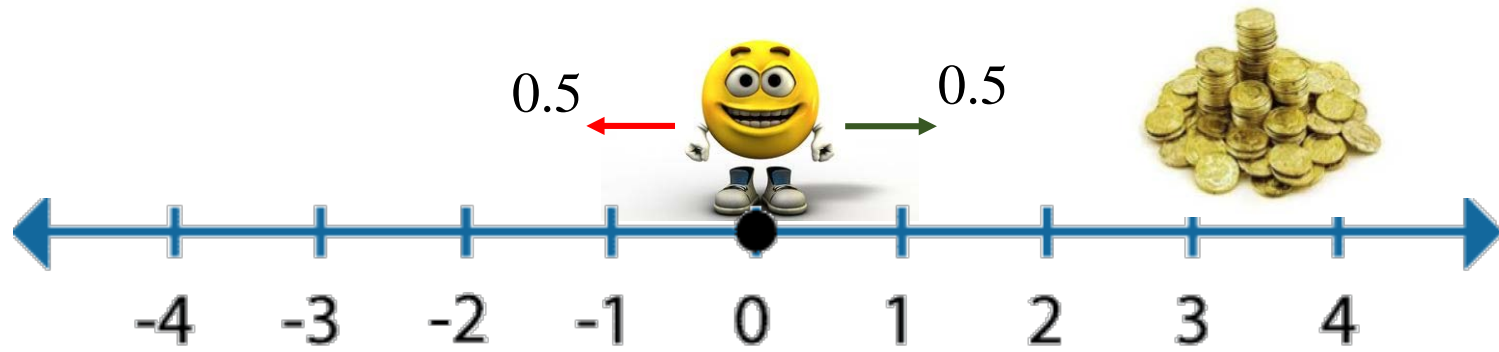
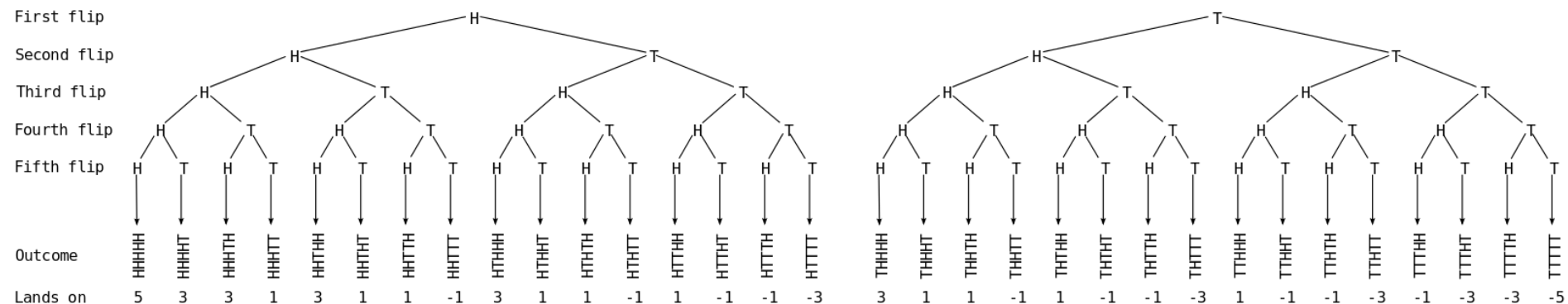
3.1.1 An one dimension random walk model

