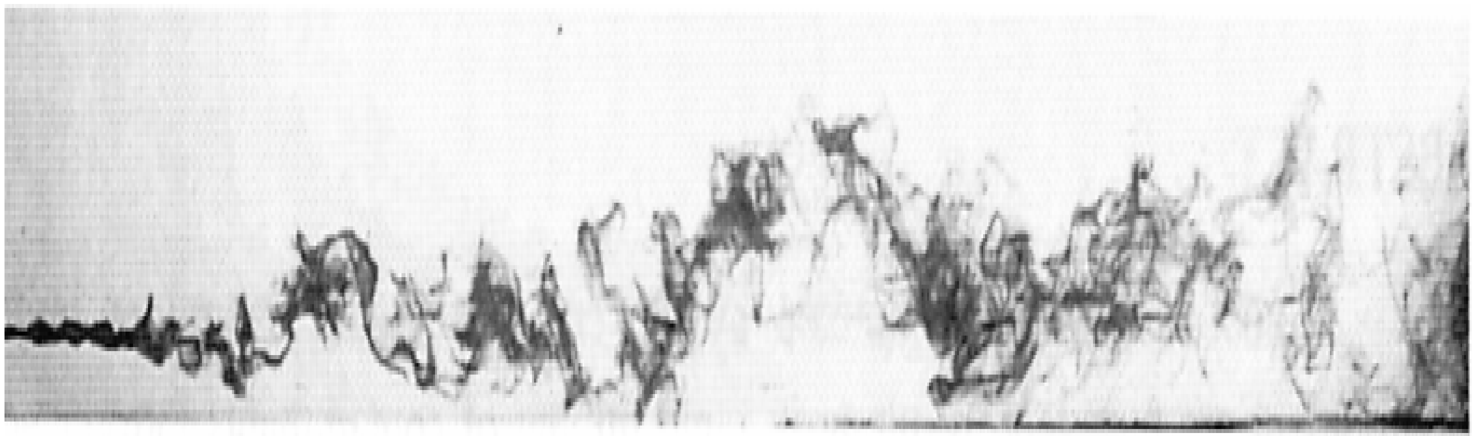
Normal and Anomalous Diffusion (Tutorial)

Loukas Vlahos vlahos@astro.auth.gr)

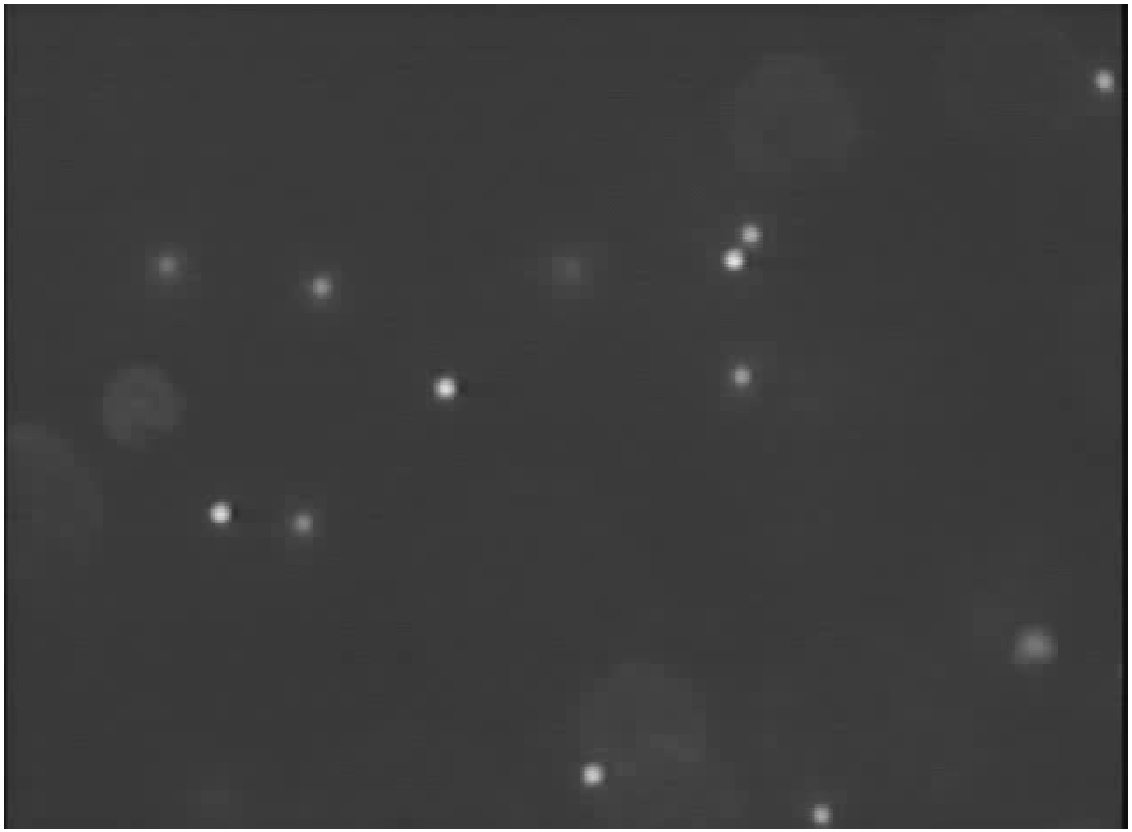
In collaboration with Heinz Isliker



Topics

- Motivation
- Brownian motion and random Walks
- Normal Diffusion
- Walks on Fractal media-traps-Levy flights
- Anomalous diffusion
- Applications and open problems

Motivation



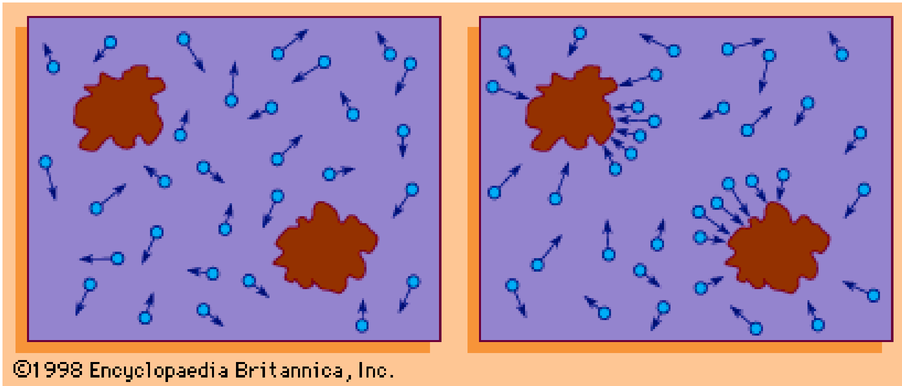
The art of doing research in physics

- We usually start with an observation of natural phenomenon
- We the have a nice idea on “How this phenomenon can be interpreted”
- We need model equations or simulation to build a solid base on the idea.
- Then the idea, started from an observation and moved on to a generic mathematical model, can become a prototype for interpreting many natural phenomena…. and this in the beauty of physics……

Back on the “Brownian motion” : the idea

- Motion of small particles suspended in a fluid due to bombardment by molecules in thermal motion (the physicist)-Einstein.
- Observed first by Jan Ingenhousz 1785, but was rediscovered by Brown in 1828.
- Pollen grains (from trees, plans) are organic substances with life in them, the erratic motion is expression of the power inherent to life (the botanologist)-Brown

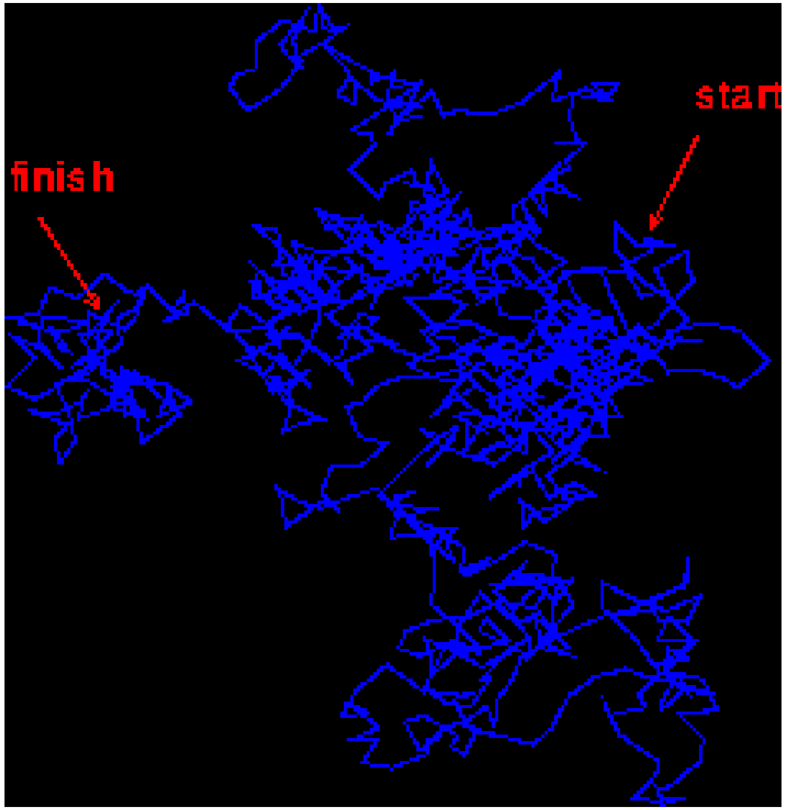
Qualitative Idea



Can we pose another question: How long it will take a drank man to go from the bar to his house?

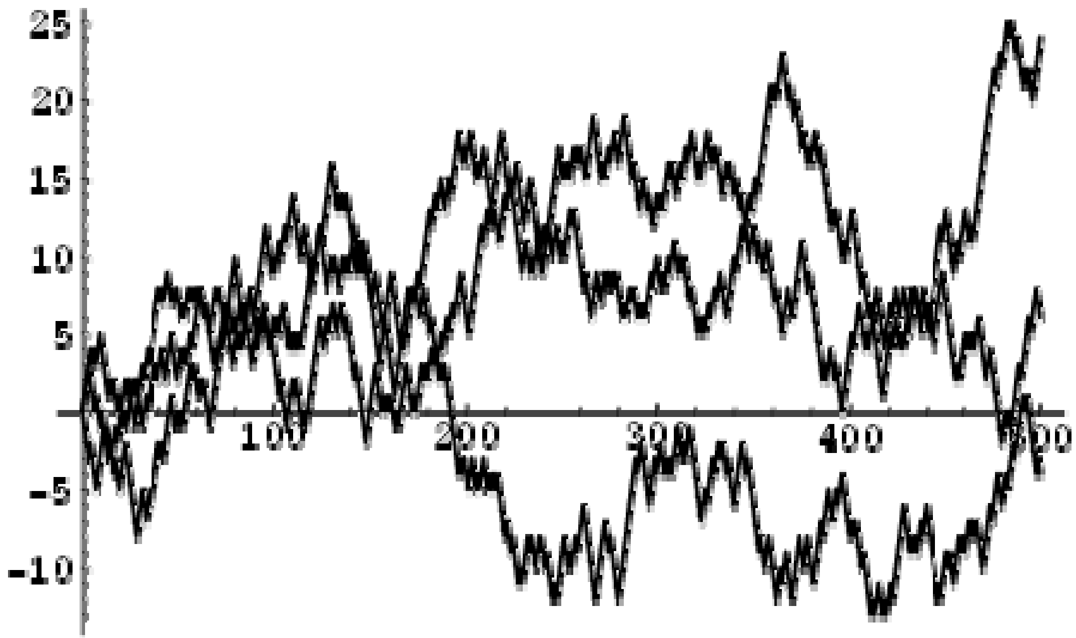
Random walk in 2D

- Choose a random value Δx in the interval [-1,1] and $\Delta y = \pm\sqrt{1-\Delta x^2}$



Question

- What will be the statistics of the distance <r(t_0)> at time t_0 after many repetitions?



