Stochastic Equations and Processes in physics and biology

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Introduction

When fluctuations and noise become important

Course outline

- Introductory lecture: probability and random variables
- Autocorrelation function, Markovian, stationary and ergodig processes, the random telegraph process
- Random walk, the ruin problem, biased random walk, diffusion equation
- The Wiener-Khinchin theorem, power spectral density, white and colored noise, Wiener process, Ornstein-Uhlenbeck process, the Langevin equation
- Ito and Stratonovich calculus, the Fokker-Planck equation
- Diffusion of a classical Brownian particle, overdamped motion, self-propelled particles and bacteria
- Collective phenomena in stochastic networks

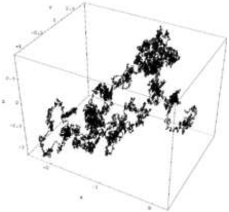
Recommended literature

- Crispin Gardiner *Stochastic Methods: A Handbook for the Natural and Social Sciences*
- Hannes Risken *The Fokker-Planck Equation*
- R.L. Stratonovich *Topics in the Theory of Random Noise*
- R. Kubo, M. Toda, N. Hashitsume, *Statistical Physics II*
- Google on *Stochastic Differential Equations Lecture Notes* gives over 1.000.000 results

Historical overview

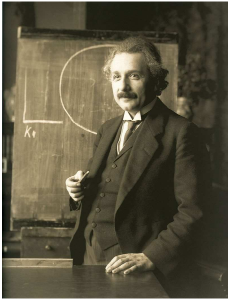
Brownian motion

Experiments by Robert Brown (1827) with grains of pollen of *Clarkia* plant (pinkfairies) suspended in water



Brownian motion

Albert Einstein (1879-1955)



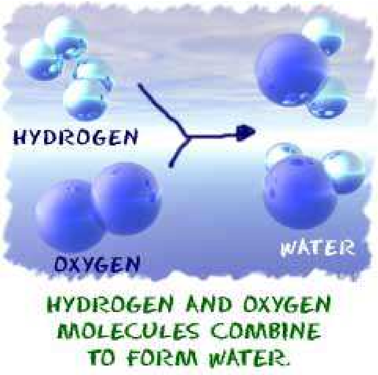
Über die von der molekular-kinetischen Theorie der Wärme geforderte Bewegung von in der ruhenden Flüssigkeiten suspendierten Teilchen, Albert Einstein Ann. Phys. (Leipzig) **17**, 549 (1905)

Brownian motion

Marian Smoluchowski (1872-1917): Polish physicist

Zur kinetischen Theorie der Brownsche Bewegung
Marian Smoluchowski, Ann. Phys. (Leipzig) **21**, 756 (1906)

Chemical reactions



Chemical reactions

Macroscopic equilibrium theory of chemical reactions:

- Cato Maximilian Guldberg (Norwegian mathematician) (left on photo)
- Peter Waage (Norwegian chemist) (right on photo)

Chemical reactions

$$\alpha A + \beta B \rightleftharpoons C$$

Reaction rates

$$r_a = s[A]^\alpha [B]^\beta \exp\left(-\frac{E_a}{kT}\right), \;\; r_d = s[C]\exp\left(-\frac{E_d}{kT}\right)$$

$s \ldots$ steric factor (correction factor w.r.t experimental values)

Law of mass action (1864-1879)

$$K = \exp\left(-\frac{(E_d - E_a)}{kT}\right) = \frac{[C]}{[A]^\alpha [B]^\beta}$$

Kinetic theory of chemical reactions

1916-1918 . . . kinetic theory of chemical reactions based on the collision theory

- Max Trautz (German chemist)
- William Cudmore McCullagh Lewis (British chemist)

Kramers theory of chemical reactions

Hendrik Anthony "Hans" Kramers (1894 - 1952): Dutch physicist

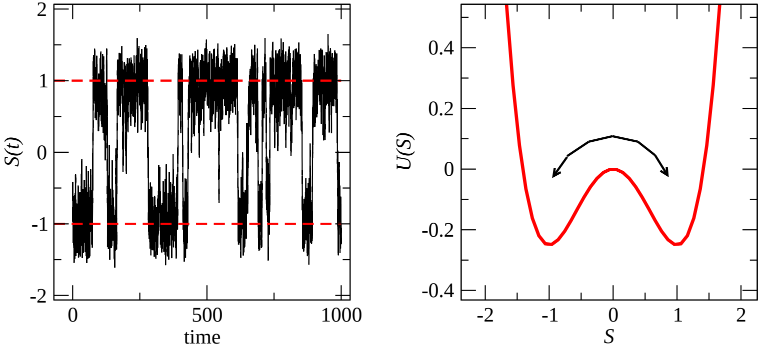
Kramers theory of chemical reactions

Two reacting chemicals: X_1 **and** X_2

$$X_1 \rightleftharpoons X_2$$

Associated bistable system: overcoming a potential barrier

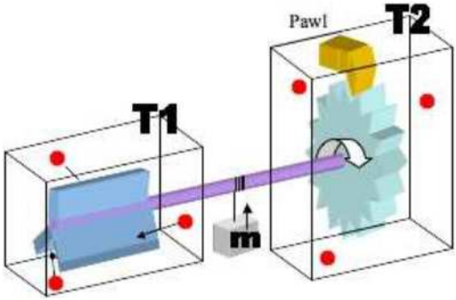
$$\dot{S}(t) = -\frac{dU(S)}{dS} + \text{noise}$$



Smoluchowski-Feynamn ratchet

Richard Phillips Feynman (1918-1988) American theoretical physicist (Nobel Prize in Physics in 1965 for contributions to the development of quantum electrodynamics)