Fair coin tossing



Head ~50%

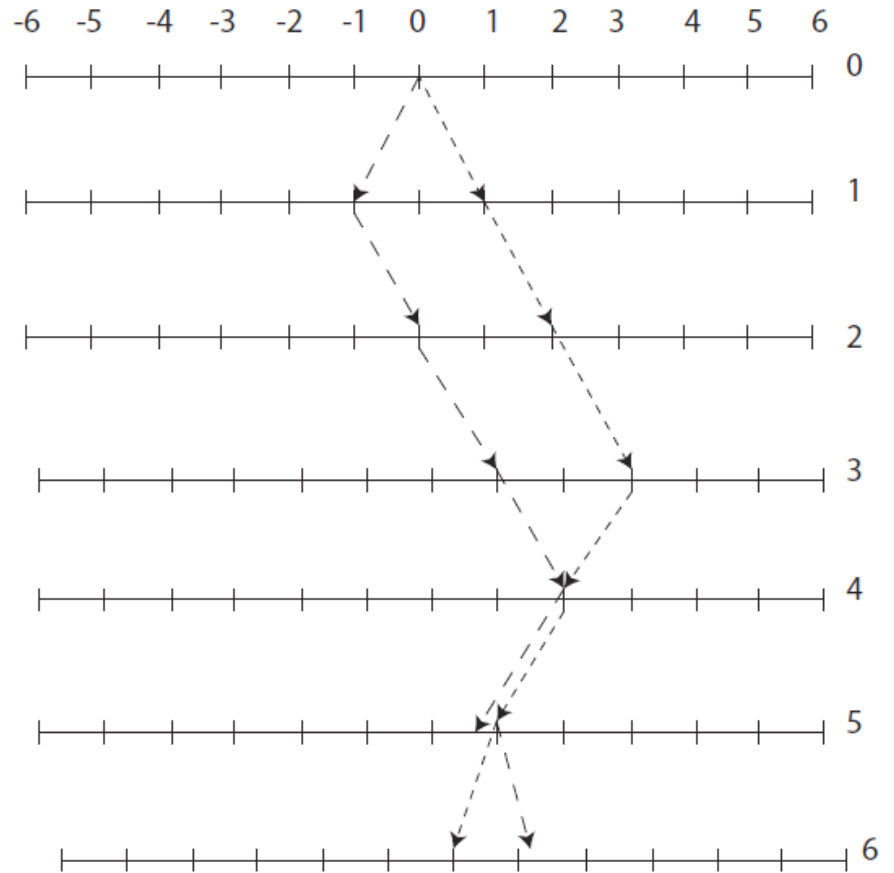
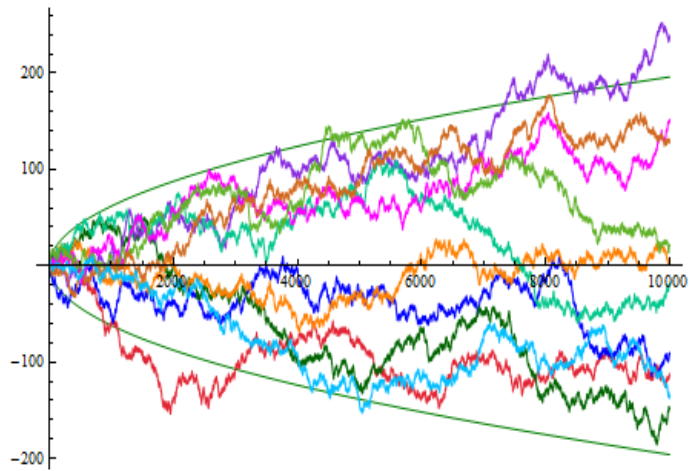
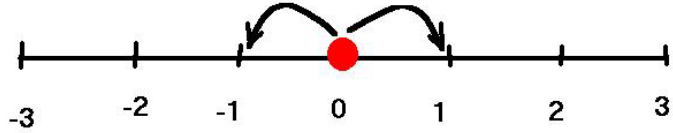
Tail ~50%



3.1.1 An one dimension random walk model

Random walk

$P=0.5$ $P=0.5$



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.