More….

$$R^2 = (\Delta x_1 + \Delta y_1 + \Delta x_2 + \Delta y_2 + \Delta x_3 + \Delta y_3 + ... + \Delta x_N + \Delta y_N)^2$$

$$= (\Delta x_1)^2 + ...(\Delta y_N)^2 + ... + 2(\Delta x_1 \Delta x_2) + ...$$

$$< R >= \sqrt{N < r^2 >} = \sqrt{N} r_{rms}$$

- If the distance of the drank man from the bar to his house is 1000m and his step is 1m then you estimate the number of steps that are necessary and assuming that it takes several seconds for each step… you can estimate how long it will take him to reach home….

Mean free path

- A typical particle moving inside a fluid with density n of molecules with radius α will travel a mean distance

$$\lambda = \langle v \rangle \tau$$

between collisions, <v> is the mean velocity and τ the collision time.

- Let us assume an ideal tube of length L and particle collision cross section α inside the fluid. Typical particle will suffer

$$N = 4\pi\alpha^2 L n$$

Collisions before exiting. From this relation we estimate the mean free path

$$\lambda = \frac{1}{4\pi\alpha^2 n}$$

Diffusion from random collisions

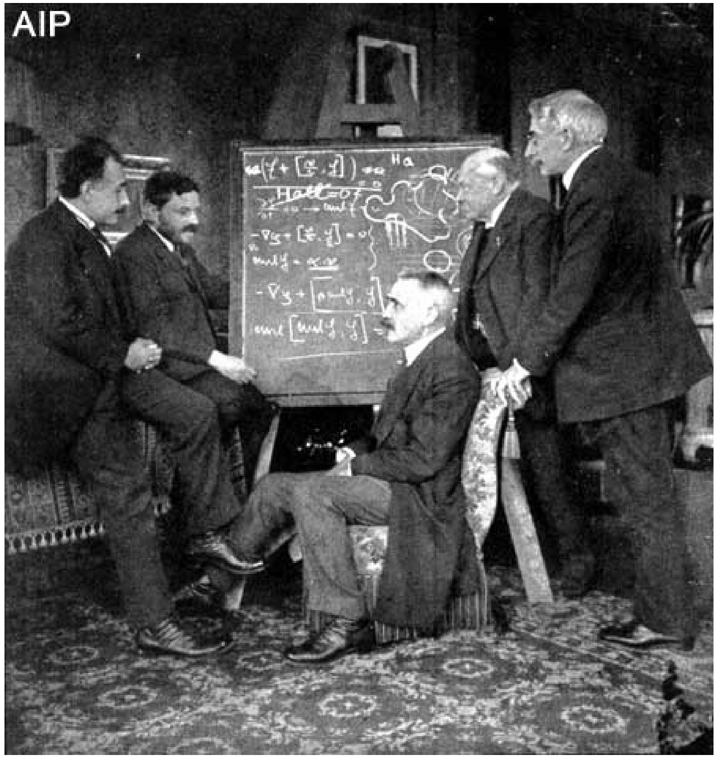
$$< R^2 >= N(< r^2 >) = (t/\tau)(< r^2 >) = Dt$$

$$D \sim < r^2 > / \tau, \quad \tau = \lambda / v_{rms}$$

Mathematical formula for Brownian motion
Langevin Formula

- Paul Langevin at 1908 modeled the Brownian motion

$$m\vec{a} = \vec{F}_i - \gamma\vec{v} + \vec{R}(t)$$



m is the mass of the particle,
v its Speed, $\gamma=6\pi\eta\alpha$,
η=dynamic viscosity,

R(t)=randomly Fluctuating force

More on Langevin's formula

$$m x\ddot{x} = m\left[\frac{d(x\dot{x})}{dt} - \dot{x}^2\right] = -\gamma x\dot{x} + xF(t)$$

$$m\left[\frac{d < x\dot{x} >}{dt} - < \dot{x}^2 >\right] = -\lambda < x\dot{x} > + < xF(t) >$$

$$< xF(t) > = < x >< F(t) > = 0$$

$$\frac{1}{2} m < \dot{x}^2 > = \frac{1}{2} kT$$

$$\left[\frac{d < x\dot{x} >}{dt} + \frac{\gamma}{m} < x\dot{x} >\right] = kT / m$$

$$< x\dot{x} > = \frac{1}{2}\frac{d}{dt} < x^2 > = \frac{kT}{a}(e^{-\gamma t/m} + 1)$$

More on Langevin's formula

$$< x^2 >= \frac{2kT}{\gamma}\left[t - \frac{m}{\gamma}(1 - e^{-\gamma t/m}) \right]$$

More on Langevin's formula

- For
- Ballistic

$$t << (\gamma / m)^{-1}$$

$$< x^2 >= \frac{kT}{2m}\gamma t^2$$

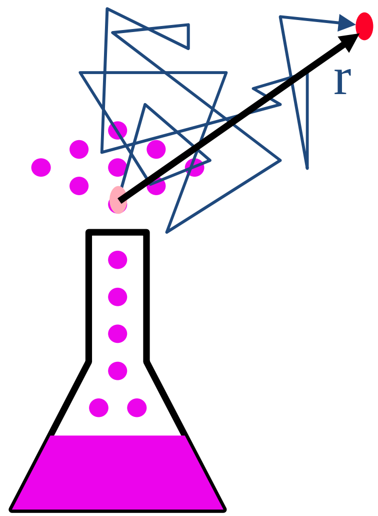
$$t >> (\gamma / m)^{-1}$$

$$Normal\ Diffusion$$

$$< x^2 >= \frac{2kT}{\gamma}t = \frac{kT}{3\pi\eta\alpha}t$$

$$< r^2 >= 3 < x^2 >= \frac{kT}{\pi\eta\alpha}t = Dt$$

Exercise 1: Perfume

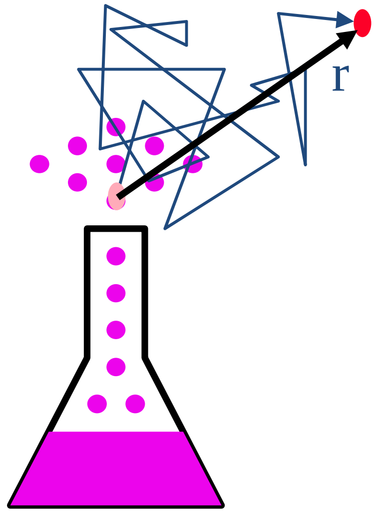


1. ***If the diffusion constant in atmosphere at 300 K is $D = 10^{-5}$ m^2/s, how far (in <u>any</u> direction) will perfume particles diffuse in 1 minute?***

2. ***Approximately how far <u>up</u> will the perfume diffuse in 1 minute?***

Exercise 1: Perfume

1.



$$r_{rms} \approx \left\langle r^2 \right\rangle^{1/2} = \sqrt{Dt}$$

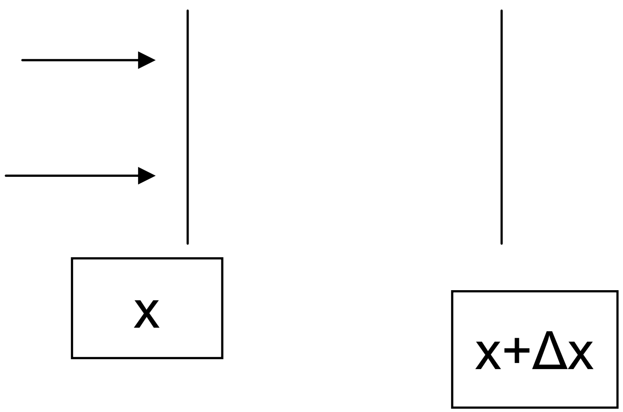
$$\approx \sqrt{\left(10^{-5}\,\mathrm{m^2/s}\right)\left(60\mathrm{s}\right)}$$

$$\approx 6\times10^{-2}\,\mathrm{m} = 6\,\mathrm{cm}$$

The Diffusion equation

- Fick's law
- The flux is proportional to the gradient in concentration

$$J = -D\frac{\partial n}{\partial x}$$

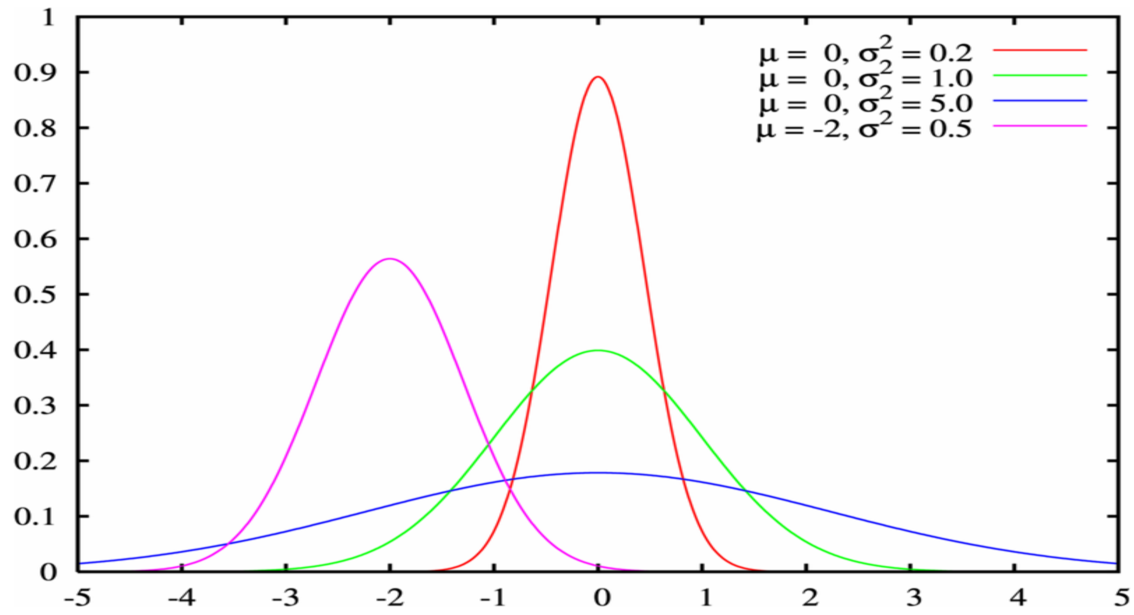


$$\frac{\partial n}{\partial t} = -D\left[\left.\frac{\partial n}{\partial x}\right|_{x} - \left.\frac{\partial n}{\partial x}\right|_{x+\Delta x}\right] = D\frac{\partial^2 n}{\partial x^2}$$

