Stochastische Prozesse in der Physik

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im Rahmen des Bachelor–Studiengangs *Physik*

Montag 15.15 bis 16.45 Uhr, Konferenzraum Wismarsche Str. 44
Montag 17.00 bis 18.30 Uhr, Konferenzraum Wismarsche Str. 44
Wintersemester 2012/13

This is a joint lecture with the International Study Programme *Master of Science in Physics* at the Institute of Physics.

In addition, everyone from other faculties who likes to learn model driven approaches rather than purely statistical ones is welcome.

Die Lehrveranstaltung begann mit der ersten Vorlesung am Montag, d. 15.10.2012 um 15.15 Uhr im Seminarraum Wismarsche Str. 44 und endete am 28.01.2013 mit einer Diskussion der Studenten-Projekte.

The Importance of Being Noisy – Stochasticity in Science

Why stochastic tools? When you asked alumni graduated from European universities moving into nonacademic jobs in society and industry what they actually need in their business, you found that most of them did stochastic things like time series analysis, data processing etc., but that had never appeared in detail in university courses.

Aim The general aim is to provide stochastic tools for understanding of random events in many beautiful applications of different disciplines ranging from econophysics up to sociology which can be used multidisciplinary.

State of the art General problem under consideration is the theoretical modeling of complex systems, i. e. many–particle systems with nondeterministic behavior. In contrast to established classical deterministic approach based on trajectories we develop and investigate probabilistic dynamics by stochastic tools such as stochastic differential equation, Fokker–Planck and master equation to get probability density distribution. The stochastic apparatus provides more understandable and exact background for describing complex systems. The idea goes back to Einstein's work on Brownian motion in 1905 which explains diffusion process as fluctuation problem by Gaussian law as a special case of Fokker–Planck equation.

Textbooks

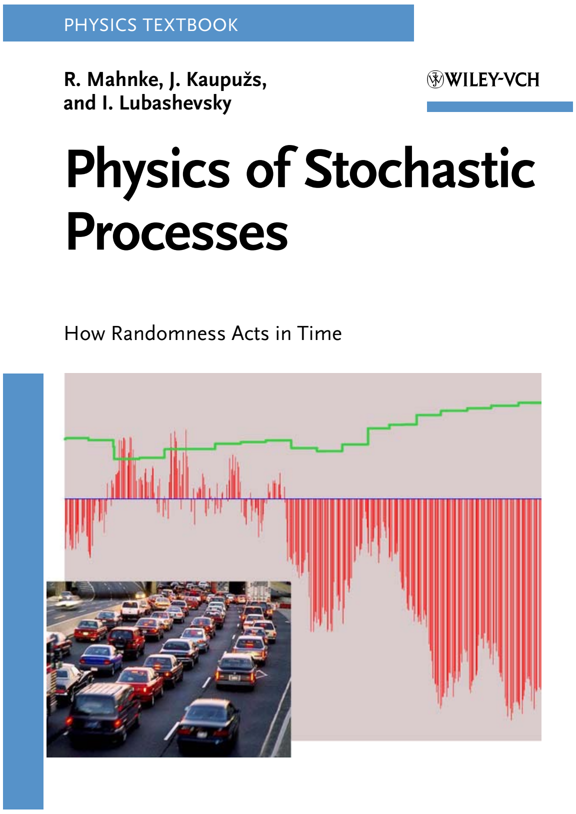

Fig. 1: R. Mahnke, J. Kaupužs and I. Lubashevsky: *Physics of Stochastic Processes*, Wiley-VCH, Weinheim, 2009.

- C. W. Gardiner: Handbook of Stochastic Methods, Springer, 2004
- V. S. Anishchenko et. al: Nonlinear Dynamics of Chaotic and Stochastic Systems, Springer, 2007
- W. Paul, J. Baschnagel: Stochastic Processes, Springer, 1999
- H. Risken: The Fokker-Planck Equation, Springer, 1984
- M. Ullah, O. Wolkenhauer: Stochastic Approaches for Systems Biology, Springer, 2011

Inhaltsverzeichnis

1 Master Equation

1.1 Markovian Stochastic Processes

Stochastic processes enter into many physical descriptions of nature. Historically first the motion of a heavy particle in a fluid of light molecules has been observed. The path of such *Brownian particle* consists of stochastic displacements due to random collisions. Such motion was studied by the Scottish botanist Robert Brown (1773 – 1858). In 1828 he discovered that the microscopically small particles into which the pollen of plants decay in an aqueous solution are in permanent irregular motion. Such a stochastic process is called *Brownian motion* and can be interpreted as discrete random walk or continuous diffusion movement.

The intuitive background to describe the irregular motion completely as stochastic process is to measure values $x_1, x_2, \ldots, x_n, \ldots$ at time moments $t_1, t_2, \ldots, t_n, \ldots$ of a time dependent random variable $x(t)$ and assume that a set of joint probability densities, called JPD–distributions

$$p_n(x_1, t_1; x_2, t_2; \ldots; x_n, t_n)\,, \qquad n = 1, 2, \ldots \tag{1}$$

exists. The same can be done by introducing the set of conditional probability densities (called CPD–distributions)

$$p_n(x_n, t_n \mid x_{n-1}, t_{n-1}; \ldots; x_1, t_1)\,, \qquad n = 2, 3, \ldots \tag{2}$$

denoting that at time t_n the value x_n can be found, if at previous times $t_{n-1}, \ldots, t_1$ the respective values $x_{n+1}, \ldots x_1$ were present. The relationship between JPD and CPD is given by

$$\begin{aligned} &p_{n+1}(x_1, t_1; \ldots; x_{n+1}, t_{n+1}) \\ &\qquad = p_{n+1}(x_{n+1}, t_{n+1} \mid x_n, t_n; \ldots; x_1, t_1)\; p_n(x_1, t_1; \ldots; x_n, t_n)\,. \end{aligned} \tag{3}$$

This stochastic description in terms of macroscopic variables will be called *mesoscopic*. Why? Typical systems encountered in the everyday life like gases, liquids, solids, biological organisms, human or technical objects consist of about 10^{23} interacting units. The macroscopic properties of matter are usually the result of collective behavior of a large number of atoms and molecules acting under the laws of quantum mechanics. To understand and control these collective macroscopic phenomena the complete knowledge based upon the known fundamental laws of microscopic physics is useless because the problem of interacting particles is much beyond the capabilities of the largest recent and future computers. The understanding of complex macroscopic systems consisting of many basic particles (in the order of atomic sizes: 10^{-10} m) requires the formulation of new concepts. One of the methods is the stochastic description taking into account the statistical behavior. Since the macroscopic features are averages over time of a large number of microscopic interactions, the stochastic description links both approaches together, the microscopic and the macroscopic one, to give probabilistic results.

Speaking about a *stochastic process* from the physical point of view we always refer to stochastic variables (random events) changing in time. A realization of a stochastic process is a trajectory $x(t)$ as function of time. Here we introduce a hierarchy of *probability distributions*

$$p_n(x_1, t_1; x_2, t_2; \ldots; x_n, t_n)\, dx_1 dx_2 \ldots dx_n\ , \qquad n = 1, 2, \ldots\ , \tag{4}$$

where $p_1(x_1, t_1)dx_1$ is known as time dependent probability of first order to measure the value x_1 (precisely, the value within $[x_1, x_1 + dx_1]$) at time t_1, $p_2(x_1, t_1; x_2, t_2)$ is the same probability of second order, up to higher–order joint distributions $p_n(x_1, t_1; \ldots; x_n, t_n)dx_1dx_2 \ldots dx_n$ to find for the stochastic variable the value x_1 at time moment t_1, the value x_2 at time t_2 and so on. Only the knowledge of such infinite hierarchy of joint probability densities $p_n(x_1, t_1; \ldots; x_n, t_n)$ (expression (1)) with $n = 1, 2, \ldots$ gives us the overall description of the stochastic process.

A stochastic process without any dynamics (like a coin throw or any hazard game) is called a temporally *uncorrelated process*. It holds that

$$p_2(x_1, t_1; x_2, t_2) = p_1(x_1, t_1)\, p_1(x_2, t_2)\ , \tag{5}$$

if random variables at different times are mutually independent. It means that each realization of a random number at time t_2 does not depend on previous time t_1, i. e., the correlation at different times $t_1 \neq t_2$ is zero. Such a stochastic process, where function $p_1(x_1, t_1) \equiv p_1(x)$ is the density of a normal distribution, is called *Gaussian white noise*. The Gaussian white noise with its rapidly varying, highly irregular trajectory is an idealization of a realistic fluctuating quantity. Due to factorization of all higher–order joint probability densities the knowledge of the normalized distribution $p_1(x_1, t_1)$ describes the process totally.

Now we are introducing dynamics via correlations between two different time moments. This basic assumption enables us to define the *Markov process*, also called *Markovian process*, by two quantities totally, namely the first–order $p_1(x_1, t_1)$ and the second–order probability density $p_2(x_1, t_1; x_2, t_2)$, or equivalently by the joint probability $p_1(x_1, t_1)$ and the conditional probability $p_2(x_2, t_2 \mid x_1, t_1)$ to find the value x_2 at time t_2, given that its value at previous time t_1 $(t_1 < t_2)$ is x_1. In contradiction to uncorrelated processes (5) discussed before, Markov processes are characterized by the following temporal relationship

$$p_2(x_1, t_1; x_2, t_2) = p_2(x_2, t_2|x_1, t_1)\, p_1(x_1, t_1)\ . \tag{6}$$

The *Markov property*

$$p_n(x_n, t_n \mid x_{n-1}, t_{n-1}; \ldots ; x_1, t_1) = p_2(x_n, t_n \mid x_{n-1}, t_{n-1}) \tag{7}$$

enables us to calculate all higher–order joint probabilities p_n for $n > 2$. To determine the fundamental equation of stochastic processes of Markov type we start with the third–order distribution $(t_1 < t_2 < t_3)$

$$\begin{aligned} p_3(x_1, t_1; x_2, t_2; x_3, t_3) &= p_3(x_3, t_3 \mid x_2, t_2; x_1, t_1)\ p_2(x_1, t_1; x_2, t_2) \\ &= p_2(x_3, t_3 \mid x_2, t_2)\ p_2(x_2, t_2 \mid x_1, t_1)\ p_1(x_1, t_1) \end{aligned} \tag{8}$$

and integrate this identity over x_2 and divide both sides by $p_1(x_1, t_1)$. We get the following result for the conditional probabilities defining a Markov process

$$p_2(x_3, t_3 \mid x_1, t_1) = \int p_2(x_3, t_3 \mid x_2, t_2)\, p_2(x_2, t_2 \mid x_1, t_1)\, dx_2\ , \tag{9}$$

called *Chapman–Kolmogorov equation.*

1.2 Repetition: Deterministic Processes

1.2.1 Deterministic Dynamics

Comparing deterministic dynamics and stochastic motion. Each dynamical system (without randomness) has a unique solution called trajectory which is either a regular or an irregular (chaotic) motion. On the other hand, a stochastic process describes temporal evolution of random events by probabilities (discrete case) or probability densities (continuous case). A stochastic trajectory is a sequence of states and times measured as time series.