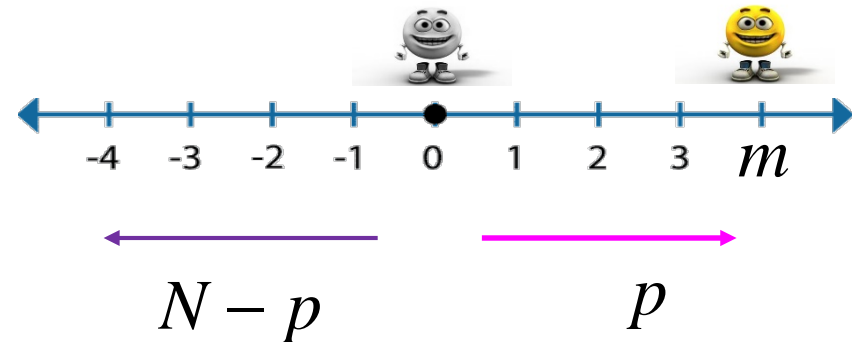
Suppose that the particle

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

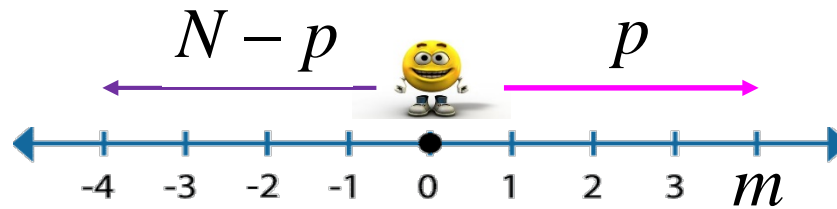
N is even \rightarrow m is even. N is odd \rightarrow m is odd

For example,

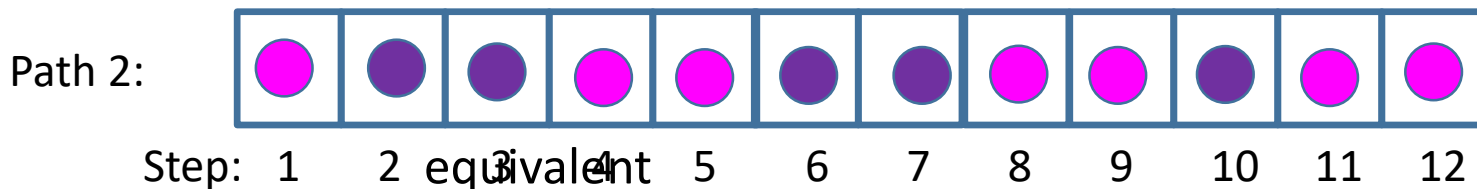
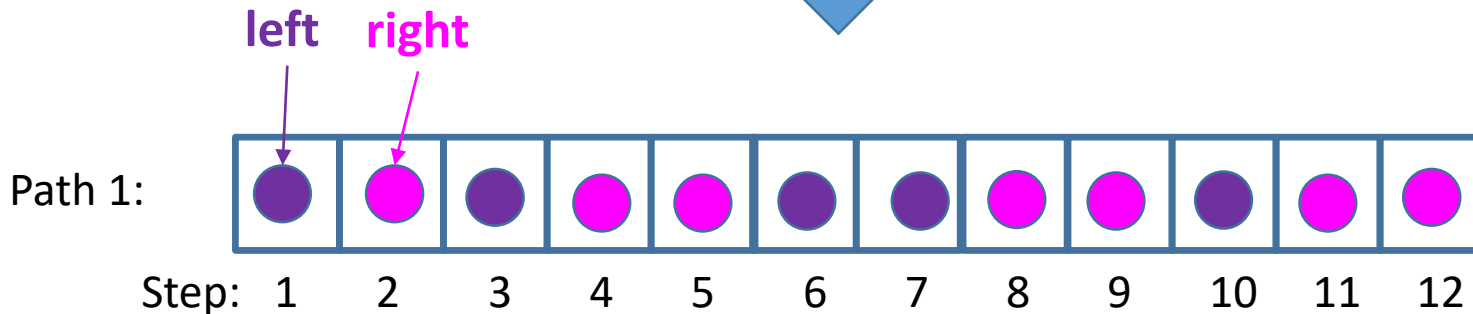
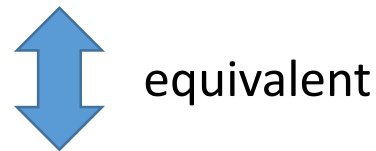
if $N=3$, the possible values of $m = -3, -1, 1, 3$.