Solution of Diffusion Equation

$$n(x,0) = \delta(x)$$

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

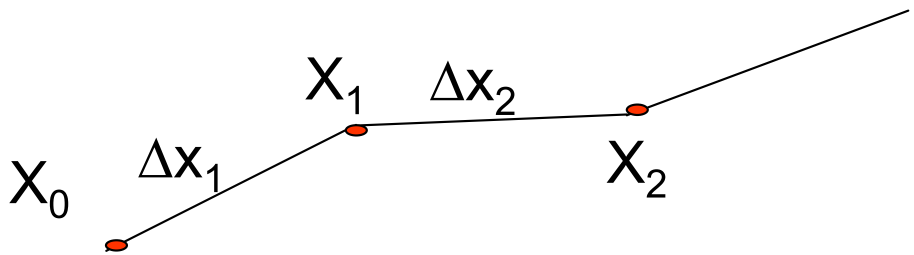


How to treat formally the classical RW

- Only position *x* of a particle is considered
- Time step Δt constant (time plays dummy role, a simple counter)
- Position of particle after n-steps (at time $t_n = n\Delta t$): x_n

$$x_n = \Delta x_n + \Delta x_{n-1} + \Delta x_{n-2} + \ \ldots \ + \Delta x_1 + x_0$$

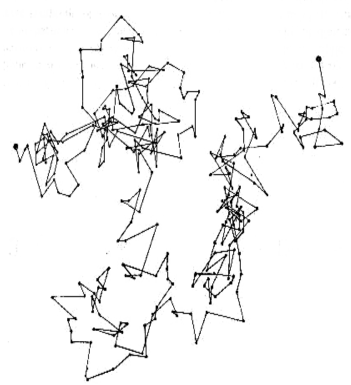
Δx_i: jump increment: random
x_0: initial position



- Need to specify
- distribution of jump increments $q(\Delta x)$: prob. to make a jump Δx
- $\longrightarrow$ RW completely specified:
problem: determine solution, i.e. probability $P(x,t_n)$ that a particle is at position *x* at time $t_n = n\,\Delta t$

How to treat formally the classical RW

- 1827: Brown observed that small particles (pollen grains) in a fluid followed an erratic zig-zag path when seen under the microscope:now called Brownian motion – prototype of random walk.
- The solution of the RW is *P(x,t)*,



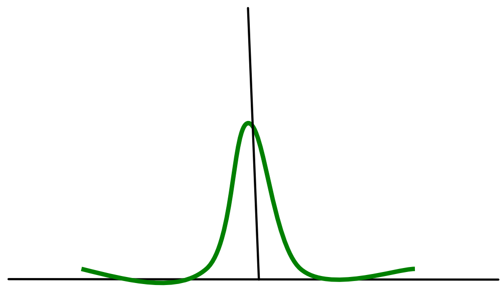
the probability for a particle to be

at position *x* at time *t*, how to determine it ?

- Problem treated by
- 1900: Bachelier (PhD student of Poincare), modelling of stock market temporal evolution.
- 1905: Einstein, modelling of Brownian motion.

Einstein's formalism

- Assume RW in 1-D position space
- Introduce time interval Δt fixed,
  Δt << observation time,
  Δt > typical interaction time for a grain fluid-molecule collision
- The dust grain makes individual and subsequent jumps Δx,
  the Δx follow a certain probability distribution $q(\Delta x)$
  (i.e. the prob. for a jump Δx (with uncertainty $d\Delta x$) is $q(\Delta x)\, d\Delta x$)
- $q(\Delta x)$ is normalized, $\int q(\Delta x)\, d\Delta x = 1$
  and let it be symmetric, for simplicity ($q(-\Delta x)=q(\Delta x)$)
- the dust grain makes only small jumps:
  $q(\Delta x)$ is non-zero only for small Δx
  (peaked and narrow)



Einstein's formalism, cont.

- We need to calculate *P(x,t)*, the prob. for a particle to be at *x* at time *t*
- Assume we knew *P(x, t-Δt)* at an earlier time t-Δt, then

$$P(x,t) = P(x-\Delta x, t-\Delta t)\, q(\Delta x)$$

the prob. to be at *x* at time *t* equals
the prob. to have been at *x-Δx* at time *t - Δt* ago and
to have made a jump *Δx* in time *Δt*

- we still must sum over all possible *Δx*,

$$P(x,t) = \int_{-\infty}^{\infty} P(x - \Delta x, t - \Delta t)\, q(\Delta x)\, d\Delta x$$

RW equation in 1-D → integral equation, to be solved for unknown *P(x,t)*

Einstein's solution for *P(x,t)*

- Einstein-Bachelier equation

$$P(x,t) = \int_{-\infty}^{\infty} P(x - \Delta x, t - \Delta t)\, q(\Delta x)\, d\Delta x$$

- Only small jumps: *q(Δx)* non-zero only for small *Δx*, also *Δt* is small) Taylor expand *P(x-Δx, t-Δt)*,

$$\begin{aligned} P(x - \Delta x, t - \Delta t) = P(x,t) \;&-\; \Delta t\, \partial_t P(x,t) + \ldots \\ &-\; \Delta x\, \partial_x P(x,t) + \frac{1}{2} \Delta x^2\, \partial_x^2 P(x,t) + \ldots \end{aligned}$$

- Insert

$$\begin{aligned} P(x,t) = \int P(x,t)\, q(\Delta x)\, d\Delta x \;&-\; \int \Delta t\, \partial_t P(x,t)\, q(\Delta x)\, d\Delta x \\ &-\; \int \Delta x\, \partial_x P(x,t)\, q(\Delta x)\, d\Delta x \\ &+\; \frac{1}{2} \int \Delta x^2\, \partial_x^2 P(x,t)\, q(\Delta x)\, d\Delta x \end{aligned}$$

- Simplify

$$\begin{aligned} P(x,t) = P(x,t) \;&-\; \Delta t\, \partial_t P(x,t) \\ &+\; \frac{1}{2} \sigma_{\Delta x}^2\, \partial_x^2 P(x,t) \end{aligned}$$

- Simple diffusion equation !

$$\partial_t P(x,t) = \frac{\sigma_{\Delta x}^2}{2 \Delta t} \partial_x^2 P(x,t)$$

Einstein's solution, cont.

- Integral equation turned to simple diffusion equation

$$\partial_t P(x,t) = \frac{\sigma^2_{\Delta x}}{2\Delta t}\partial_x^2 P(x,t)$$

with diffusion constant $D = \frac{\sigma^2_{\Delta x}}{2\Delta t}$

- In infinite system, when particles all start at *x=0* (*P(x,0)=δ(x)*) solution is known,

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

i.e. Gaussian, with time dependent variance $\sigma^2 = 2Dt$

- Mean square displacement:

$$\langle x^2(t)\rangle = \int x^2 P(x,t) = 2Dt$$

(just the variance of the Gaussian, per definition)

) normal diffusion

Normal diffusion should be the usual case

- Consider definition of RW

$$x_n = \Delta x_n + \Delta x_{n-1} + \Delta x_{n-2} + \ \dots \ + \Delta x_1 + x_0$$

- Central Limit Theorem (CLT) of probability theory:
  if all increments Δx_i
  - have finite mean μ and variance σ^2
  - are mutually independent
  - and their number is large

  then x_n has Gaussian distribution (here $\mu=0$, $x_0=0$),

$$P(x,t_n) = \frac{1}{\sqrt{2\pi t_n \sigma^2/\Delta t}} e^{-\frac{x^2}{2 t_n \sigma^2/\Delta t}}$$

- with variance $t_n\sigma^2/\Delta t$ (n=$t_n/\Delta t$)
  (of course the $\langle x^2(t_n)\rangle = \int x^2\, P(x,t_n)\, dx = \text{variance} = t_n\sigma^2/\Delta t$
- MSD: → prop. to t_n) diffusion always normal
- Assumptions of CLT somehow natural: normal diffusion should be the usual case !