1.2.2 Mathematical Pendulum: Dynamics

Text and presentation by MSc. Martins Brics.

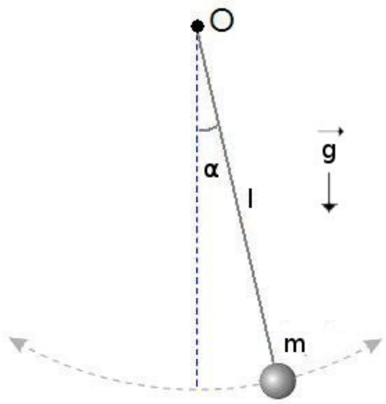

Fig. 2: Mathematical pendelum

Lets calculate total mechanical energy E of mathematical pendulum (see Fig. 2)

$$E = E_{kin} + E_{pot} = \frac{mv^2}{2} + mgl(1 - \cos\alpha) = \frac{L^2}{2I} + mgl(1 - \cos\alpha)\,, \quad (10)$$

where E_{kin} is kinetic energy, E_{pot} is potential energy (potential energy is assumed to be 0, when $\alpha = 2\pi n$, $n \in \mathbb{Z}$), m is mass of pendulum, v is speed of pendulum, l is length of pendulum, $I = ml^2$ is moment of inertia, $L = mvl = I\dot{\alpha}$ is angular momentum $p_\alpha \equiv L$.

So Hamiltonian for mathematical pendulum is

$$H(\alpha, p_\alpha) \equiv H(\alpha, L) = \frac{L^2}{2I} + mgl(1 - \cos\alpha). \tag{11}$$

The equations of motion with initial conditions are

$$\frac{d\alpha}{dt} = \frac{\partial H}{\partial L} = \frac{L}{I}, \tag{12}$$

$$\frac{dL}{dt} = -\frac{\partial H}{\partial \alpha} = -mgl\sin\alpha, \tag{13}$$

$$L(t=0) = L_0\ ; \alpha(t=0) = \alpha_0\ . \tag{14}$$

To get phase plane solution we can simply use energy conservation equation (10) or divide equations (12) and (13) and solve first order order differential equations (ODE).

Lets use energy conservation. Then

$$E = \frac{L_0^2}{2I} + mgl(1 - \cos\alpha_0) = \frac{L^2}{2I} + mgl(1 - \cos\alpha)\ , \tag{15}$$

$$L = \pm\sqrt{2IE - 2Imgl(1 - \cos\alpha)}\ . \tag{16}$$

For simpler analysis lets introduce dimensionless quantities defined as $\tilde{E} = E/2mgl$, $\tilde{L} = L/\sqrt{mglI}$, $\tilde{t} = t\sqrt{mgl/I} = t\sqrt{g/l}$.

The dimensionless analog of equation (16) reads

$$\tilde{L} = \pm 2\sqrt{\tilde{E} - \frac{1}{2}(1 - \cos\alpha)} = \pm 2\sqrt{\tilde{E} - \sin^2\frac{\alpha}{2}}\ . \tag{17}$$

From equation (17), because $0 \leq \sin^2\alpha \leq 1$, we see that there are two possibilities; either trajectory in phase plane are closed lines (there exist α for which L=0) or not (see Fig. 3). The first situation corresponds to oscillations and it is when $\tilde{E} < 1$. The second situation corresponds to rotation and it is when $\tilde{E} > 1$.

Lets rewrite equations of motion also in dimensionless form.

$$\frac{d\alpha}{d\tilde{t}} = \tilde{L}, \tag{18}$$

$$\frac{d\tilde{L}}{d\tilde{t}} = -\sin\alpha, \tag{19}$$

$$\tilde{L}(\tilde{t} = 0) = \tilde{L}_0\ ;\ \alpha(\tilde{t} = 0) = \alpha_0\ . \tag{20}$$

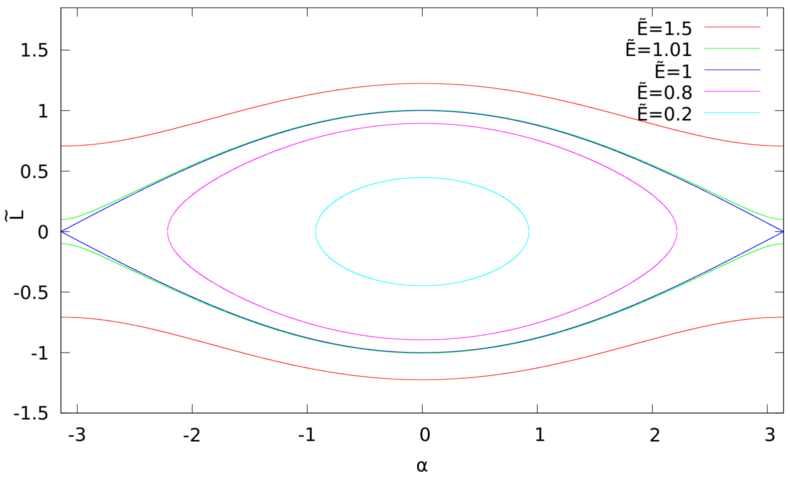

Fig. 3: Phase plane solution for mathematical pendulum

If we insert equation (17) into (18) we get.

$$\frac{d\alpha/2}{d\tilde{t}} = \pm\sqrt{\tilde{E} - \sin^2\frac{\alpha}{2}}, \tag{21}$$

$$\alpha(\tilde{t} = 0) = \alpha_0 \; . \tag{22}$$

And if we integrate with MAPLE, we get

$$\tilde{t} = \pm\frac{\mathrm{sgn}(\cos\frac{\alpha}{2})}{\sqrt{\tilde{E}}}\mathrm{EllipticF}\left(\sin\frac{\alpha}{2}, \frac{1}{\sqrt{\tilde{E}}}\right) \mp \frac{\mathrm{sgn}(\cos\frac{\alpha_0}{2})}{\sqrt{\tilde{E}}}\mathrm{EllipticF}\left(\sin\frac{\alpha_0}{2}, \frac{1}{\sqrt{\tilde{E}}}\right) \tag{23}$$

As Elliptic functions of first kind are no elementary functions, this do not help a lot, so better use numerical solvers. But there are two cases when elliptic integral disappears, when $\tilde{E} = 1$ and $\alpha \ll 1$.

- When $\tilde{E} = 1$, then we equations (21) simplifies to

$$\frac{d\alpha/2}{d\tilde{t}} = \pm\cos\frac{\alpha}{2} \tag{24}$$

and if we integrate we get

$$\tilde{t} = \pm\mathrm{arctanh}(\sin\frac{\alpha}{2}) + C \; . \tag{25}$$

If we use initial conditions and express α, we get

$$\alpha = 2\arcsin(\tanh(\operatorname{sgn}(\tilde{L}_0)\tilde{t} + \operatorname{arctanh}(\sin\frac{\alpha_0}{2}))) \ , \tag{26}$$

$$\tilde{L} = 2\operatorname{sgn}(\tilde{L}_0)\sqrt{1 - \tanh^2(\operatorname{sgn}(\tilde{L}_0)\tilde{t} + \operatorname{arctanh}(\sin\frac{\alpha_0}{2}))} \tag{27}$$

This is rotation or oscillation with infinite period.

- When $\tilde{E} \ll 1$, $sin\frac{\alpha}{2} \approx \frac{\alpha}{2}$ and then equations 21 simplifies to

$$\frac{d\alpha/2}{d\tilde{t}} = \pm\sqrt{\tilde{E} - \left(\frac{\alpha}{2}\right)^2} \tag{28}$$

And if we integrate we get

$$\tilde{t} = \pm \arcsin\frac{\alpha}{2\sqrt{\tilde{E}}} + C \tag{29}$$

If we use initial conditions and express α, we get

$$\alpha = 2\sqrt{\tilde{E}}\sin\left[\operatorname{sgn}(\tilde{L}_0)\tilde{t} + \arcsin\frac{\alpha_0}{2\sqrt{\tilde{E}}}\right] \tag{30}$$

$$\tilde{L} = \operatorname{sgn}(\tilde{L}_0)2\sqrt{\tilde{E}}\cos\left[\operatorname{sgn}(\tilde{L}_0)\tilde{t} + \arcsin\frac{\alpha_0}{2\sqrt{\tilde{E}}}\right] \tag{31}$$

These are harmonic oscillations.