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

3.1.2 Explicit solution



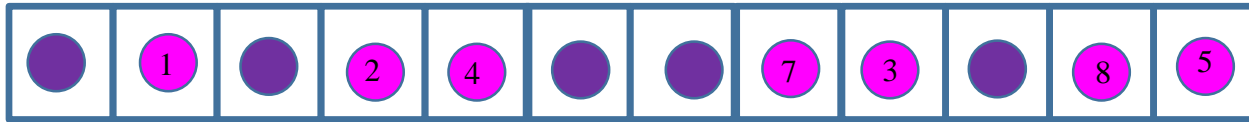
To find out the number of paths with p steps to the right and $N - p$ to the left.



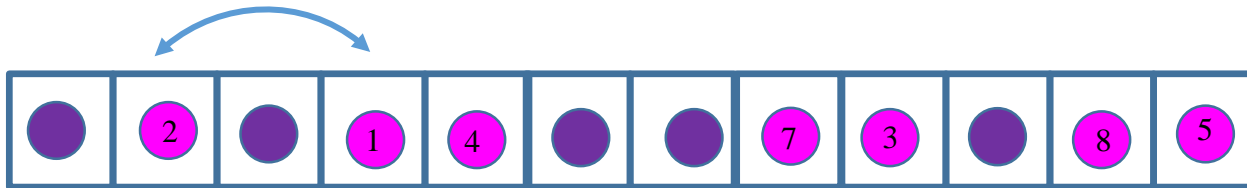
The number of choices with p indistinguishable pink ball in N boxes

3.1.2 Explicit solution

Consider p distinguishable balls, which can be placed in N boxes in the following number of ways:



$$N(N-1)(N-2)\cdots(N-p+1) = \frac{N!}{(N-p)!}$$



Interchanging distinguishable balls does not change the pattern. There are $p!$ permutations of p balls.

排列

3.1.2 Explicit solution

number of ways p
distinguishable balls
can be placed in N
boxes

=

number of full
box empty box
patterns

×

number of full
permutations of
distinguishable
balls within a
pattern

$$\frac{N!}{(N-p)!} = C_p^N \times p!$$



binomial coefficient

$$C_p^N = \frac{N!}{p!(N-p)!}$$

$$(x+y)^N = \sum_{p=0}^N C_p^N x^{N-p} y^p$$

3.1.2 Explicit solution

- The total number of possible path is 2^N
- the probability that a particle at a point m steps to the right of its origin after total N steps.