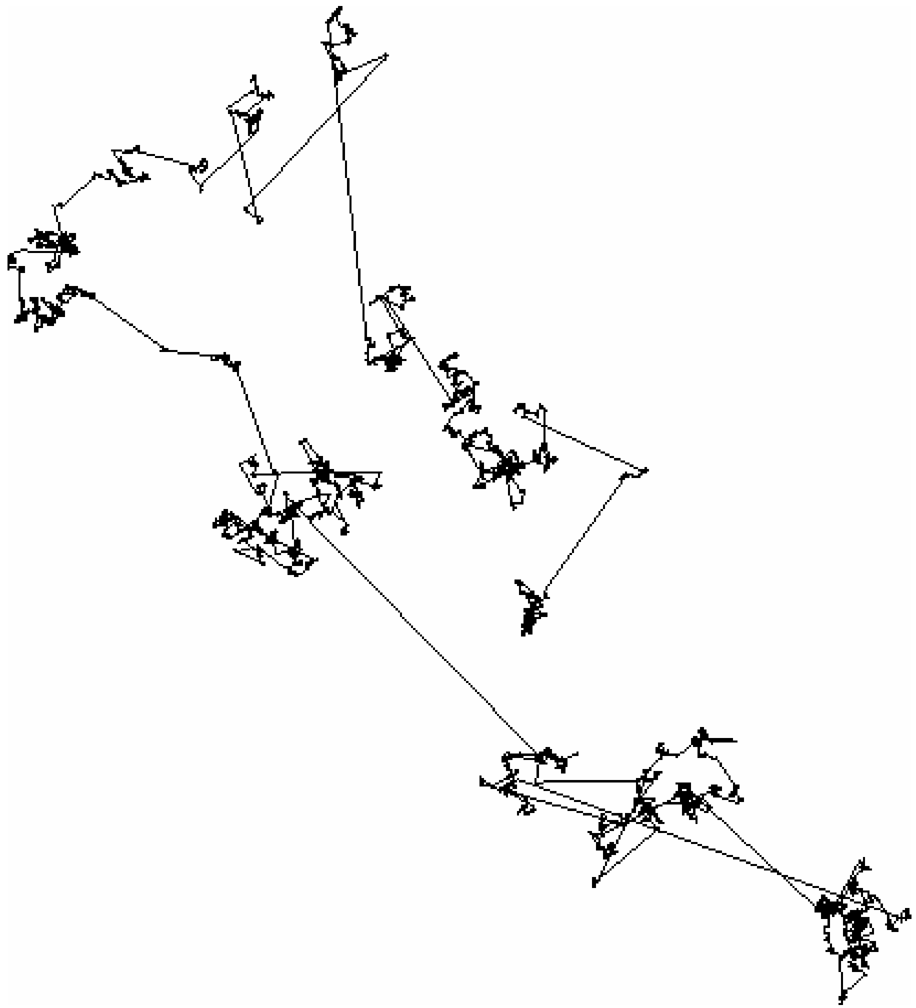
Normal Diffusion

- 1. The mean square displacement

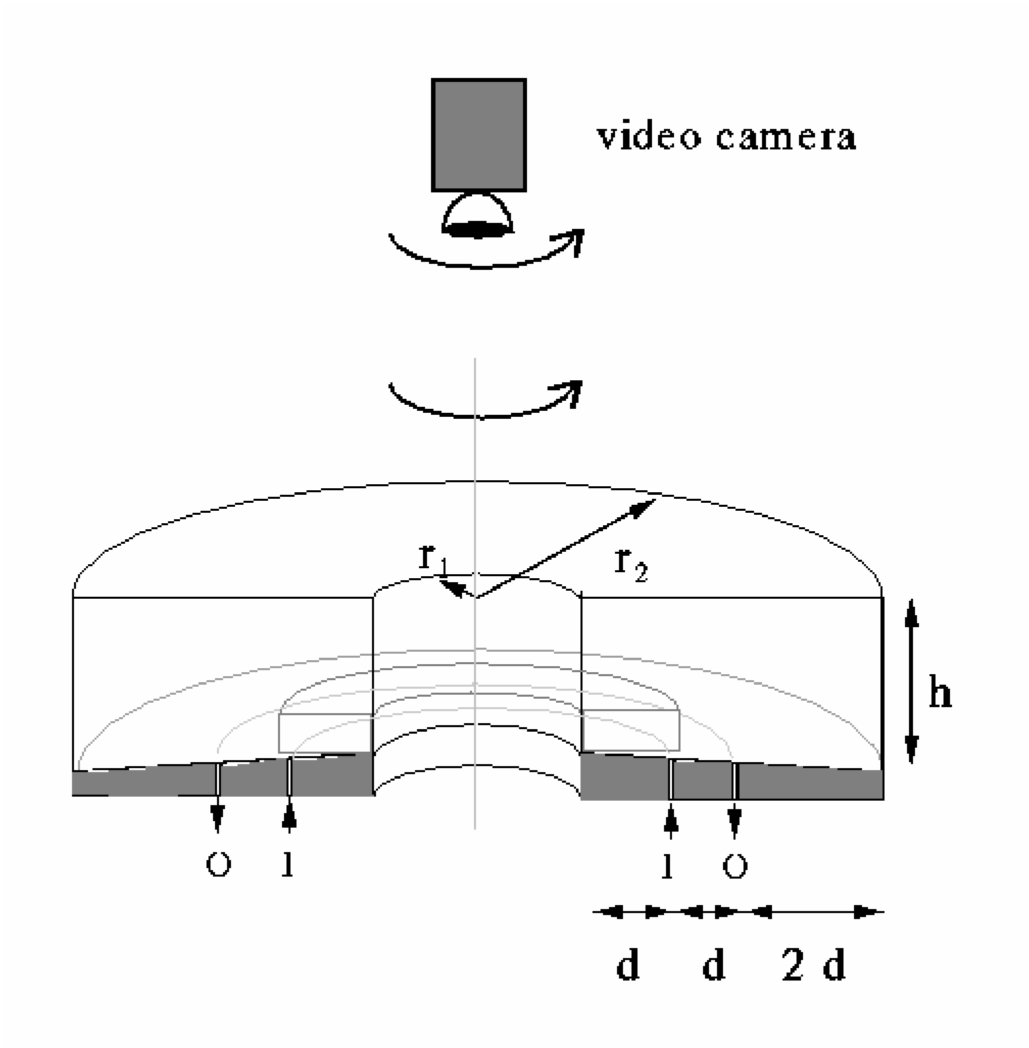
$$< r^2 >= Dt \quad or \quad D = \frac{< r^2 >}{t}$$

- 2. P(x,t)--Gaussian (normal) distributions .
- 3. Diffusion equation
- 4. Langevin's beautiful and simple formula can model the normal diffusion