1.2.3 Mathematical Pendulum: Stationary solutions

Stationary solutions of Eqs. (12, 13) do not change in time. To find them we have to set time derivatives to zero, e. g. $\frac{d\alpha}{d\tilde{t}} = 0$ and $\frac{d\tilde{L}}{d\tilde{t}} = 0$

$$0 = \tilde{L}_{st}, \tag{32}$$
$$0 = -\sin\alpha_{st}, \tag{33}$$

If we limit angle to $0 \leq \alpha < 2\pi$ the solution are two stationary solutions:

$$\boldsymbol{x}_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \boldsymbol{x}_2 = \begin{pmatrix} \pi \\ 0 \end{pmatrix} \ , \tag{34}$$

where I used vector notation:

$$\boldsymbol{x} = \begin{pmatrix} \alpha \\ \tilde{L} \end{pmatrix} . \tag{35}$$

Lets analyze stability of them. To do so lets introduce small perturbations $\delta\tilde{L}$ for angular impulse and $\delta\alpha$ for angle: $\alpha = \alpha_{st}+\delta\alpha$, $\tilde{L} = \tilde{L}_{st}+\delta\tilde{L}$. Inserting this into Eqs. of motion (18) and (19) we obtain Eq. for perturbations

$$\frac{d\delta\alpha}{d\tilde{t}} = \tilde{L}_{st} + \delta\tilde{L}, \tag{36}$$

$$\frac{d\delta\tilde{L}}{d\tilde{t}} = -\sin(\alpha_{st} + \delta\alpha), \tag{37}$$

Expanding in Taylor series up to first order we get

$$\frac{d\delta\alpha}{d\tilde{t}} = \delta\tilde{L}, \tag{38}$$

$$\frac{d\delta\tilde{L}}{d\tilde{t}} = -\cos(\alpha_{st})\delta\alpha, \tag{39}$$

or in Matrix notation

$$\frac{d}{d\tilde{t}} \begin{pmatrix} \delta\alpha \\ \delta\tilde{L} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\cos(\alpha_{st}) & 0 \end{pmatrix} \begin{pmatrix} \delta\alpha \\ \delta\tilde{L} \end{pmatrix} = \mathbf{J}(\boldsymbol{x}_i) \begin{pmatrix} \delta\alpha \\ \delta\tilde{L} \end{pmatrix} , \tag{40}$$

where $\mathbf{J}(\boldsymbol{x}_i)$ in general case is Jacobian matrix. This is a linear system. The solutions of this system are

$$\begin{pmatrix} \delta\alpha \\ \delta\tilde{L} \end{pmatrix} = C_1 \boldsymbol{v_1} e^{\lambda_1 t} + C_2 \boldsymbol{v_2} e^{\lambda_2 t} , \tag{41}$$

where $C1$ and $C2$ are coefficients and $\boldsymbol{v_1}$, $\boldsymbol{v_2}$ and λ_1, λ_2 are eigenvectors and eigenvalues of matrix $\mathbf{J}(\boldsymbol{x}_i)$.The perturbation will grow if $\Re\lambda_i > 0$.

To find eigenvalues we have to solve Eq. $\det(\mathbf{J}(\boldsymbol{x}_i) - \lambda\mathbf{I}) = 0$.

- For stationarity solution $\boldsymbol{x}_1$ we find

  $$\lambda_1 = \imath \quad \lambda_2 = -\imath. \tag{42}$$

  The eigenvalue are purely imaginary, so this describes oscillations with constant amplitude. This is stable solution.

- For stationarity solution $\boldsymbol{x}_2$ we find

  $$\lambda_1 = 1 \quad \lambda_2 = -1. \tag{43}$$

  This is clearly unstable solution.

1.2.4 Linear stability analysis

In general case to preform stability analysis of stationary solution for system of nonlinear first order differential Eq. written in vector form $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$ you first have to

1. find stationary solutions: $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}_{st})$.
2. Calculate Jacobian matrix $\mathbf{J}$ with elements $J_{ij} = \frac{\partial f_i}{\partial x_j}$.
3. Evaluate Jacobian matrix at stationary solution $\mathbf{J}(\boldsymbol{x}_{st}) = \mathbf{J}|_{\boldsymbol{x}=\boldsymbol{x}_{st}}$.
4. Calculate eigenvalues of Jacobian matrix evaluated at stationary point $\det(\mathbf{J}(\boldsymbol{x}_i) - \lambda\mathbf{I}) = 0$.
5. Analyze eigenvalues:
   - if real part of all eigenvalues are negative, then solution is stable.
   - if real part of one or more eigenvalues is positive, then solution is unstable.
   - if eigenvalues are purely imaginary, there is no conclusion (then we have a borderline case between stability and instability; such cases in general require an investigation of the higher order terms we neglected in linear stability analysis). If after applying stability analysis of higher order we still have the same analysis then we have undamped osculations with constant amplitude around stationery solution as in case of Mathematical Pendulum (Sec. 1.2.2). Such solutions are still called stable. As it is quite difficult you can try to solve Eq. numerically to see if it is stable or unstable.

1.2.5 Lorenz Model

Lorenz model (see system of Eqn. (44)) was originally derived by *Edward N. Lorenz* as approximation to Rayleigh-Benard convection cells model which describe the dynamical behavior of convection rolls in fluid layers that are heated from below. Variables x, y, z are velocities in x, y and z direction, and parameter σ is Prandtl number, $r = R_a/R_c$ where where R_a is the Raleigh number and R_c is the critical value of R_a, and b is just geometrical factor. Note that all parameters are positive numbers.

$$\begin{cases} \dfrac{dx}{dt} = \sigma(y-x) \\ \dfrac{dy}{dt} = rx - y - xz \\ \dfrac{dz}{dt} = xy - bz \end{cases} \tag{44}$$

Lets start with fixed point analysis.

For simplicity lets introduce vector $\boldsymbol{x}$ and vector function $\boldsymbol{f}(\boldsymbol{x})$

$$\boldsymbol{x} = \begin{pmatrix} x \\ y \\ x \end{pmatrix} \qquad \boldsymbol{f}(\boldsymbol{x}) = \begin{pmatrix} \sigma(y-x) \\ rx - y - xz \\ xy - bz \end{pmatrix} \qquad \frac{d\boldsymbol{x}}{dt} = \dot{\boldsymbol{x}}\ ,$$

so now Lorenz equation we can write just as $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$. To find fixed points we need to solve $\boldsymbol{f}(\boldsymbol{x}) = 0$.

$$\begin{cases} 0 = \sigma(y-x) \\ 0 = rx - y - xz \\ 0 = xy - bz \end{cases} \tag{45}$$

Despite nonlinearity of Lorenz system it is quit easy because first equation of (45) gives us that for fixed $x = y$. And we find that

$$\boldsymbol{x}_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \qquad \boldsymbol{x}_2 = \begin{pmatrix} \sqrt{(r-1)b} \\ \sqrt{(r-1)b} \\ r-1 \end{pmatrix} \qquad \boldsymbol{x}_3 = \begin{pmatrix} -\sqrt{(r-1)b} \\ -\sqrt{(r-1)b} \\ r-1 \end{pmatrix} \tag{46}$$

Note that $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$ are only valid for $r > 1$, this implies, that $r = 1$ should be bifurcation point.

Now we should explore stability of fixed points. But because Lorenz system is invariant under transformation $(x, y, z) \leftrightarrow (-x, -y, z)$ we have to analyze only properties of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, because fixed point $\boldsymbol{x}_3$ has the same properties as $\boldsymbol{x}_2$. As this system is complicated lets do only **linear stability analysis**.

Linear stability analysis tells us, if real parts of all eigenvalues of the Jacobian matrix $\boldsymbol{J}(\boldsymbol{x})$ ($J_{ij} = \frac{\partial f_i}{\partial x_j}$) at fixed point are negative then fixed point is stable. For Lorenz system Jacobian matrix is

$$\boldsymbol{J}(\boldsymbol{x}) = \begin{pmatrix} -\sigma & \sigma & 0 \\ r-z & -1 & -x \\ y & x & -b \end{pmatrix} \tag{47}$$

- Stability of $\boldsymbol{x}_1$:

  For fixed point $\boldsymbol{x}_1$ Jacobian matrix is

  $$\boldsymbol{J}(\boldsymbol{x}_1) = \begin{pmatrix} -\sigma & \sigma & 0 \\ r & -1 & 0 \\ 0 & 0 & -b \end{pmatrix} \tag{48}$$

  To calculate eigenvalues λ of Jacobian matrix we need to solve equation $\mathrm{Det}(\boldsymbol{J}(\boldsymbol{x}_1) - \lambda I) = 0$, where I is 3x3 is identity matrix.

  $$\mathrm{Det}(\boldsymbol{J}(\boldsymbol{x}_1) - \lambda I) = \begin{vmatrix} -\sigma-\lambda & \sigma & 0 \\ r & -1-\lambda & 0 \\ 0 & 0 & -b-\lambda \end{vmatrix} = -(b+\lambda)\begin{vmatrix} -\sigma-\lambda & \sigma \\ r & -1-\lambda \end{vmatrix} =$$
  $$= -(b+\lambda)[(\sigma+\lambda)(1+\lambda) - r\sigma] = -(b+\lambda)[\lambda^2 + (\sigma+1)\lambda - \sigma(r-1)] \tag{49}$$

  And if we solve

  $$-(b+\lambda)[(\sigma+\lambda)(1+\lambda)-r\sigma] = -(b+\lambda)[\lambda^2+(\sigma+1)\lambda-\sigma(r-1)] = 0 \tag{50}$$

  we get that

  $$\lambda_1 = -b \qquad \lambda_{2,3} = -\frac{1}{2}\left[(\sigma+1) \pm \sqrt{(\sigma+1)^2 + 4\sigma(r-1)}\right] \tag{51}$$

  We see that real part of λ_1 and λ_2 are always negative, but for $r > 1$ as we expected λ_3 becomes negative.

  So for $r < 1$ fixed point $\boldsymbol{x}_1$ is stable, but for $r > 1$ is unstable.

- Stability of $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$:

  For fixed point $\boldsymbol{x}_2$ Jacobian matrix is

  $$\boldsymbol{J}(\boldsymbol{x}_2) = \begin{pmatrix} -\sigma & \sigma & 0 \\ 1 & -1 & -\sqrt{(r-1)b} \\ \sqrt{(r-1)b} & \sqrt{(r-1)b} & -b \end{pmatrix} \tag{52}$$

To calculate eigenvalues λ of Jacobian matrix we need to solve equation $\mathrm{Det}(\boldsymbol{J}(\boldsymbol{x}_1) - \lambda I) = 0$, where I 3x3 is identity matrix. If we expand Determinant we get third order equation for λ

$$\lambda^3(1 + b + \sigma)\lambda^2 + b(r + \sigma)\lambda + 2b\sigma(r - 1) = 0 \tag{53}$$

but analytical solutions of equation 53 (to get them I used MAPLE and later also Mathematica) are long and complicated expressions. But nerveless we can tray to plot them. Lets start to analyze most popular case $\Re(\lambda) = f(r)$ for $b = 8/3$, $\sigma = 10$. As you can see in Fig. 4 real part of eigenvalues is positive for $0 < r < 1$, somewhere about 13.3 and for $r > 24.73$. The better look for behavior for $13 < r < 14$ you can see in Fig- 5. But now it looks like singularity (two eigenvalues go to $+\infty$ and one to $-\infty$), what is not possible.