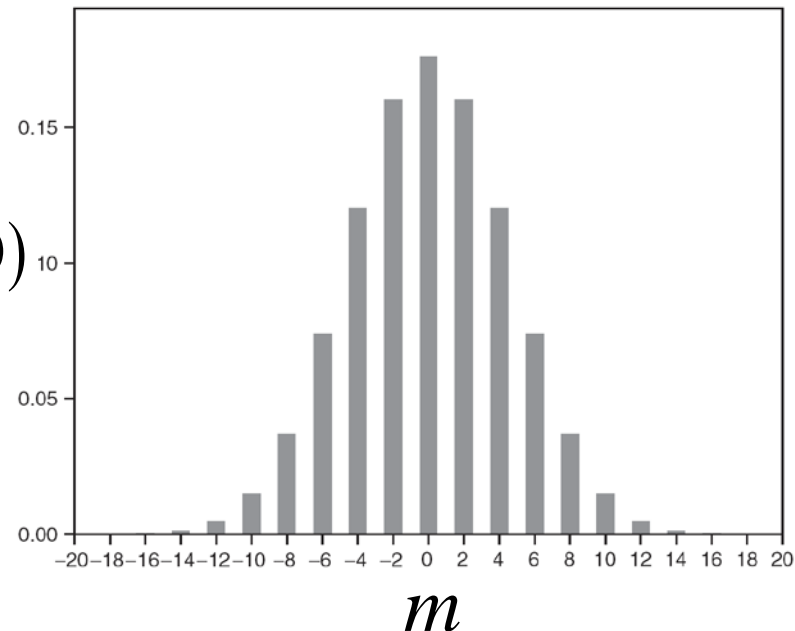
$$w(m, N) = \frac{C_p^N}{2^N}$$

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

The sum of all probabilities is unity

$$\begin{aligned} \sum_{m=-N}^N w(m, N) &= \sum_{p=0}^N C_p^N \left(\frac{1}{2}\right)^N \\ &= \sum_{p=0}^N C_p^N \left(\frac{1}{2}\right)^{N-p} \left(\frac{1}{2}\right)^p \\ &= \left(\frac{1}{2} + \frac{1}{2}\right)^N = 1 \end{aligned}$$

$w(m, 20)$

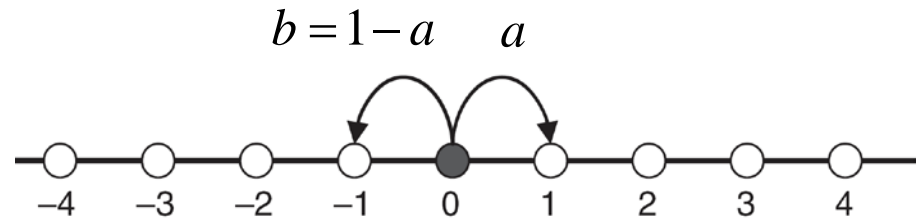


3.1.2 Explicit solution

Characteristic functions

- the **characteristic function** of any real-valued random variable defines its **probability distribution**.

Let $\lambda(\theta) = ae^{i\theta} + be^{-i\theta}$



$$\lambda^2(\theta) = (ae^{i\theta} + be^{-i\theta})^2 = a^2 e^{i2\theta} + 2abe^{i0} + b^2 e^{-i2\theta}$$

$m=2$ $m=0$ $m=-2$

$P_N(m)$	$P_2(2)$	$P_2(0)$	$P_2(-2)$
	$= a \cdot a$	$= 2a \cdot b$	$= b \cdot b$

these coefficients are the probability

characteristic function $\lambda(\theta) = ae^{i\theta} + be^{-i\theta} = \langle e^{i\theta x} \rangle$ $x = \pm 1$

mean

3.1.2 Explicit solution

To extract the coefficient analytically, for example as $m=2$

$$\lambda^2(\theta) = (ae^{i\theta} + be^{-i\theta})^2 = a^2e^{i2\theta} + 2abe^{i0} + b^2e^{-i2\theta}$$

$$P_2(2) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \lambda^2(\theta) e^{-i2\theta} d\theta \quad \text{Fourier transform}$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} (a^2e^{i2\theta} + 2abe^{i0} + b^2e^{-i2\theta}) e^{-i2\theta} d\theta$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} (a^2e^{i0\theta} + 2abe^{-i2\theta} + b^2e^{-i4\theta}) d\theta$$

$$= \frac{1}{2\pi} \left(a^2 \int_{-\pi}^{\pi} d\theta + 2ab \int_{-\pi}^{\pi} e^{-i2\theta} d\theta + b^2 \int_{-\pi}^{\pi} e^{-i4\theta} d\theta \right)$$