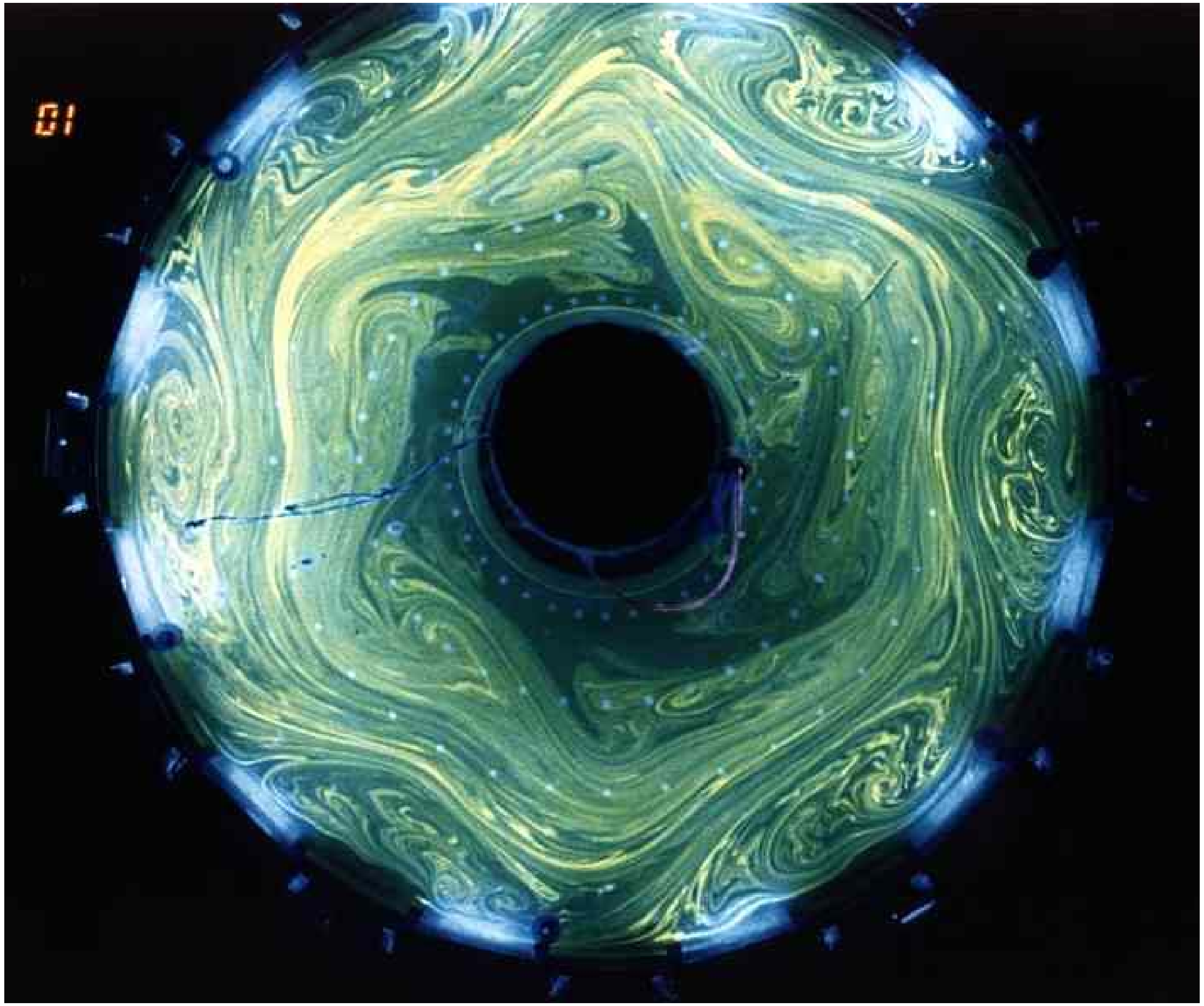
Anomalous....Diffusion



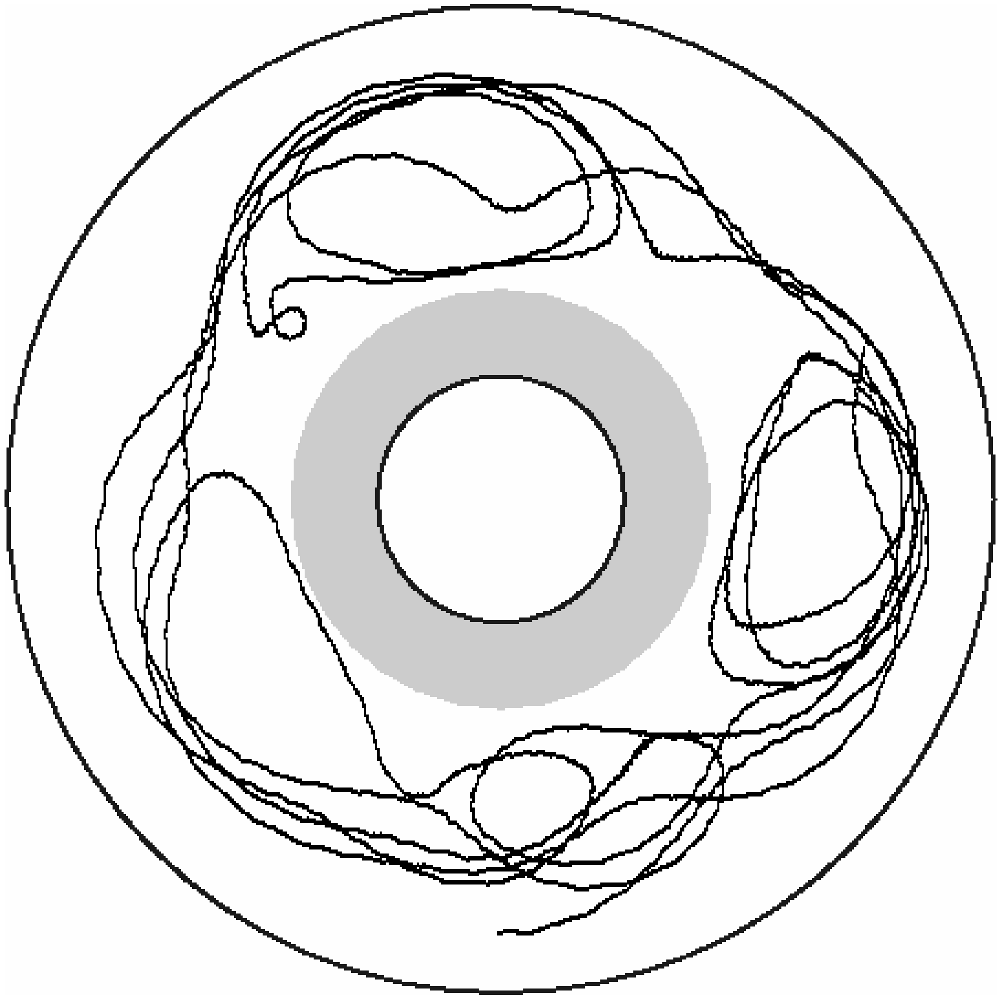
An experiment



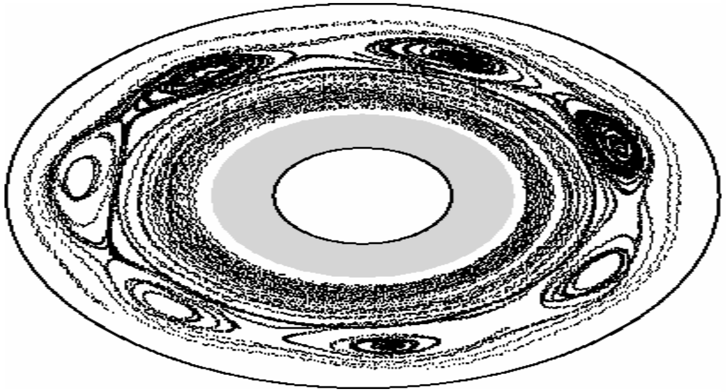
What we see

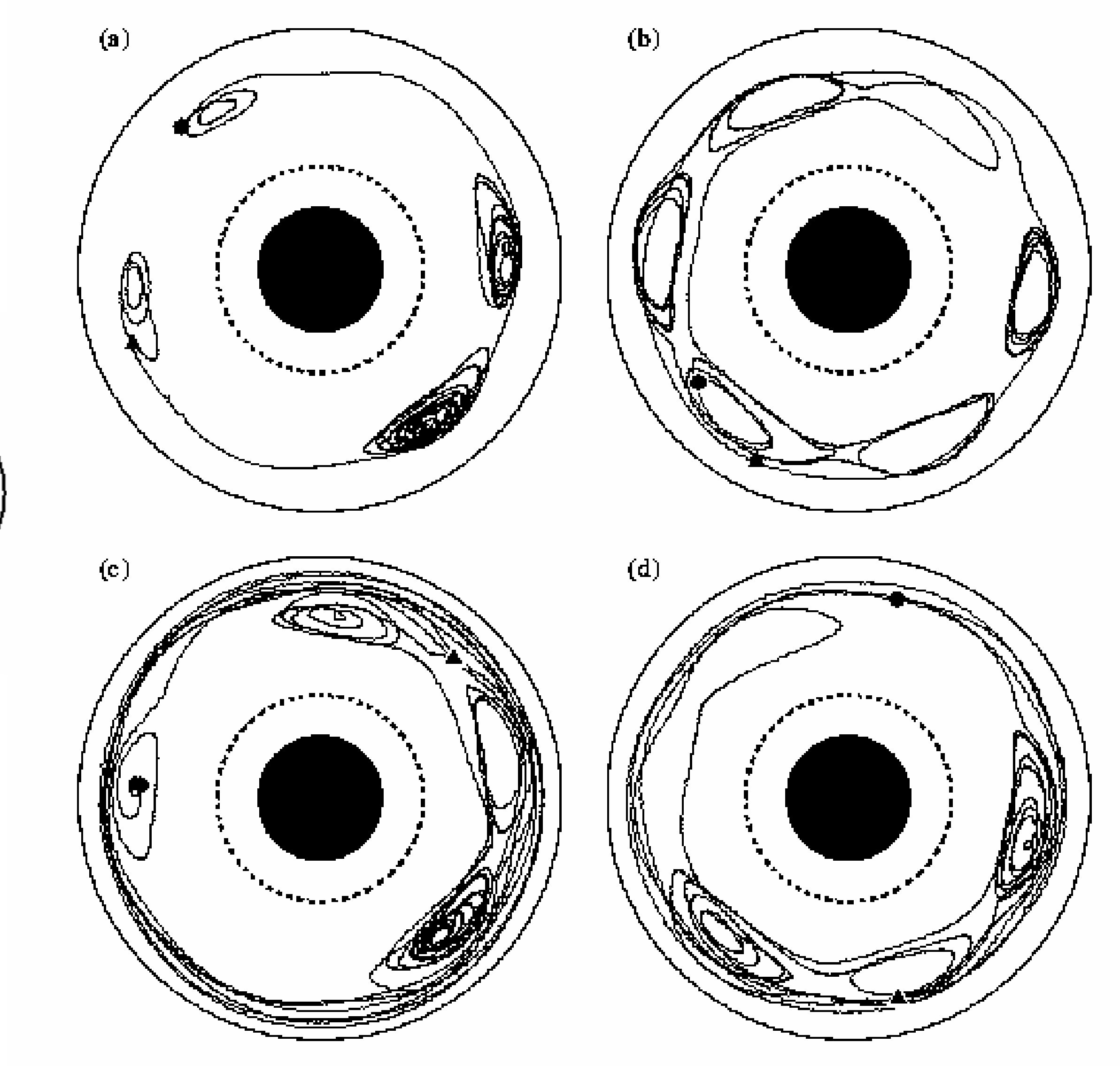


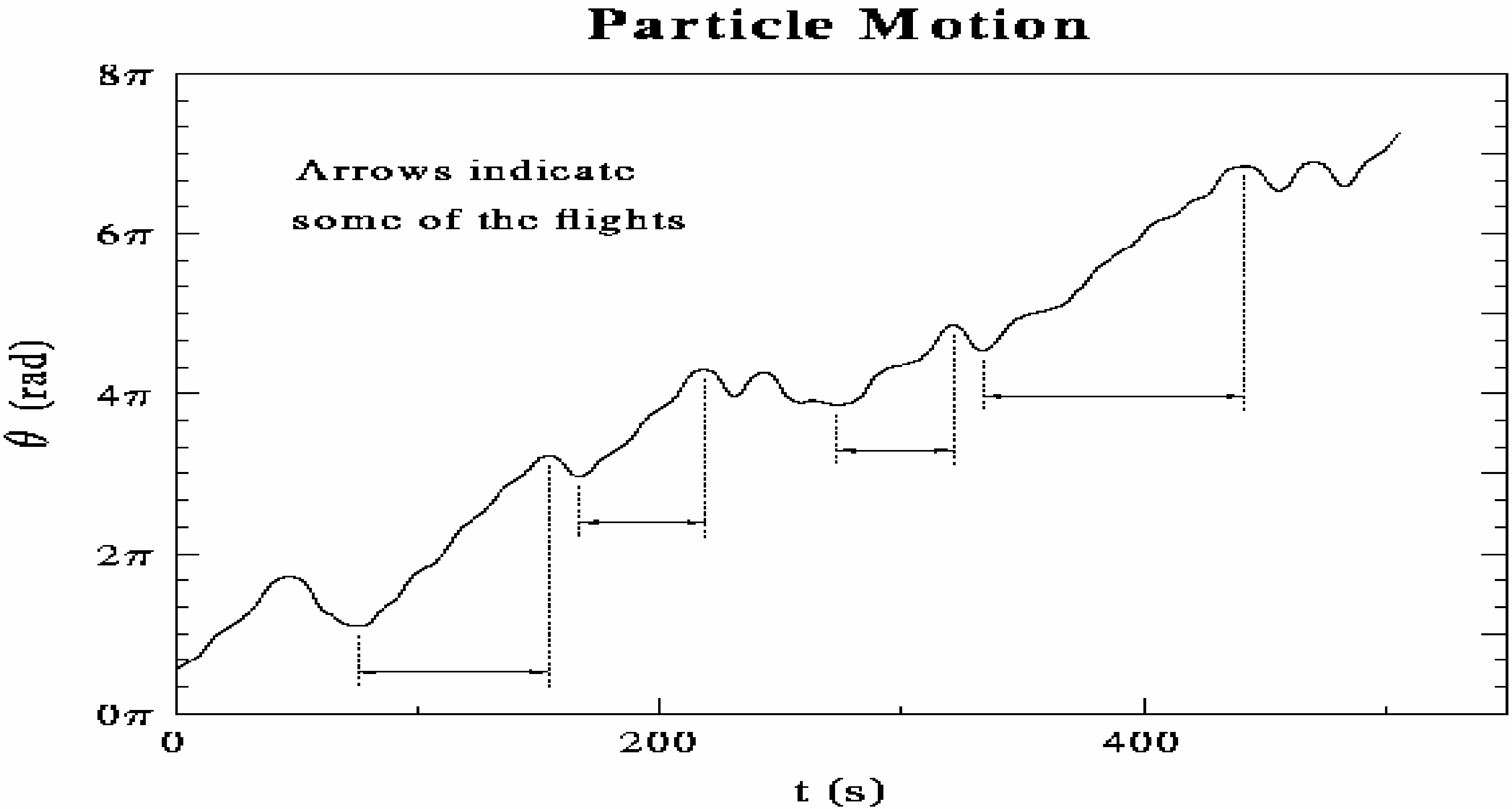
“Strange” walk



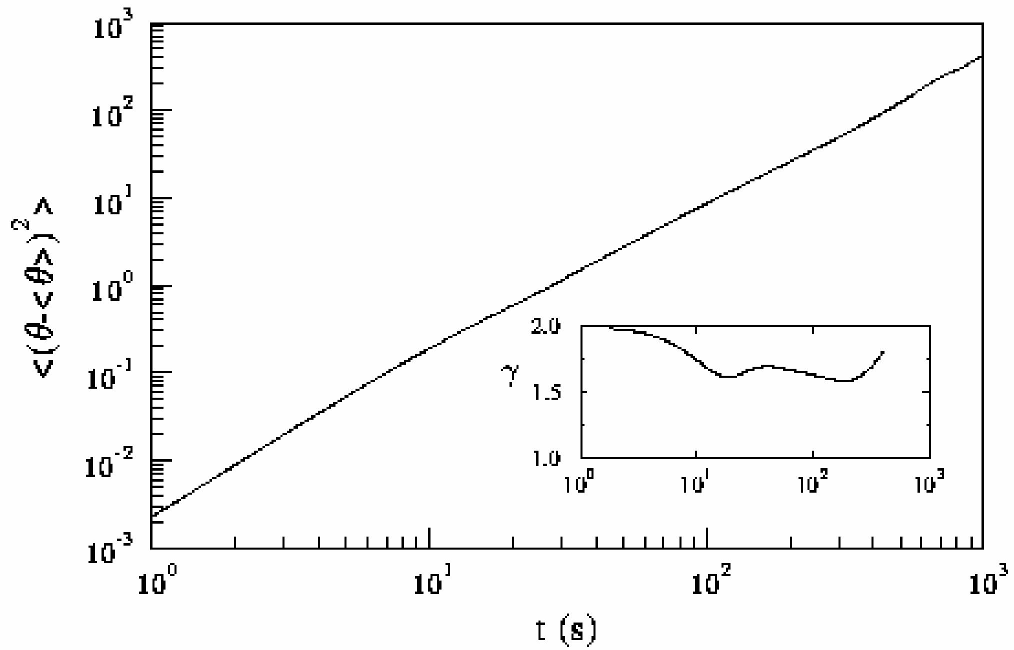
Trajectories inside the annulus



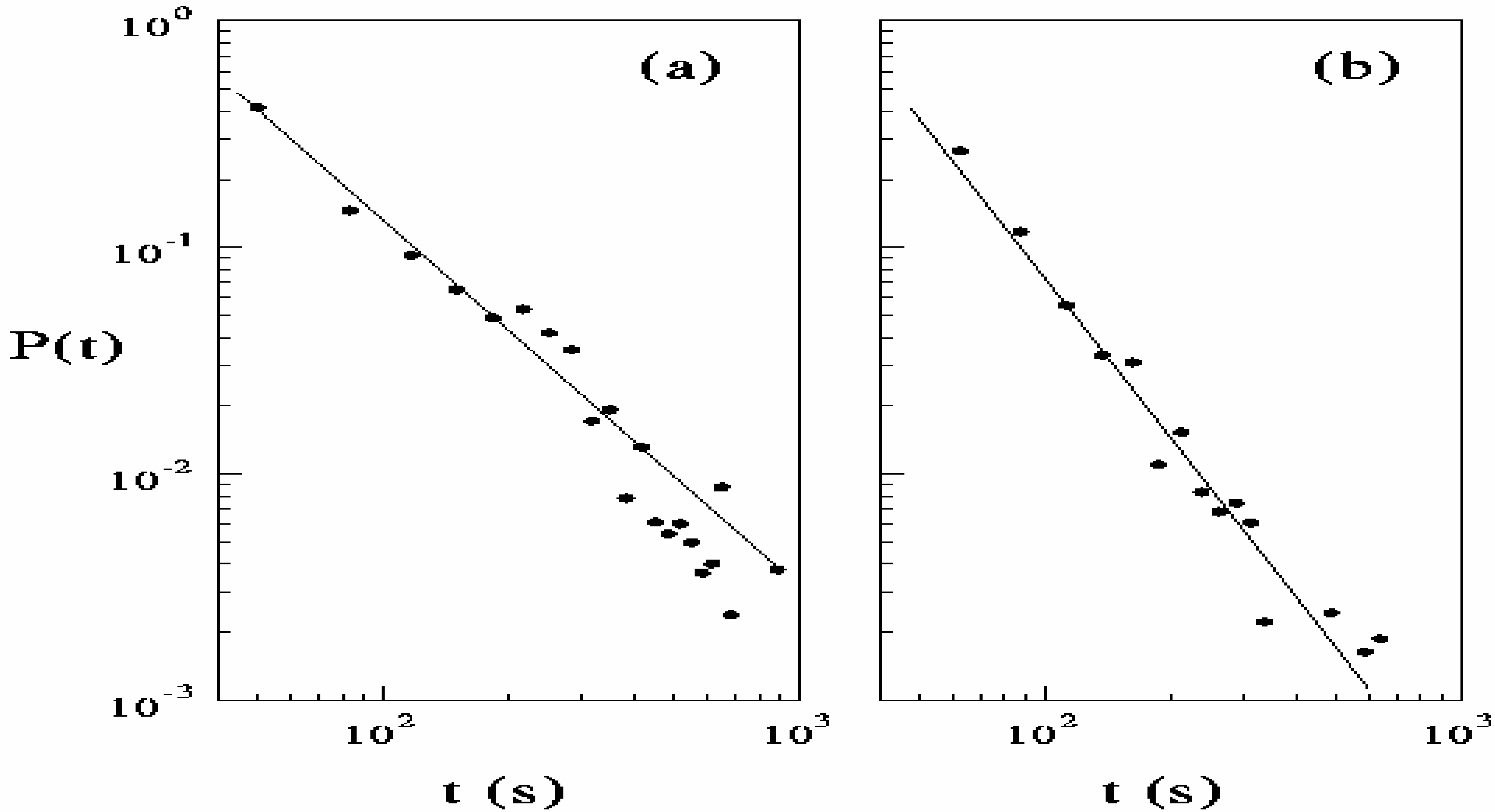



Particle Motion