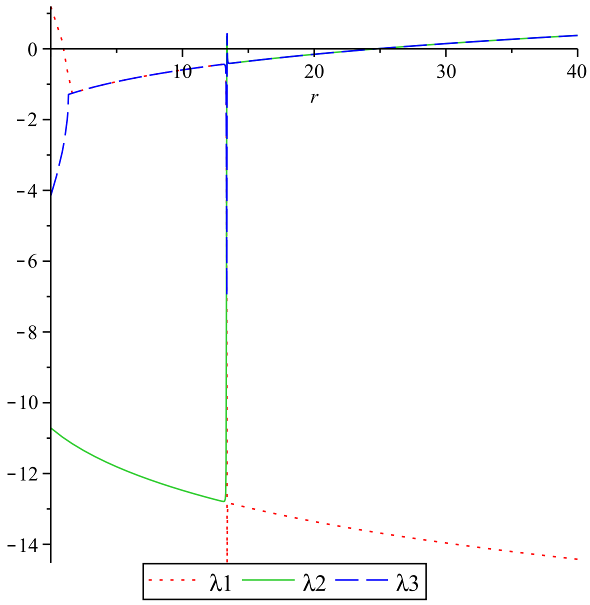

Fig. 4: $\Re(\lambda) = f(r)$ for $b = 8/3$, $\sigma = 10$, plotted with maple

And if we tray to look numerically if fixed points in this region are reallyunstable (see Fig. 6.) we see that they actually are stable. So positive real parts of eigenvectors around 13.3 must be just numerical errors from maple, and the same calculations with Mathematica (see Fig. 7) confirms this. So Mathematica for this test is better choice.

If we now change σ and b we get similar picture to 7 or 8 - there is critical value for $r > 1$ when system becomes unstable or there is no such value.

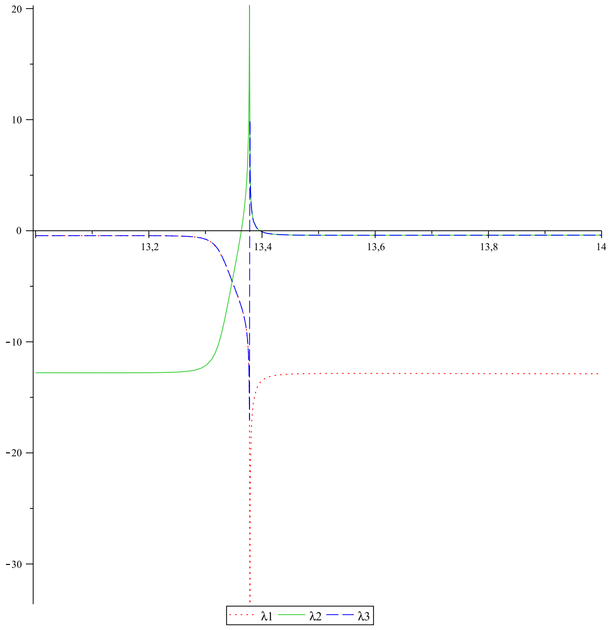

Fig. 5: $\Re(\lambda) = f(r)$ for $b = 8/3$, $\sigma = 10$, plotted with maple in smaller range

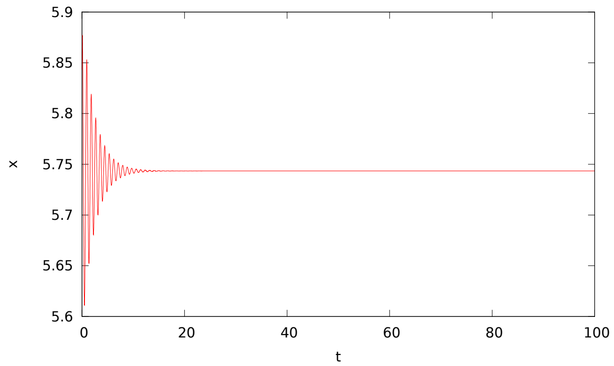

Fig. 6: Stability analysis of $\boldsymbol{x}_2$ for $b = 8/3$, $\sigma = 10$, $r = 13.78$

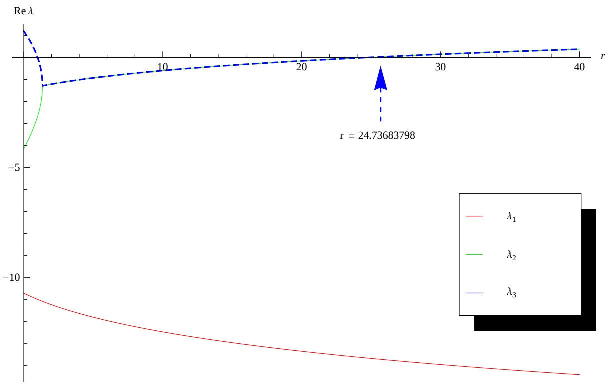

Fig. 7: $\Re(\lambda) = f(r)$ for $b = 8/3$, $\sigma = 10$, plotted with mathematica

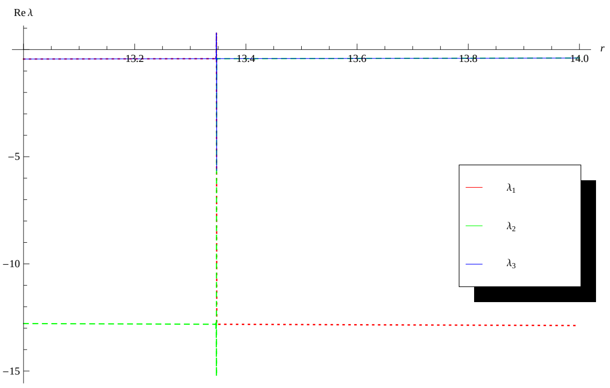

Fig. 8: $\Re(\lambda) = f(r)$ for $b = 8/3$, $\sigma = 1$, plotted with mathematica

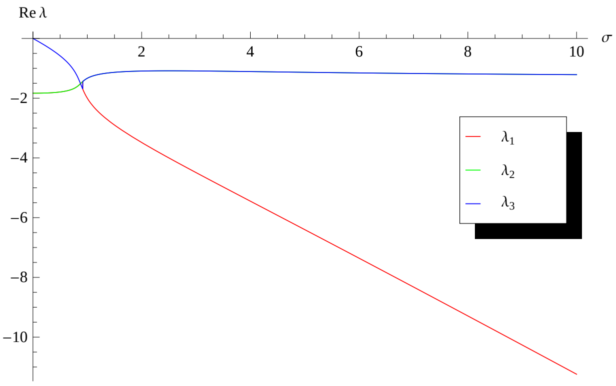

Fig. 9: $\Re(\lambda) = f(\sigma)$ for $b = 8/3$, $r = 2$, plotted with mathematica

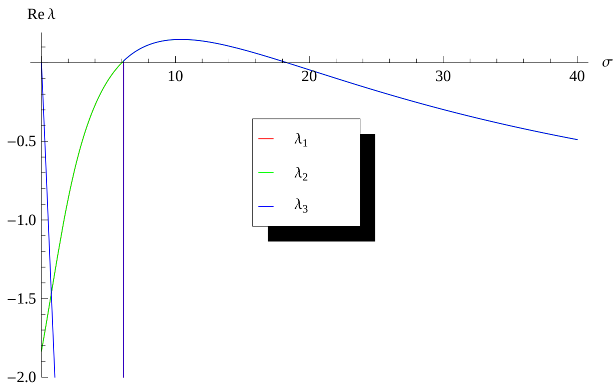

Fig. 10: $\Re(\lambda) = f(\sigma)$ for $b = 8/3$, $r = 30$, plotted with mathematica

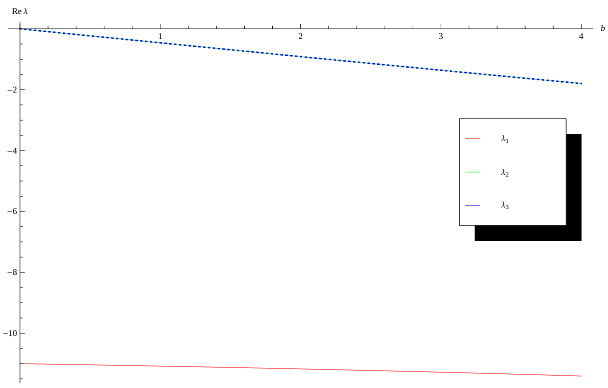

Fig. 11: $\Re(\lambda) = f(b)$ for $\sigma = 10$, $r = 2$, plotted with mathematica

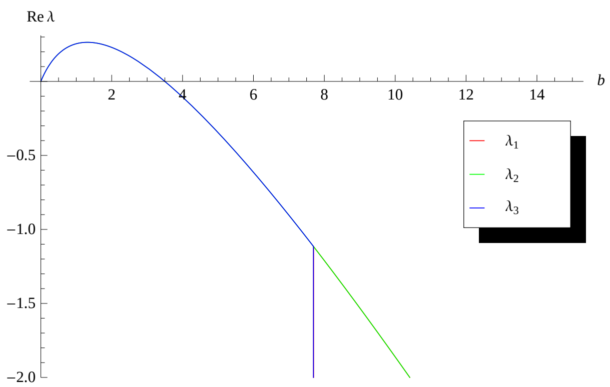

Fig. 12: $\Re(\lambda) = f(b)$ for $\sigma = 10$, $r = 30$, plotted with mathematica

If we now look at $\Re(\lambda) = f(\sigma)$ for fixed r and b. We always get similar Figs. to (9) or (10) - there is interval when system becomes unstable or there is no such interval.

If we now look at $\Re(\lambda) = f(b)$ for fixed r and σ. We always get similar Figs. to (11) or (12) - the system is stable, or there is interval $0 < b < b_{max}$ when system is unstable.

But generally it possible to find analyzing numerical solutions or analytical expressions, that if

$$r = r_H = \frac{\sigma(\sigma + b + 3)}{\sigma - b - 1} \qquad \sigma > b + 1 \tag{54}$$

we get eigenvalues are

$$\lambda_1 = -1 - b - s \qquad \lambda_2 = \imath \frac{\sqrt{2}\sqrt{bs + bs^2}}{\sqrt{s - 1 - b}} \qquad \lambda_3 = -\imath \frac{\sqrt{2}\sqrt{bs + bs^2}}{\sqrt{s - b - 1}} \tag{55}$$

and we see that $\Re(\lambda_1) < 0$ and $\Re(\lambda_{2,3}) = 0$. So this should be the critical point (in fig. 7 $r_H = 24.73683798$) when $\boldsymbol{x}_2$ becomes unstable.