$$= a^2$$

3.1.2 Explicit solution

Generally, we extract the coefficient via Fourier transform

$$\begin{aligned} P_N(m) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \lambda^N(\theta) e^{-i\theta m} d\theta \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} (ae^{i\theta} + be^{-i\theta})^N e^{-i\theta m} d\theta \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{k=0}^N C_k^N a^{N-k} e^{i\theta(N-k)} b^k e^{-i\theta k} e^{-i\theta m} d\theta \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{k=0}^N C_{N-k}^N a^{N-k} e^{i\theta(N-k)} b^k e^{-i\theta k} e^{-i\theta m} d\theta \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{p=0}^N C_p^N a^p e^{i\theta p} b^{N-p} e^{-i\theta(N-p)} e^{-i\theta m} d\theta \\ &= \frac{1}{2\pi} \sum_{p=0}^N C_p^N a^p b^{N-p} \int_{-\pi}^{\pi} e^{i\theta(2p-N-m)} d\theta \end{aligned}$$

$$C_p^N = C_{N-p}^N$$

$$p = N - k$$

3.1.2 Explicit solution

we notice

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i\theta(2p-N-m)} d\theta = \begin{cases} 0, & \text{if } p \neq (N+m)/2 \\ 1, & \text{if } p = (N+m)/2 \end{cases}$$

Thus, we have

$$P_N(m) = C_p^N a^p b^{N-p}, \quad p = (N+m)/2$$

Specifically,

$$P_N(m) = w(m, N) = \frac{C_p^N}{2^N}$$

when $a = b = 1/2$

General Characteristic function

- probability density function (PDF) $p(x)$.
- displacement x is continuous.
- the characteristic function is given by

$$\lambda(k) = \langle e^{ikx} \rangle = \int_{-\infty}^{\infty} p(x) e^{ikx} dx$$

$$\lambda(\theta) = ae^{i\theta} + be^{-i\theta} = \langle e^{i\theta x} \rangle$$

Fourier transform of $p(x)$.

- One important property of the characteristic function

$$\lambda(0) = \int_{-\infty}^{\infty} p(x) dx = 1$$

3.1.2 Explicit solution

General random walk model

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

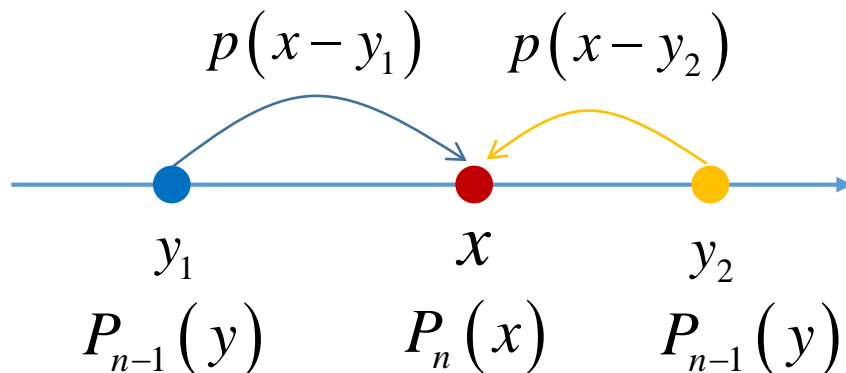
$$P_n(x) = \int_{-\infty}^{\infty} P_{n-1}(y) p(x-y) dy$$
$$= P_{n-1}(x) * p(x)$$

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.



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

3.1.2 Explicit solution

Let us define

$$P_n(k) = \int_{-\infty}^{\infty} P_n(x) e^{ikx} dx$$



$$P_n(k) = P_{n-1}(k) \lambda(k)$$



$$P_n(k) = P_{n-1}(k) \lambda(k) = P_{n-2}(k) \lambda^2(k) = \dots = \lambda^n(k)$$



$$P_n(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} P_n(k) e^{-ikx} dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} \lambda^n(k) e^{-ikx} dx$$

convolution theorem

$$f(x) * g(x) = \int_{-\infty}^{\infty} f(y) g(x-y) dy$$
$$F[f(x) * g(x)] = \frac{1}{2\pi} f(k) \cdot g(k)$$