Arrows indicate
some of the flights
8π
6π
4π
2π
0π
θ (rad)
0
200
400
t (s)

$$< r^2 > \sim Dt^{1.6}$$

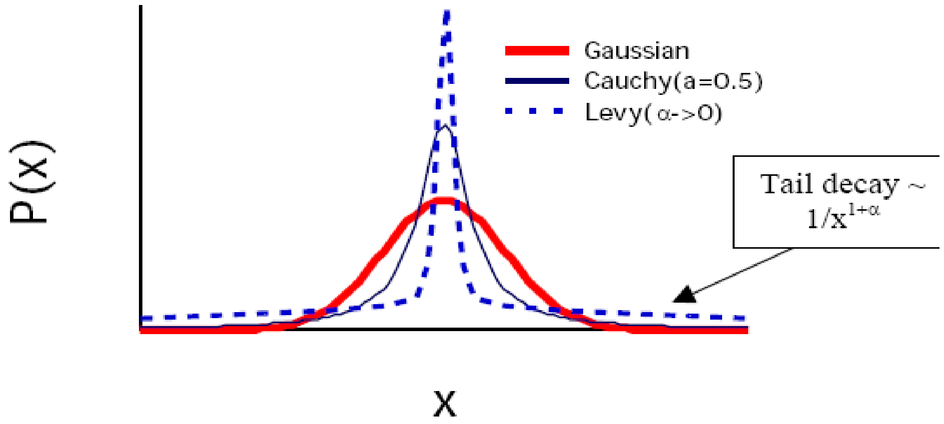


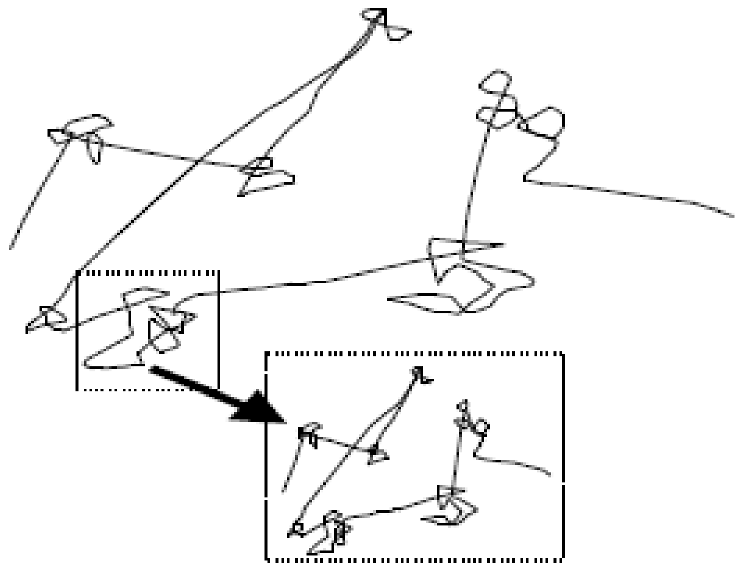
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
$<(\theta-<\theta>)^2>$
10^0
10^1
10^2
10^3
t (s)
2.0
1.5
1.0
γ



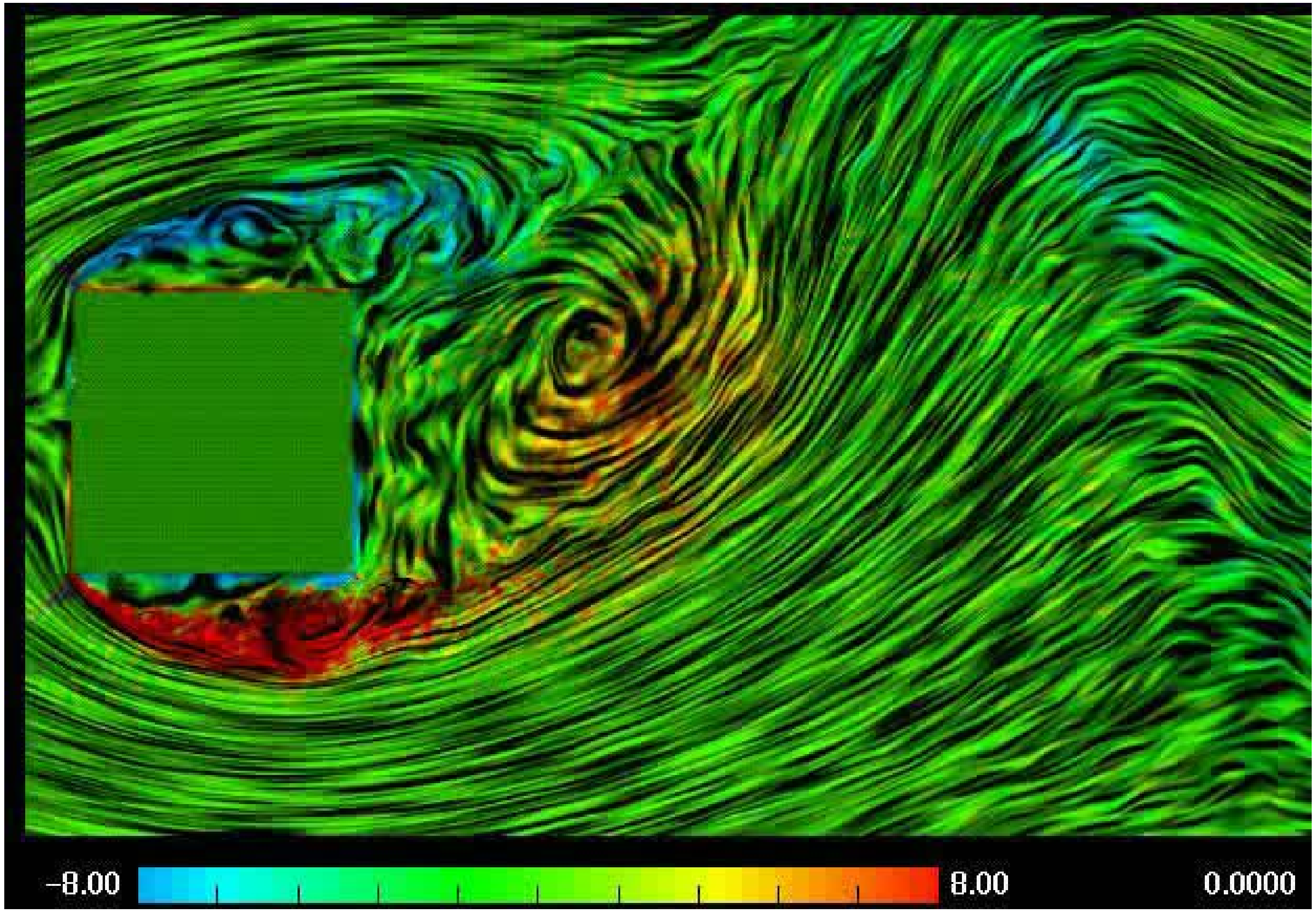
(a)
(b)
P(t)
10^0
10^{-1}
10^{-2}
10^{-3}
10^2
10^3
t (s)