So if $\sigma < b + 1$, then $\boldsymbol{x}_2$ is stable if $1 < r$ and if $\sigma > b + 1$, then $\boldsymbol{x}_2$ is stable if $1 < r < r_H$ (see equation 54).

But linear stability theory only says about long time solution if initial conditions are close to fixed points. So to fully understand we have to calculate Lyaponov exponents for all initial conditions. This is hard and can be only done numerically. So instead of that I tried to explore phase plane solution dependence on initial conditions and r for fixed b and σ. So I chose 2 sytems with $b = 8/3$, $\sigma = 10$ and $b = 8/3$, $\sigma = 1$.

- if $b = 8/3$, $\sigma = 1$

  Then independent of initial conditions if $r > 1$ the solution converges to $\boldsymbol{x}_2$ (see figures 13 and 14) or when $r < 1$ the solution converges to $\boldsymbol{x}_1$. So bifurcation diagram for this case is simple and you can see in figure 15 (as it is symmetrical for -x only positive values are showed).

- if $b = 8/3$, $\sigma = 10$

  Then we have much more interesting situation.

  - If $0 < r < 1$ then independent of initial condition system converges to $\boldsymbol{x}_1$.

- if $1 < r < 13.92$ then independent of initial condition system converges to $\boldsymbol{x}_2$ or $\boldsymbol{x}_3$
- if $13.93 < r < 24.0$ then if initial condition are close to $\boldsymbol{x}_2$ or $\boldsymbol{x}_3$ system converges to $\boldsymbol{x}_2$ or $\boldsymbol{x}_3$, but if not system start to rotate around one fixed point and then switch rotation around other fixed point. Switching happens irregularly until it comes finally enough close to one of attractors and then converges quit fast. Two trajectories from initial conditions which are close can be very different (see figures 16 and 17) but at $\lim_{t\to\infty}$ they are either $\boldsymbol{x}_2$ or $\boldsymbol{x}_3$. This is called **transient chaos**.
- if $24.1 < r < 24.73$ then if initial condition are close to $\boldsymbol{x}_2$ or $\boldsymbol{x}_3$ system converges to $\boldsymbol{x}_2$ or $\boldsymbol{x}_3$, but if not system start to rotate around one fixed point and then switch rotation around other fixed point. Switching happens irregularly and steady state is never reached (see fig. 18,19 and 20). This is called **strange attractor**.
- if $24.74 < r < 313$ Independent of initial conditions we can observe strange attractor (21 and 24). In this region limit cycles also are observed.
- $r > 313$ There is no more strange attracts only limit cycles (see fig.22, 23 and 25)

The bifurcation diagram you can see in Fig. (26).

As system is attracted to one point, phase space volume is not conserved and we have a **dissipative system**.

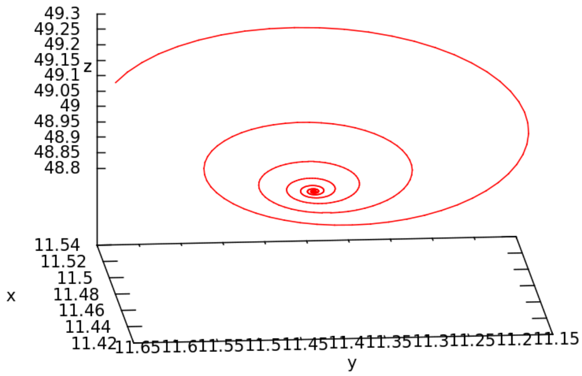

Fig. 13: Phase space trajectories for $b = 8/3$, $\sigma = 1$, $r = 50$ with initial conditions $x_0 = x_2 + 0.1$, $y_0 = y_2 + 0.1$, $z_0 = z_2 + 0.1$ and x_2, y_2, z_2 are components of $\boldsymbol{x}_2$

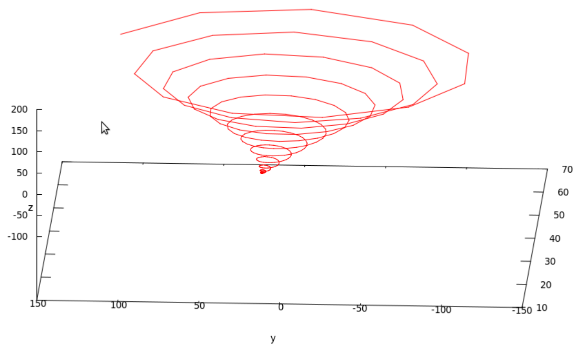

Fig. 14: Phase space trajectories for $b = 8/3$, $\sigma = 1$, $r = 50$ with initial conditions $x_0 = x_2 + 50$, $y_0 = y_2 + 50$, $z_0 = z_2 + 50$ and x_2, y_2, z_2 are components of $\boldsymbol{x}_2$

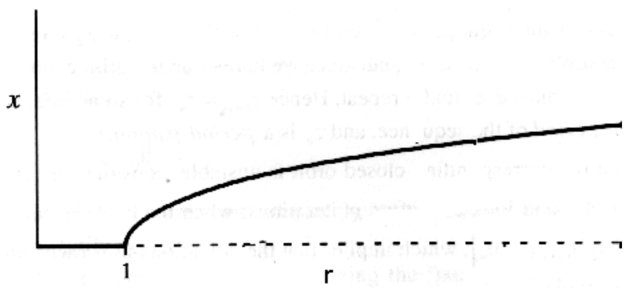

Fig. 15: Bifurcation diagram for $b = 8/3$, $\sigma = 1$

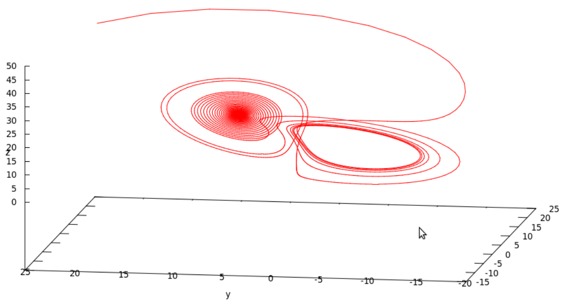

Fig. 16: Phase space trajectories for $b = 8/3$, $\sigma = 10$, $r = 20$ with initial conditions $x_0 = 24.69$, $y_0 = 24.69$, $z_0 = 38.9$

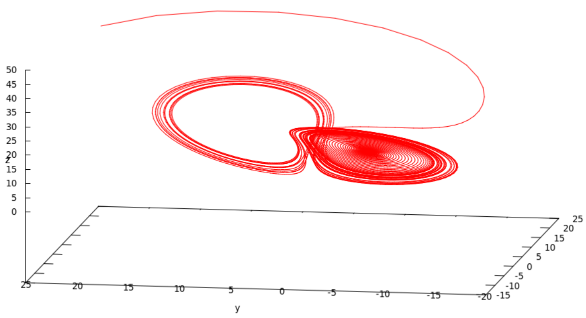

Fig. 17: Phase space trajectories for $b = 8/3$, $\sigma = 10$, $r = 20$ with initial conditions $x_0 = 24.69$, $y_0 = 24.69$, $z_0 = 39.1$

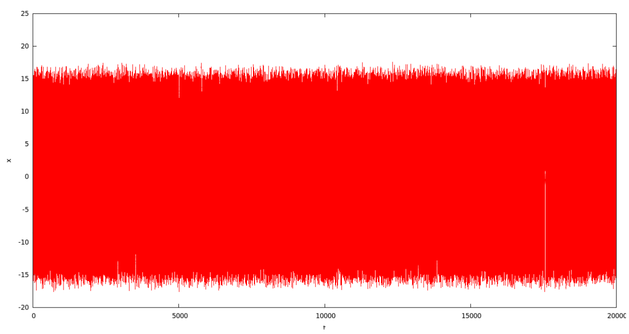

Fig. 18: x=f(t) for $b = 8/3$, $\sigma = 10$, $r = 24,5$ with initial conditions $x_0 = 24.69$, $y_0 = 24.69$, $z_0 = 39.1$

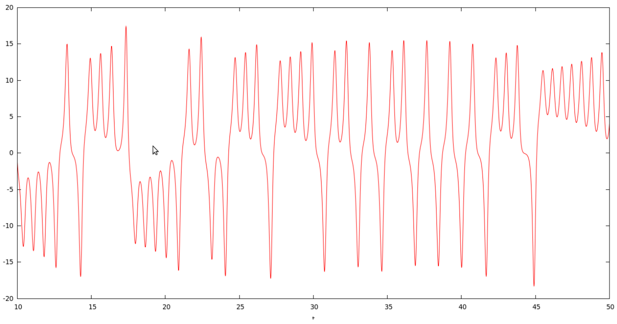

Fig. 19: x=f(t) for $b = 8/3$, $\sigma = 10$, $r = 24,5$ with initial conditions $x_0 = 24.69$, $y_0 = 24.69$, $z_0 = 39.1$ in smaller time range

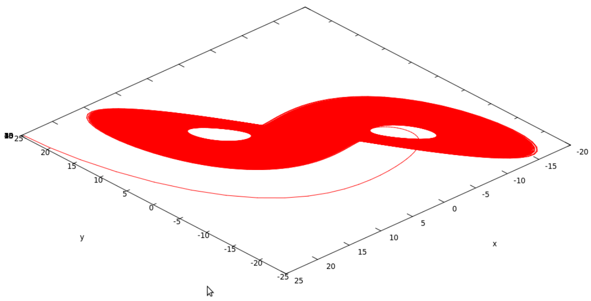

Fig. 20: Phase space trajectories for $b = 8/3$, $\sigma = 10$, $r = 24,5$ with initial conditions $x_0 = 24.69$, $y_0 = 24.69$, $z_0 = 39.1$

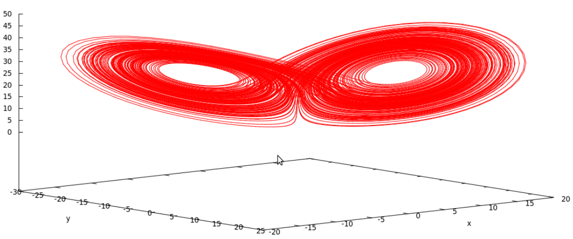

Fig. 21: Phase space trajectories for $b = 8/3$, $\sigma = 10$, $r = 28$ with initial conditions $x_0 = 1$, $y_0 = 5$, $z_0 = 10$