$$P_n(x) = P_{n-1}(x) * p(x)$$

$$\lambda(k) = \int_{-\infty}^{\infty} p(x) e^{ikx} dx$$

3.1.3 Mean, Variance, and the Generating function

The expected value of function f is defined by

$$\langle f \rangle = \sum_{m=-N}^N f(m) w(m, N)$$

$$\langle p \rangle = \sum_{m=-N}^N p(m) w(m, N) = \sum_{p=0}^N p C_p^N \left(\frac{1}{2} \right)^N$$

n -th moment $\langle m^n \rangle = \sum_{m=-N}^N m^n w(m, N) = \sum_{m=-N}^N m^n C_p^N \left(\frac{1}{2} \right)^N$ where $p = (N + m)/2$

$\langle m \rangle$ mean displacement

$\langle m^2 \rangle$ mean square displacement or variance

3.1.3 Mean, Variance, and the Generating function

In order to evaluate the various moments, we introduce the **generating function**


$$G(u) = \sum_{p=0}^N u^p w(m, N)$$

or
$$G(u) = \sum_{p=0}^N u^p C_p^N \left(\frac{1}{2}\right)^N = \sum_{p=0}^N C_p^N u^p \left(\frac{1}{2}\right)^{N-p} \left(\frac{1}{2}\right)^p = (1+u)^N \left(\frac{1}{2}\right)^N$$

Example: to calculate $\langle m \rangle$

$$G'(u) = \sum_{p=0}^N p u^{p-1} w(m, N) \Rightarrow G'(1) = \sum_{p=0}^N p w(m, N) = \langle p \rangle$$


$$G(u) = (1+u)^N \left(\frac{1}{2}\right)^N \Rightarrow G'(1) = N/2$$

 $\langle p \rangle = N/2$

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

$$\langle p \rangle = \frac{1}{2} \sum_{p=0}^N (N + m) w(m, N)$$

$$= \frac{1}{2} \sum_{p=0}^N N w(m, N) + \frac{1}{2} \sum_{p=0}^N m w(m, N) = \frac{N}{2} + \frac{\langle m \rangle}{2}$$

 $\langle m \rangle = 0$

3.1.3 Mean, Variance, and the Generating function

Example: $\langle m^2 \rangle^{1/2} = ?$

$$G'(u) = \sum_{p=0}^N p u^{p-1} w(m, N) \quad G''(u) = \sum_{p=0}^N p(p-1) u^{p-2} w(m, N)$$

$$G''(1) = \sum_{p=0}^N p(p-1) w(m, N) = \langle p(p-1) \rangle = \langle p^2 \rangle - \langle p \rangle$$

$$G(u) = (1+u)^N \left(\frac{1}{2}\right)^N \quad \Rightarrow \quad G''(u) = N(N-1)(1+u)^{N-2} \left(\frac{1}{2}\right)^N$$

$$G''(1) = \frac{N(N-1)}{4} \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \quad \langle p^2 \rangle = \langle p \rangle + \frac{N(N-1)}{4} = \frac{N^2}{4} + \frac{N}{4}$$
$$G''(1) = \langle p^2 \rangle - \langle p \rangle$$

$$m = 2p - N$$

$$\langle m^2 \rangle = \langle (2p - N)^2 \rangle = 4\langle p^2 \rangle + N^2 - 4N\langle p \rangle = N^2 + N + N^2 - 4N \frac{N}{2} = N$$

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

3.1.3 Mean, Variance, and the Generating function

Generally, the n th-moment $\langle x^n \rangle = \int_{-\infty}^{\infty} p(x) x^n dx$

Its characteristic function

$$\begin{aligned}\lambda(k) &= \langle e^{ikx} \rangle = \int_{-\infty}^{\infty} p(x) e^{ikx} dx = \int_{-\infty}^{\infty} dx p(x) \left(1 + ikx - \frac{k^2 x^2}{2!} + i \frac{k^3 x^3}{3!} + \dots \right) \\ &= \sum_{n=0}^{\infty} \frac{i^n k^n}{n!} \langle x^n \rangle\end{aligned}$$