Levy walks and anomalous diffusion





Flow over an obstacle



Langevin type Equations

$$m\frac{d\vec{v}}{dt} = \vec{F}_i - \gamma\vec{v} + \vec{R}(\vec{x},t)$$

$$\frac{d\vec{x}}{dt} = \vec{v}$$

- Strange kinetics-motion in a spatio-temporal complex environment

A ‘**Turbulent**’ Magnetic Field Model

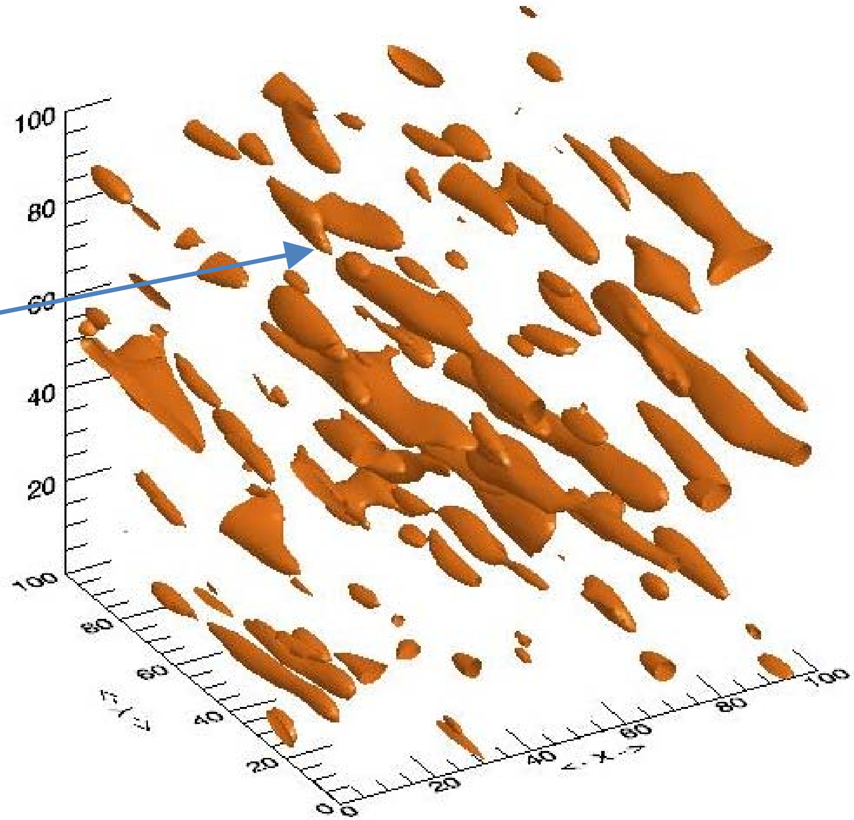
$\mathbf{A}\,(\mathbf{x},t) = \Sigma_{\mathbf{k}}\, \mathbf{a}_{\mathbf{k}} \cos(\mathbf{k}\bullet\mathbf{x} - \omega(\mathbf{k})t + \phi_{\mathbf{k}})$

$\langle|\mathbf{a}_{\mathbf{k}}|^2\rangle \sim (1 + \mathbf{k}^T S \mathbf{k})^{-\nu}$

random $\phi_{\mathbf{k}}$

$\mathbf{B} = \nabla \times \mathbf{A}$

$\mathbf{E} = -\,\partial_t \mathbf{A} + \eta(\mathbf{j})\,\mathbf{j}$



threshold j_c

Electromagnetic forces on charged particles

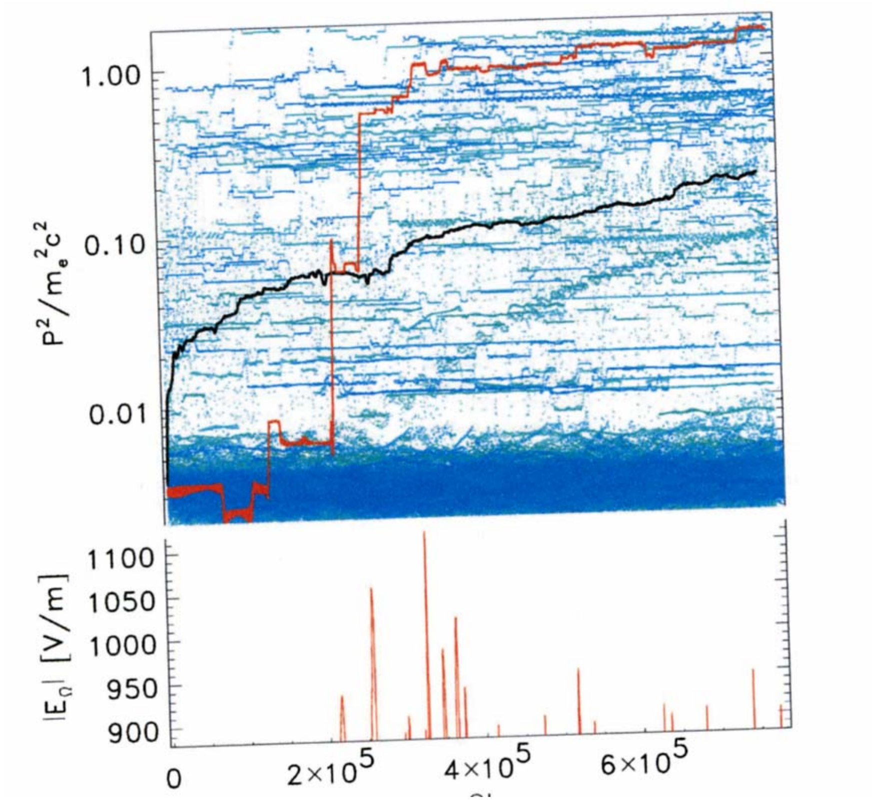
- We can follow the evolution of an ensemble of electrons in the presence of electromagnetic waves

$$m\frac{dv}{dt} = -\gamma v + q[\vec{E}(x,t) + \frac{\vec{v}\times\vec{B}(x,t)}{c}]$$

$$\frac{d\vec{r}}{dt} = \vec{v}$$

Electron motion in turbulent plasmas

- The particle along its orbit meets strong localized E-fields. The motion is long flights interrupted by short and localized E-fields inside the plasma.
- A typical example of anomalous diffusion in energy space---particle acceleration.



Conditions for anomalous diffusion

- Central Limit Theorem (CLT) tries to make all diffusion normal
- For anomalous diffusion, we must violate at least one of its necessary conditions:
  (i) mean and/or variance of increments Δx_i must be infinite, or
  (ii) increments Δx_i must be mutually dependent, or
  (iii) the total number of increments must be small, or
  (iv) the time step Δt is not constant, anymore, but also random
- Point (iv) is what exactly is done in Continuous Time Random Walk (CTRW)
- Point (i) is realized by choice of particular distributions of increments $q(\Delta x)$, the Levy-distributions, with power-law tails:
  $q(\Delta x) \approx \Delta x^{-\alpha}$ (for Δx large)
  (Levy distributions make though sense only in the frame of CTRW)
- Point (iii): small number of steps: less than 30
  (with one step we would not talk about RW anymore)
- Point (ii) is an interesting possibility, could physically often be motivated – has it been tried ?

Continuous Time Random Walk (CTRW)

- Only position is considered (as in classical RW)
- Position of particle after *n*-steps (at time t_n): x_n

$$x_n = \Delta x_n + \Delta x_{n-1} + \Delta x_{n-2} + \ \dots \ + \Delta x_1 + x_0$$

Δx_i: jump increment; x_0: initial position
$\longrightarrow$ as in classical RW

- New in CTRW: time t_n after *n* steps:

$$t_n = \Delta t_n + \Delta t_{n-1} + \Delta t_{n-2} + \ \dots \ + \Delta t_1$$

Δt_i : time needed to perform *i*th step: now random
) also t_n random

- Need now to specify distribution of jump increments Δx and of temporal increments Δt :
  $q(\Delta x, \Delta t)$: probability to make a jump Δx and to spend a time Δt in the jump
- $\longrightarrow$ RW completely specified:
  problem: determine solution, i.e. prob. $P(x,t)$ that particle is at position x at time t

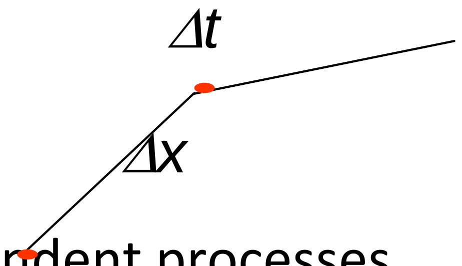
The distribution of increments

- General form $q(\Delta x, \Delta t)$: joint pdf, that specifies both the distribution of Δx and Δt (Δx and Δt might be mutually dependent)
- In practice, two cases are important and were investigated so far, related to different interpretation of what Δt represents:

1. consider Δt to be a waiting or trapping time

$$q(\Delta x, \Delta t) = q(\Delta x)\, q(\Delta t)$$

Δx and Δt are independent:
- waiting/being trapped and spatial jumping are independent processes
- $q(\Delta x)$ and $q(\Delta t)$ can be specified independently of each other

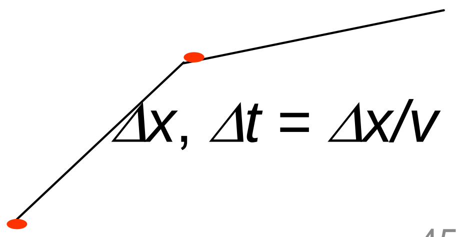


1. Consider Δt to be the time spent in the spatial increment:
assume a constant velocity v, then

$$\Delta t = \Delta x / v$$

i.e. Δt is given by Δx and v, and

$$q(\Delta x, \Delta t) = \delta(\Delta t - \Delta x/v)\, q(\Delta x)$$



The distribution of increments, cont.