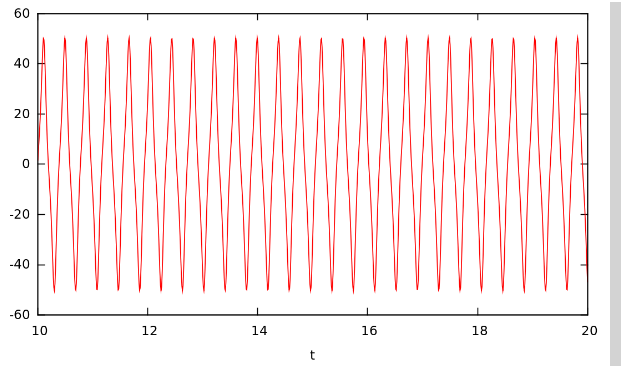

Fig. 22: x=f(t) for $b = 8/3$, $\sigma = 10$, $r = 350$ with initial conditions $x_0 = 1$, $y_0 = 5$, $z_0 = 10$

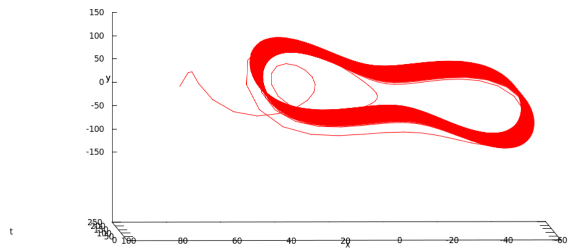

Fig. 23: Time evolution of projection of phase space trajectories to plane xy for $b = 8/3$, $\sigma = 10$, $r = 350$ with initial conditions $x_0 = 1$, $y_0 = 5$, $z_0 = 10$

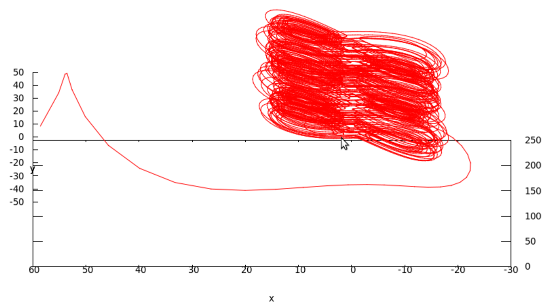

Fig. 24: Time evolution of projection of phase space trajectories to plane xy for $b = 8/3$, $\sigma = 10$, $r = 28$ with initial conditions $x_0 = 1$, $y_0 = 5$, $z_0 = 10$

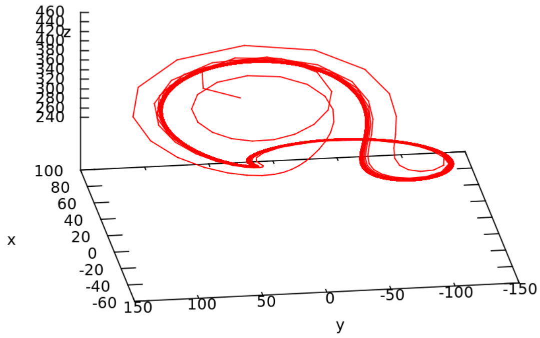

Fig. 25: Phase space trajectories for $b = 8/3$, $\sigma = 10$, $r = 350$ with initial conditions $x_0 = 1$, $y_0 = 5$, $z_0 = 10$

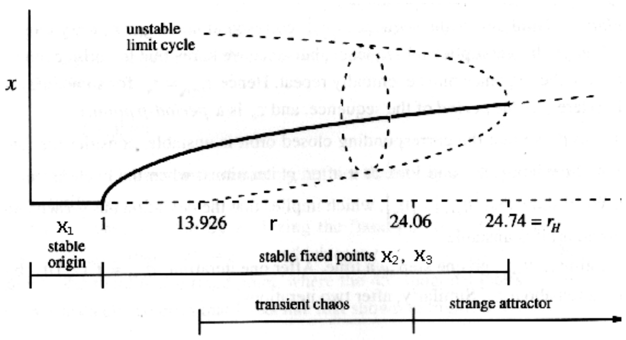

Fig. 26: Bifurcation diagram for $b = 8/3$, $\sigma = 10$

1.3 Derivation of Master Equation

As already stated the Markov process is uniquely determined through the distribution $p_1(x,t)$ at time t and the conditional probability $p_2(x',t' \mid x,t)$, also called transition probability from x at t to x' at later t', to determine the whole hierarchy p_n $(n \geq 3)$ by the Markov property (7). Also these two functions cannot be chosen arbitrarily, they have to fulfill two consistency conditions, namely the Chapman–Kolmogorov equation (9)

$$p_2(x'',t'' \mid x,t) = \int p_2(x'',t'' \mid x',t')\, p_2(x',t' \mid x,t)\, dx' \;, \tag{56}$$

the Markov relationship (6)

$$p_1(x',t') = \int p_2(x',t'|x,t)\, p_1(x,t)\, dx \;, \tag{57}$$

and the normalization condition

$$\int p_1(x',t')\, dx' = 1 \;. \tag{58}$$

The history in a Markov process, given by (7), is very short, only one time interval from t to t' plays any role. If the trajectory has reached x at time t, the past is forgotten, and it moves toward x' at t' with a probability depending on x, t and x', t' only. The entire information relevant for the future is thus contained in the present. A Markov process is a stochastic process for which the future depends on the past and the present only through the present. It has no memory. In an ordinary case where the space of states x is locally homogeneous this gives sense to transform the Chapman–Kolmogorov equation (9) in an equivalent differential equation in the short time limit $t' = t + \tau$ with small τ tending to zero. The short time behavior of the transition probability $p_2(\cdot \mid \cdot)$ should be written as series expansion with respect to time interval τ in the form

$$p_2(x,t+\tau \mid x'',t) = [1 - \bar{w}(x,t)\tau]\, \delta(x-x'') + \tau w(x,x'',t) + \mathcal{O}(\tau^2) \;. \tag{59}$$

The new quantity $w(x,x'',t) \geq 0$ is the transition rate, the probability per time unit, for a jump from x'' to $x \neq x''$ at time t. This transition rate w multiplied by the time step τ gives the second term in the series expansion describing transitions from another state x'' to x. The first term (with the delta function) is the probability that no transitions takes place during time interval τ. Based on the normalization condition

$$\int p_2(x,t+\tau \mid x'',t)\, dx = 1 \tag{60}$$

it follows that

$$\bar{w}(x,t) = \int w(x'',x,t)\,dx'' \ . \tag{61}$$

The ansatz (59) implies that a realization of the random variable after any time interval τ retains the same value with a certain probability or attains a different value with the complementary probability. A typical trajectory $x(t)$ consists of straight lines $x(t) = \text{const}$ interrupted by jumps. 1994).

From Chapman–Kolmogorov equation (9) together with (59) we get

$$\begin{aligned} p_2(x,t+\tau \mid x',t') &= \int p_2(x,t+\tau \mid x'',t) p_2(x'',t \mid x',t')\,dx'' \\ &= \int \left[1 - \bar{w}(x,t)\tau\right] \delta(x-x'') p_2(x'',t \mid x',t')\,dx'' \\ &\quad + \int \tau w(x,x'',t) p_2(x'',t \mid x',t')\,dx'' + \mathcal{O}(\tau^2) \ . \end{aligned} \tag{62}$$

With (61) and after taking the short time limit $\tau \to 0$ one obtains the following differential equation

$$\begin{aligned} \frac{\partial}{\partial t} p_2(x,t \mid x',t') &= \int w(x,x'',t) p_2(x'',t \mid x',t')\,dx'' \\ &\quad - \int w(x'',x,t) p_2(x,t \mid x',t')\,dx'' \ . \end{aligned} \tag{63}$$

In order to rewrite the derived equation in a form well known in physical concepts we get after multiplication by $p_1(x',t')$ and integration over x' the differential formulation of the Chapman–Kolmogorov equation

$$\frac{\partial}{\partial t} p_1(x,t) = \int w(x,x',t) p_1(x',t)\,dx' - \int w(x',x,t) p_1(x,t)\,dx' \tag{64}$$

called *master equation* in the (physical) literature.

The name 'master equation' for the above probability balance equation is used in a sense that this differential expression is a general, fundamental or basic equation. For a homogeneous in time process the transition rates $w(x,x',t)$ are independent of time t and therefore $w(x,x',t) = w(x,x')$. The short time transition rates w have to be known from the physical context, often like an intuitive ansatz, or have to be formulated based on a reasonable hypothesis or approximation. With known transition rates w and given initial distribution $p_1(x,t=0)$ the master equation (64) gives the resulting evolution of the probability p_1 over an infinitely long time period.

1.4 Master Equation and its Solution

The basic equation of stochastic Markov processes called *master equation* is usually written as gain–loss equation (64) for the probabilities $p(x,t)$ in the form

$$\frac{\partial p(x,t)}{\partial t} = \int \left\{ w(x,x')p(x',t) - w(x',x)p(x,t) \right\} dx' \ . \tag{65}$$

This very general equation can be interpreted as local balance for the probability densities which have to fulfill the global normalization condition

$$\int p(x,t)\, dx = 1 \tag{66}$$

at each time moment t, also at the beginning for the initial distribution $p(x,t=0)$. The linear master equation (65) with known transition rates per unit time $w(x,x')$ is a so–called Markov evolution equation showing the relaxation from a chosen starting distribution $p(x,t=0)$ to some final probability distribution $p(x,t\to\infty)$. The linearity of the master equation is based on the assumption that the underlying dynamics is Markovian. The transition probabilities w do not depend on the history of reaching a state, so that the transition rates per unit time are indeed constants for a given temperature or total energy.

If the state space of the stochastic variable is a discrete one, often considering natural numbers within a finite range $0 \le n \le N$, the master equation for the time evolution of the probabilities $p(n,t)$ is written as

$$\frac{dp(n,t)}{dt} = \sum_{n' \neq n} \left\{ w(n,n')p(n',t) - w(n',n)p(n,t) \right\} \ , \tag{67}$$

where $w(n',n) \ge 0$ are rate constants for transitions from n to other $n' \neq n$. Together with the initial probabilities $p(n,t=0)$ $(n = 0,1,2,\ldots,N)$ and the boundary conditions at $n=0$ and $n=N$ this set of equations governing the time evolution of $p(n,t)$ from the beginning at $t=0$ to the long–time limit $t\to\infty$ has to be solved. The meaning of both terms is clear. The first (positive) term is the inflow current to state n due to transitions from other states n', and the second (negative) term is the outflow current due to opposite transitions from n to n'.