We obtain n -th moments using characteristic function

$$\langle x^n \rangle = (-i)^n \left. \frac{d^n \lambda(k)}{dk^n} \right|_{k=0}$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

Theory by Einstein, experiment by Perrin

Einstein

- Assume that the macroscopic resistance on the particle is proportional to the velocity - by classical hydrodynamics
- showed diffusion obey the statistical law

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

the diffusion coefficient D is given by

$$D = kT / f$$

T : absolute temperature; K : Boltzmann's constant

f : the coefficient of resistance

$$f = 6\pi\mu a \quad (\text{Stokes' law})$$

μ : viscosity coefficient; a : particle size

3.1.4 To determine Boltzmann's constant from Brownian Motion

The modern theory of the Brownian motion

Langevin's equation $m \frac{d\mathbf{v}}{dt} = -f\mathbf{v} + \mathbf{F}(t)$

where \mathbf{v} the velocity of the particle and m mass. The random force follows Fluctuation-dissipation relation


$$\langle \mathbf{F}_i(t) \cdot \mathbf{F}_i(t') \rangle = 6fk_B T \delta(t - t')$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

To solve $m \frac{d\mathbf{v}}{dt} = -f\mathbf{v} + \mathbf{F}(t)$


multiply with \mathbf{x} , and take the ensemble average


$$m \left\langle \mathbf{x} \cdot \frac{d\mathbf{v}}{dt} \right\rangle = -f \langle \mathbf{x} \cdot \mathbf{v} \rangle + \langle \mathbf{x} \cdot \mathbf{F}(t) \rangle$$


$$m \left(\frac{d \langle \mathbf{x} \cdot \mathbf{v} \rangle}{dt} - \langle v^2 \rangle \right) = -f \langle \mathbf{x} \cdot \mathbf{v} \rangle + \langle \mathbf{x} \cdot \mathbf{F}(t) \rangle$$

$$\langle \mathbf{x} \cdot \mathbf{F}(t) \rangle = 0$$

Not correlated


$$\frac{d \langle \mathbf{x} \cdot \mathbf{v} \rangle}{dt} + \frac{f}{m} \langle \mathbf{x} \cdot \mathbf{v} \rangle - \langle v^2 \rangle = 0$$


$$\langle \mathbf{x} \cdot \mathbf{v} \rangle = ce^{-\frac{f}{m}t} + \frac{m}{f} \langle v^2 \rangle \rightarrow \frac{m}{f} \langle v^2 \rangle \text{ stationary solution}$$

3.1.4 To determine Boltzmann's constant from Brownian Motion

$$\langle x^2 \rangle = \frac{1}{3} \langle r^2 \rangle = 2Dt$$

$$\langle \mathbf{x} \cdot \mathbf{v} \rangle = \frac{1}{2} \frac{d \langle \mathbf{x} \cdot \mathbf{x} \rangle}{dt} = \frac{1}{2} \frac{d \langle r^2 \rangle}{dt} = \frac{1}{2} \frac{d(6Dt)}{dt} = 3D$$

$$\langle \mathbf{x} \cdot \mathbf{v} \rangle = \frac{m}{f} \langle v^2 \rangle$$

$$\frac{1}{2} m \langle v^2 \rangle = \frac{1}{2} f \langle \mathbf{x} \cdot \mathbf{v} \rangle = \frac{3}{2} fD$$

$$\frac{1}{2} m \langle v^2 \rangle = \frac{3}{2} kT$$

energy equipartition principle

Boltzmann constant

$$k = D \frac{f}{T} = D \frac{6\pi\mu a}{T}$$

$$f = 6\pi\mu a$$

作业：Ex. 4 Page 90

修正：Eq.(24) 应该为

$$J_p(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \Gamma(k+p+1)} \left(\frac{x}{2}\right)^{2k+p}$$