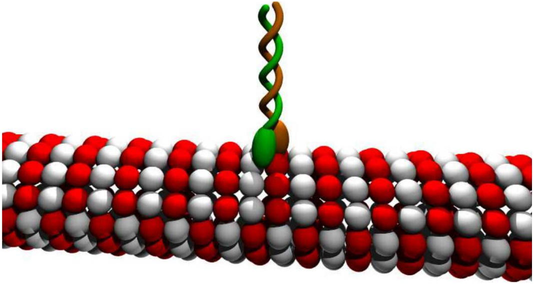
Smoluchowski-Feynamn ratchet



No rotation if in equilibrium $T_1 = T_2$

Biological examples of Rectified Brownian motion

Kinesin moves along microtubule filaments



weight: $>$ 100 KD (1 Da = 1.6 $\times 10^{-27}$ kg), size: up to 100 nm

Forward motion of kinesin as rectified Brownian Motion

Kinesin's Biased Stepping Mechanism: Amplification of Neck Linker Zippering, **W. H. Mather and R. F. Fox, Biophys J. (2006) 91(7): 2416–2426.**

- Two sources of energy:
  (1) Neck linker zippering $e \sim 2kT$ and
  (2) binding of ATP $e \gg kT$, Pulling force $\sim 1.0 \dots 7.0$ pN
- Directed cargo transport is the result of the diffusional displacement of the heads, biased by small-energy zippering and fueled by large-energy ATP binding.

Conditions for rectified Brownian Motion

- **Broken spatial symmetry**
- **Fluctuations (noise)**
- **Out of equilibrium due to external energy supply**

Example

Flashing ratchet (on and off ratchets)

Self-propelled (active) particles

Examples

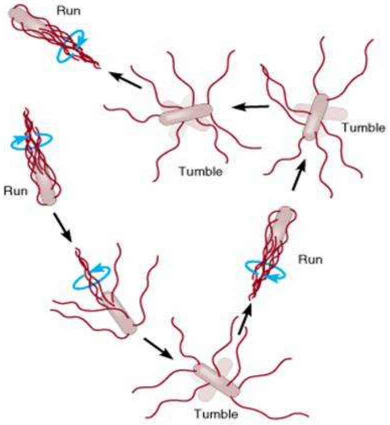
- Molecular motors (complex proteins inside a cell)
- Bacteria with flagellas, such as *E.coli*, *H.pylori* or sperm cells
- Insects, birds, fishes, humans, etc.
- Artificial active particles, such as *Janus* particles

Types of active motion

- Run-and-tumble, motion
- Active Brownian motion

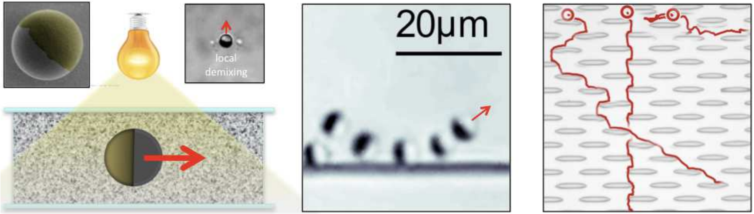
Self-propelled (active) particles

Run-and-tumble motion (picture by Dr. G. Kaiser)

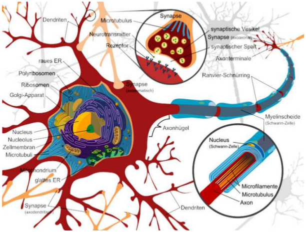


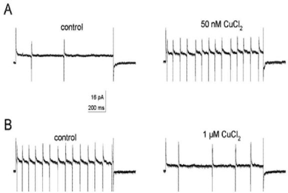
Active Brownian particles (Janus particle)

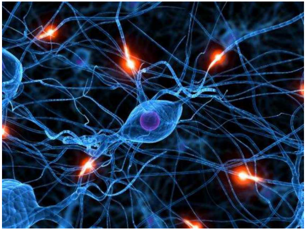
(picture by Prof. Clemens Bechinger)



Spiking Neurons and Neural Networks

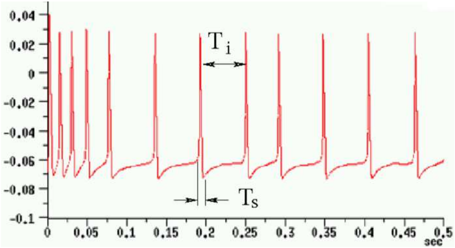






- Each neuron receives signals from other neurons through dendrites
- An electrical pulse is fired along the axon if the integral input signal exceeds a threshold

Neuron as an excitable system



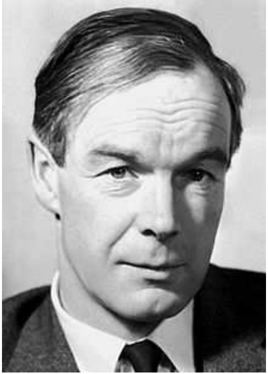
- Spike duration T_s are fixed
- Inter-spike intervals T_i are random

Models of the electrical activity of a neuron

- Hodgkin-Huxley model is an electric circuit model of a neuron (3D dynamical system, electric circuit based model 1952)
- The FitzHugh-Nagumo model (2D dynamical system (1961))
- Integrate-and-fire models (1D models)

Hodgkin-Huxley model

Alan Lloyd Hodgkin (left) and Andrew Fielding Huxley (right): Nobel Prize in Physiology and Medicine 1963



Origin of fluctuations

- Molecular motion: thermal fluctuations
- Chemical reactions: thermal fluctuations and finite-size effects
- Neurons: random synaptic input from other neurons, quasi-random release of neurotrasmitter by the synapses, random switching of ion channels
- Weather: complexity, chaos