Now let us define *stationarity*, sometimes called *steady state*, as a time independent distribution $p^{st}(n)$ by the condition $dp(n,t)/dt|_{p=p^{st}} = 0$. Therefore the stationary master equation is given by

$$0 = \sum_{n' \neq n} \left\{ w(n,n')p^{st}(n') - w(n',n)p^{st}(n) \right\} \ . \tag{68}$$

This equation states the obvious fact, that in the stationary or steady state regime the sum of all transitions into any state n must be balanced by the sum of all transitions from n into other states n'. Based on the properties of the transition rates per unit time the probabilities $p(n,t)$ tend in the long–time limit to the uniquely defined stationary distribution $p^{st}(n)$, for which in open systems a constant probability flow is possible. This fundamental property of the master equation may be stated as

$$\lim_{t \to \infty} p(n,t) = p^{st}(n) \ . \tag{69}$$

Now we are discussing the question of in a system without external exchange. The condition of equilibrium in closed isolated systems is much stronger than the former condition of stationarity (68). Here we demand as an additional constraint a balance between each pair of states n and n' separately. This so–called *detailed balance* relation is written for the equilibrium distribution $p^{eq}(n)$ as

$$0 = w(n,n')p^{eq}(n') - w(n',n)p^{eq}(n) \ . \tag{70}$$

It always holds for one–step processes in one–dimensional systems with closed boundaries further considered in our paper. Of course, each equilibrium state is by definition also stationary. If the initial probability vector $p(n,t=0)$ is strongly nonequilibrium, many probabilities $p(n,t)$ change rapidly as soon as the evolution starts (short–time regime), and then relax more slowly towards equilibrium (long–time behavior). The final state called thermodynamic equilibrium is reached in the limit $t \to \infty$.

Using linear algebra we want to solve the master equation analytically by an expansion in eigenfunctions. This method gives us a general solution of the time dependent probability vector $p(n,t)$ expressed by eigenvectors and eigenvalues. In a first step we introduce the master equation, written as a set of coupled linear differential equations (67), in a compact matrix form

$$\frac{d\,\mathbf{P}(t)}{dt} = \mathbf{W}\,\mathbf{P}(t) \ , \tag{71}$$

with a probability vector $\mathbf{P}(t) = \{p(n,t) \mid n = 0, \ldots, N\}$ and an undecomposable asymmetric transition matrix $\mathbf{W} = \{W(n,n') \mid n,n' = 0, \ldots, N\}$.

The elements of the matrix are given by

$$W(n,n') = w(n,n') - \delta_{n,n'} \sum_{m\neq n} w(m,n) \tag{72}$$

and obey the following two properties

$$W(n,n') \geq 0 \quad \text{for } n \neq n' \ , \tag{73}$$

$$\sum_n W(n,n') = 0 \quad \text{for each } n' \ . \tag{74}$$

Known from matrix theorythere are a number of consequences based on both properties. Especially the transition matrix $\mathbf{W}$ has a single zero eigenvalue whose eigenvector is the equilibrium probability distribution. In general, other eigenvalues can be complex and they always have negative real part. In our special case where the detailed balance (70) holds all eigenvalues are real, as discussed further on.

The solution $\mathbf{P}(t)$ of the master equation (71) with given initial vector $\mathbf{P}(0)$ may be written formally as

$$\mathbf{P}(t) = \mathbf{P}(0)\ \exp(\mathbf{W}\, t)\ , \tag{75}$$

(where $\exp(\mathbf{W}\, t) = \sum_{m=0}^{\infty} (\mathbf{W}\, t)^m / m!$) but this does not help us to find $\mathbf{P}(t)$ explicitly.

The familiar method is to make $\mathbf{W}$ symmetric and thereby diagonalizable and then to construct the solution as superposition of eigenvectors $\mathbf{u}_\lambda$ related to (zero or negative) eigenvalues λ in the form

$$\mathbf{P}(t) = \sum_\lambda c_\lambda \mathbf{u}_\lambda\ \mathrm{e}^{\lambda\, t}\ . \tag{76}$$

with up to now unknown coefficients c_λ. Using the condition of detailed balance (70) we transform the matrix $\mathbf{W} = \{W(n,n')\}$ to a new symmetric transition matrix $\widetilde{\mathbf{W}} = \{\widetilde{W}(n,n')\}$ with elements given by

$$\widetilde{W}(n,n') \stackrel{\text{def}}{=} W(n,n') \sqrt{\frac{p^{eq}(n')}{p^{eq}(n)}} = \widetilde{W}(n',n)\ . \tag{77}$$

Both matrices $\mathbf{W}$ and $\widetilde{\mathbf{W}}$ have the same eigenvalues λ_i. Due to the symmetry of matrix $\widetilde{\mathbf{W}}$, all eigenvalues are real. They may be labeled in order of decreasing algebraic values, so that $\lambda_0 = 0$ and $\lambda_i < 0$ for $1 \leq i \leq N$.

Denoting the normalized eigenvectors by $\mathbf{u}_i$ and $\widetilde{\mathbf{u}}_i$ respectively, defined by the eigenvalue equations

$$\sum_{n'} W(n,n')\, u_i(n') = \lambda_i\, u_i(n) \qquad ; \qquad \mathbf{W}\,\mathbf{u}_i = \lambda_i\,\mathbf{u}_i \tag{78}$$

$$\sum_{n'} \widetilde{W}(n,n')\, \widetilde{u}_i(n') = \lambda_i\, \widetilde{u}_i(n) \qquad ; \qquad \widetilde{\mathbf{W}}\,\widetilde{\mathbf{u}}_i = \lambda_i\,\widetilde{\mathbf{u}}_i \tag{79}$$

and related by the transformation $u_i(n) = \sqrt{p^{eq}(n)}\;\widetilde{u}_i(n)$ to each other, we are ready to construct the time dependent solution of the fundamental master equation (71). According to superposition formula (76), where coefficients c_λ are calculated from the initial condition $p(n,0)$ at $t=0$, the solution is then

$$p(n,t) = \sqrt{p^{eq}(n)}\,\sum_{i=0}^{N} \widetilde{u}_i(n)\;\mathrm{e}^{\lambda_i t}\left[\sum_{m=0}^{N} \widetilde{u}_i(m)\frac{p(m,0)}{\sqrt{p^{eq}(m)}}\right] \;, \tag{80}$$

or

$$p(n,t) = \sum_{i=0}^{N} u_i(n)\;\mathrm{e}^{\lambda_i t}\left[\sum_{m=0}^{N} u_i(m)\frac{p(m,0)}{p^{eq}(m)}\right] \;. \tag{81}$$

This solution plays a very important role in the stochastic description of Markov processes and can be found in different notations (e. g. as integral representation) in many textbooks.

As time increases to infinity ($t \to \infty$) only the term $i=0$ in the solution survives and the probabilities tend to equilibrium $\mathbf{P}(t) \to \mathbf{P}^{eq}$, written as

$$p(n,t) = p^{eq}(n) + \sum_{i=1}^{N} u_i(n)\;\mathrm{e}^{\lambda_i t}\left[\sum_{m=0}^{N} u_i(m)\frac{p(m,0)}{p^{eq}(m)}\right] \;. \tag{82}$$

In the long–time limit all remaining modes $c_\lambda \mathbf{u}_\lambda\, \mathrm{e}^{\lambda\, t}$ decay exponentially. In the short–time regime due to combinations of modes with different signs there is the possibility of growing and subsequent shrinking of transient states as probability current from initial distribution $\mathbf{P}(0)$ to equilibrium $\mathbf{P}^{eq}$ via intermediates $\mathbf{P}(t)$.

Master equation dynamics can be studied either by solving the basic equation analytically with implementation of numerical methods or by simulating the stochastic process as a large number of subsequent jumps from state to state with the given transition rates. Both methods have different advantages and disadvantages. One important point is the choice of the appropriate time interval called numerical integration step or waiting time in simulation technique. The step size required for a given accuracy is usually smaller when time t is closer to zero, and can be enlarged as t grows. Therefore only a numerical algorithm with an adaptive step size should be used.

1.5 One-step Master Equation for Finite Systems

We are speaking about a one–dimensional stochastic process if the state space is characterized by one variable only. Often this discrete variable is a particle number $n \geq 0$ describing the amount of molecules in a box or the size of an aggregate. In chemical physics such aggregation phenomena like formation and/or decay of clusters are of great interest. To determine the relaxation dynamics of clusters of size n we take a particularly simple Markov process with transitions between neighboring states n and $n' = n \pm 1$. This situation is called a *one–step process*. In biophysics, if the variable n represents the number of living individuals of a particular species, the one–step process is often called *birth–and–death process* to investigate problems in population dynamics. The detailed balance relation (70) can be proven for the one–step process, so that in our case the aforesaid (see Section 1.4) is completely correct.

Setting the transition rates $w(n, n-1) = w_+(n-1)$, $w(n, n+1) = w_-(n+1)$, and therefore also $w(n+1, n) = w_+(n)$, $w(n-1, n) = w_-(n)$, now the forward master equation (67) reads

$$\begin{aligned} \frac{dp(n,t)}{dt} &= w_+(n-1)\, p(n-1,t) + w_-(n+1)\, p(n+1,t) \\ &\quad - \left[w_+(n) + w_-(n)\right]\, p(n,t) \; . \end{aligned} \tag{83}$$

In general the forward and backward transition rates $w_+(n), w_-(n)$ are nonlinear functions of the random variable n; the physical dimension of $w_\pm$ is one over time (s^{-1}). The master equation is always linear in the unknown probabilities $p(n,t)$ to be at state n at time t. It has to be completed by the boundary conditions. The nonlinearity refers only to the transition coefficients. Further on we will pay attention to particles as aggregates in a closed box or vehicular jams on a circular road. Therefore in finite systems the range of the discrete variable n is bounded between 0 and N $(n = 0, 1, 2, \ldots, N)$.

The general one–step master equation (83) is valid for $n = 1, 2, \ldots, N-1$, but meaningless at the boundaries $n = 0$ and $n = N$. Therefore we have to add two boundary equations as closure conditions

$$\frac{dp(0,t)}{dt} = w_-(1)\,p(1,t) - w_+(0)\,p(0,t)\ , \tag{84}$$

$$\frac{dp(N,t)}{dt} = w_+(N-1)\,p(N-1,t) - w_-(N)\,p(N,t)\ . \tag{85}$$

To solve the set of equations we rewrite (83) as balance equation

$$\frac{dp(n,t)}{dt} = J(n+1,t) - J(n,t) \tag{86}$$

with probability current defined by

$$J(n,t) = w_-(n)\,p(n,t) - w_+(n-1)\,p(n-1,t)\ . \tag{87}$$

In the stationary regime, remember (68), all flows (87) have to be independent of n and therefore equal to a constant current of probability: $J(n+1) = J(n) = J$. In open systems the stationary solution is no longer unique, it depends on the current J.