- ‘Waiting/trapping model’:
  increments $q(\Delta x)\ q(\Delta t)$
  first version of CTRW historically introduced (1965, Montroll & Weiss)
  most published investigations/applications easiest to treat mathematically
  can though model only sub-diffusion not useful for our intended applications in confined plasma

$$\langle x^2(t)\rangle \propto t^\gamma, \text{ with } \gamma < 1$$

- ‘velocity model’:
  increments $\delta(\Delta t - \Delta x/v)\ q(\Delta x)$
  (introduced by Shlesinger & Klafter 1989) can model super-diffusion
  we focus mostly on the velocity model, in the following

$$\langle x^2(t)\rangle \propto t^\gamma, \text{ with } \gamma > 1$$

The CTRW equation I

- To treat the CTRW analytically, we need to derive its equation:

  waiting/trapping model: equation introduced in 1965 by Montroll and Weiss

  velocity model: equation introduced in 1989 by Shlesinger & Klafter
- Basically: generalize the Bachelier-Einstein equation

$$P(x,t) = \int_{-\infty}^{\infty} P(x - \Delta x, t - \Delta t)\, q(\Delta x)\, d\Delta x$$

- [Still, the equation must determine the probability *P(x,t)* for a particle to be at position *x* at time *t*]
- [CTRW can also be implemented numerically as a Monte-Carlo simulation: let the computer trace the particles which make their random jumps]

The CTRW equation II

- Generalize the Bachelier Einstein equation

$$P(x,t) = \int_{-\infty}^{\infty} P(x-\Delta x, t-\Delta t)\, q(\Delta x)\, d\Delta x$$

- New symbol *Q*. Idea: connect *Q(x,t)* to *Q(x-Δ x,t-Δ t)* in the past:

  Q(x,t) = Q(x-Δx, t-Δt) £ prob. to make a jump *Δx* in time *Δt*

  i.e.

  Q(x,t) = Q(x-Δx, t-Δt) £ δ(Δt - Δx/v) q(Δx)

  Prob. to be at *x* at time *t* equals probability to have been at time *t - Δt* at position *x - Δx*, and to have made a spatial jump *Δx* that took a time *Δt*

- Still need to sum over all possible *Δx, Δt*

$$Q(x,t) = \int dx \int_{0}^{t} dt\, Q(x-\Delta x, t-\Delta t)\, \delta(\Delta t - \Delta x / v)\, q(\Delta x)$$

very close generalization of Bachelier-Einstein

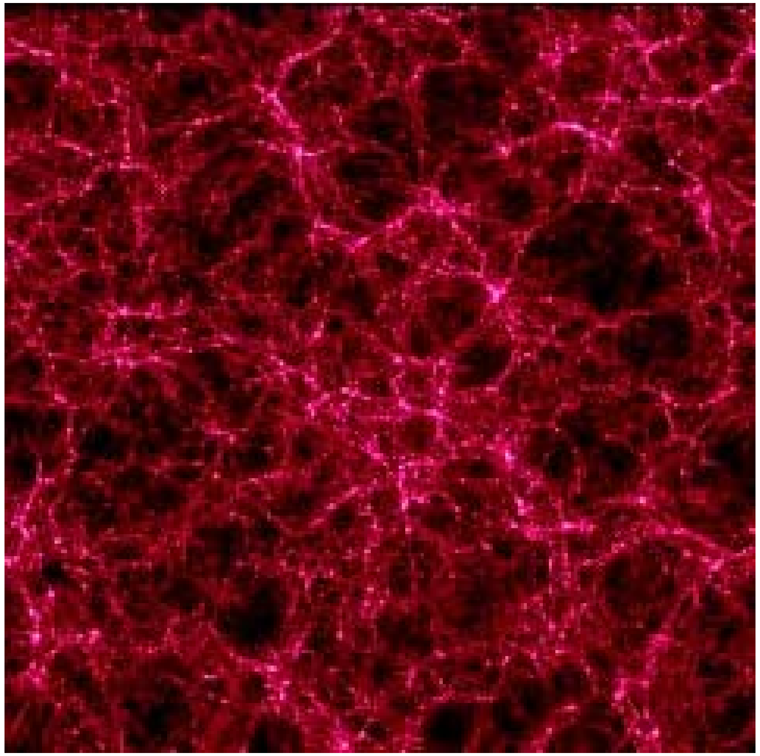
Still open problems on anomalous diffusion

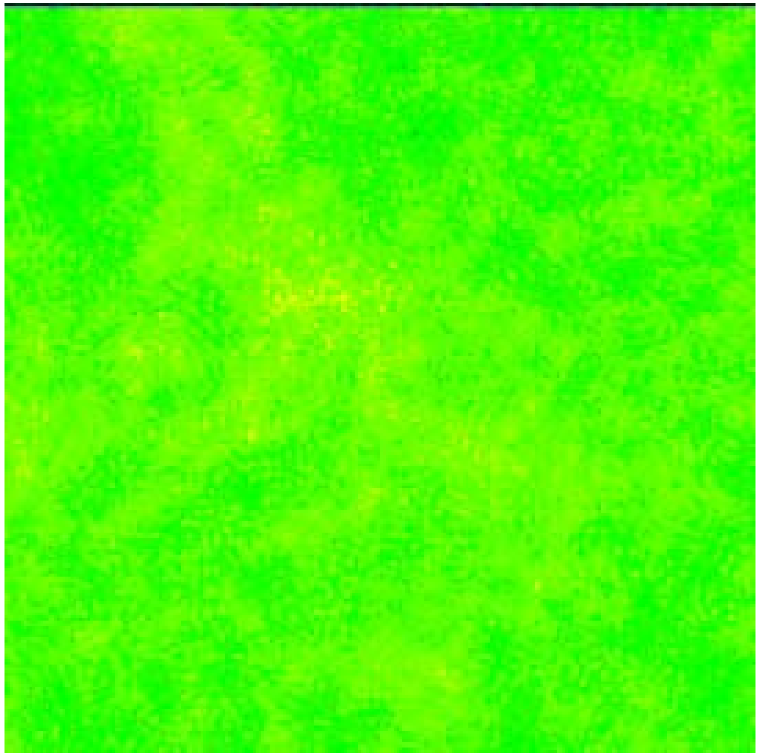
- Interaction of non-equilibrium media with particles

$$< r^2 > \sim t^a \quad a > 1 \quad super-diffusion$$
$$a < 1 \quad sub-diffusion$$

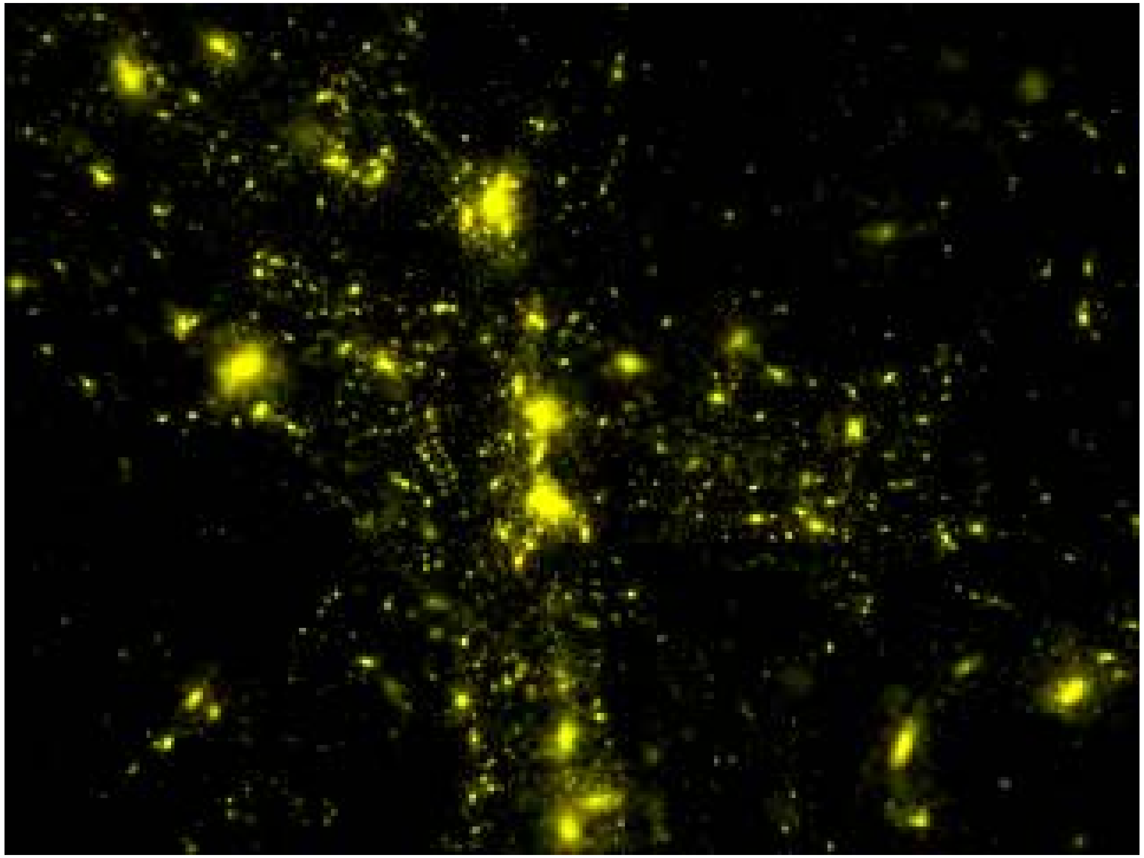
- Fractal forcing as drivers
- Spatial inhomogeneities and diffusion
- Diffusion in the entire phase space (x,v)

An open problem….Diffusion of Cosmic Rays through a fractal Universe: Moving through voids and localized action on gallaxies





Charged particle's voyage inside the universe



Conclusions

- We have discussed the importance of random walk in nature and its relation to normal diffusion in stable systems.
- We have discussed a prototype of stochastic differential equations-The Langevin equation.
- We introduced the notions of anomalous diffusion-Levy flights and continuous random walk- all these are important for turbulent systems.