In finite systems with $n = 0, 1, 2, \dots, N$ one finds a situation with zero flux $J = 0$, which corresponds to steady state with a detailed balance relationship similar to (70). Therefore the stationary distribution $p^{st}(n)$ fulfills the recurrence relation

$$p^{st}(n) = \frac{w_+(n-1)}{w_-(n)} p^{st}(n-1)\ . \tag{88}$$

By applying the iteration successively we get the relation

$$p^{st}(n) = p^{st}(0) \prod_{m=1}^{n} \frac{w_+(m-1)}{w_-(m)}\ , \tag{89}$$

which determines all probabilities $p^{st}(n)$ $(n = 1, 2, \dots, N)$ in terms of the first unknown one $p^{st}(0)$. Taking into account the normalization condition

$$\sum_{n=0}^{N} p^{st}(n) = 1 \qquad \text{or} \qquad p^{st}(0) + \sum_{n=1}^{N} p^{st}(n) = 1 \tag{90}$$

the stationary probability distribution $p^{st}(n)$ in finite systems is finally written as

$$p^{st}(n) = \begin{cases} \dfrac{\displaystyle\prod_{m=1}^{n} \frac{w_+(m-1)}{w_-(m)}}{\displaystyle 1 + \sum_{k=1}^{N} \prod_{m=1}^{k} \frac{w_+(m-1)}{w_-(m)}} & n = 1, 2, \ldots, N \\ \\ \dfrac{1}{\displaystyle 1 + \sum_{k=1}^{N} \prod_{m=1}^{k} \frac{w_+(m-1)}{w_-(m)}} & n = 0\ . \end{cases} \tag{91}$$

It is often convenient to write the stationary solution (89) in the exponential form

$$p^{st}(n) = p^{st}(0) \exp\left\{-\Phi(n)\right\}\ , \tag{92}$$

where, in analogy to physical systems, the function

$$\Phi(n) = \sum_{m=1}^{n} \ln\left(\frac{w_-(m)}{w_+(m-1)}\right) \tag{93}$$

is called the potential.

The obtained result (91) based on the zero–flux relationship (88) is a unique solution for the stationary probability distribution in finite systems with closed boundaries. For an isolated system the stationary solution of the master equation p^{st} is identical with the thermodynamic equilibrium p^{eq}, where the detailed balance holds, which for one–step processes reads

$$w_-(n)\, p^{eq}(n) = w_+(n-1)\, p^{eq}(n-1)\ . \tag{94}$$

The condition of detailed balance states a physical principle. If the distribution p^{eq} is known from equilibrium statistical mechanics and if one of the transition rates is also known (e. g. w_+ by a reasonable ansatz), the equation (94) provides the opportunity to formulate the opposite transition rate w_- in a consistent way. By this procedure the nonequilibrium behavior is adequately described by a sequence of (quasi–)equilibrium states. The relaxation from any initial nonequilibrium distribution tends always to the known final equilibrium. In physical systems the equilibrium distribution usually is represented in an exponential form

$$P^{eq}(n) \propto \exp\left[-\Omega(n)/(k_B T)\right] \tag{95}$$

where $\Omega(n)$ is the thermodynamic potential depending on the stochastic variable n, k_B is the Boltzmann constant, and T is the temperature. Eq. (95) is comparable with (92) where $\Phi(n) = \Omega(n)/(k_B T)$.

1.6 Stochastic Decay in Finite Systems

Up to now we have considered Markov processes in a more general framework without defining the states of the system as well as the rates for the transitions between these states precisely. The particular case, where the states are characterized by a single particle number n and the rates by a one–step backward transition $w_-(n)$ only, is called *decay process.*

In a first step we present an example of traffic flow considered as Markov process. We want to investigate the dissolution of a queue of cars standing in front of traffic lights. When the lights switch to green, the first car starts to move. After a certain time interval (waiting time $\tau = \text{const} > 0$) the next vehicle accelerates to pass the stop line and so on. In our model we consider the decay of traffic congestion without taking into account any influence of external factors like ramps or intersections on driver's behavior. The stochastic variable $n(t)$ is the number of cars which are bounded in the jam at time t. A queue or platoon of n vehicles is also called car cluster of size n.

When the initial jam size is finite, given by the value $n(t = 0) = n_0$ the trajectory $n(t) = n_0, n_0 - 1, \ldots, 2, 1, 0$ consists of unit jumps at random times. The jam starting with size n_0 becomes smaller and smaller and dissolves completely. This one–step stochastic process is a death process only, sometimes called *Poisson process.*

Defining $p(n,t)$ as the probability to find a jam of size n at time t, the master equation for the dissolution process reads

$$\frac{\partial}{\partial t} p(n,t) = w_-(n+1)p(n+1,t) - w_-(n)p(n,t) \tag{96}$$

with the decay rate per unit time assumed as

$$w(n',n) = w(n-1,n) \equiv w_-(n) = \frac{1}{\tau} \; . \tag{97}$$

In this approximation the experimentally known waiting time constant τ is a given control parameter in our escape model. It is a reaction time of a driver, about 1.5 or 2 seconds, to escape from the jam when the road in front of his car becomes free. Therefore the transition rate (97) is a constant $w_- = 1/\tau$ independent of jam size n.

For the described process of jam shrinkage ($n_0 \geq n \geq 0$), starting with cluster size $n = n_0$ and ending with $n = 0$, we thus obtain the following master equation including boundary conditions (compare (83) – (85))

$$\frac{\partial}{\partial t} p(n_0, t) = -\frac{1}{\tau}\, p(n_0, t) \;, \tag{98}$$

$$\frac{\partial}{\partial t} p(n, t) = \frac{1}{\tau}\, [p(n+1, t) - p(n, t)] \;, \qquad n_0 - 1 \geq n > 0 \;, \tag{99}$$

$$\frac{\partial}{\partial t} p(0, t) = \frac{1}{\tau}\, p(1, t) \tag{100}$$

and initial probability distribution $p(n, t = 0) = \delta_{n,n_0}$. The delta–function means that at the beginning the vehicular queue consists of exactly n_0 cars.

In order to find the explicit expression of the probability distribution $p(n, t)$ we have to solve the set of equations (98) – (100). This can be done analytically starting with the first equation, getting $p(n_0, t) = \exp(-t/\tau)$ as exponential decay function, inserting the solution into the next equation for $p(n_0 - 1, t)$, solving it and continue iteratively up to $p(0, t)$. The general solution of the probability $p(n, t)$ to observe a car cluster of size n at time t is

$$p(n, t) = \frac{(t/\tau)^{n_0 - n}}{(n_0 - n)!}\, e^{-t/\tau} \;, \qquad 0 < n \leq n_0 \;, \tag{101}$$

$$p(0, t) = 1 - \sum_{m=0}^{n_0 - 1} \frac{(t/\tau)^m}{m!}\, e^{-t/\tau} \;. \tag{102}$$

As already mentioned (90), the probabilities are always normalized to unity, which can be proven by summation $\sum_{n=0}^{n_0} p(n, t)$ inserting (101, 102) to get one. The time evolution of the probability $p(n, t)$ has been calculated from Eqs. (101) and (102) for an initial queue length $n_0 = 50$.

The average or expectation value $\langle n \rangle$ of the cluster size n is usually given by

$$\langle n \rangle(t) \equiv \sum_{n=0}^{n_0} n\, p(n, t) = \sum_{n=1}^{n_0} n\, p(n, t) \tag{103}$$

and can be calculated using the known probabilities (101) to get the exact result

$$\langle n \rangle(t) = n_0\, Q(n_0 - 1, t) - \frac{t}{\tau}\, Q(n_0 - 2, t) \tag{104}$$

where $Q(n, t)$ is an abbreviation called Poisson term

$$Q(n, t) \stackrel{\text{def}}{=} e^{-t/\tau} \sum_{m=0}^{n} \frac{(t/\tau)^m}{m!} \;. \tag{105}$$

The variance or second central moment $\langle\langle n\rangle\rangle(t)$ which measures the fluctuations is given by

$$\langle\langle n\rangle\rangle = \langle(n - \langle n\rangle)^2\rangle = \langle n^2\rangle - \langle n\rangle^2 \tag{106}$$

and can be also calculated as follows

$$\begin{aligned}\langle\langle n\rangle\rangle(t) = n_0 &\left[n_0\, Q(n_0-1,t) - \frac{2t}{\tau}\, Q(n_0-2,t)\right](1 - Q(n_0-1,t)) \\ &+ \left(\frac{t}{\tau}\right)^2 \left[Q(n_0-3,t) - Q^2(n_0-2,t)\right] + \frac{t}{\tau}\, Q(n_0-2,t)\ .\end{aligned} \tag{107}$$

In some approximation, where we set $Q(n,t)$ (105) to one, the mean value (104) reduces to a linearly decreasing function in time

$$\langle n\rangle(t) \approx n_0 - t/\tau\ , \tag{108}$$

whereas the variance (107) to a linearly increasing behavior

$$\langle\langle n\rangle\rangle(t) \approx t/\tau\ . \tag{109}$$

In the case of linear mean value approximation (108) the time required, that the jam dissolves totally, is given by

$$t_{\text{end}} = n_0\tau\ . \tag{110}$$

Equations (108) and (109), however, do not describe the final stage of dissolution of any finite car cluster. In this case, taking the limit $t \to \infty$ in the time dependent results (101) and (102), we have

$$\lim_{t\to\infty} p(n,t) = \delta_{n,0}\ . \tag{111}$$

If we do not consider the final stage of dissolution of a large cluster, i. e., if t is remarkably smaller than t_{end} (110), then the probability $p(0,t)$ that the cluster is completely dissolved is very small. This allows us to obtain correct results for $n > 0$ by the following alternative method.

Let us define the generating function $G(z,t)$ by

$$G(z,t) \stackrel{\text{def}}{=} \sum_n z^n p(n,t)\ . \tag{112}$$

According to the actually considered situation, the particular term $p(0,t)$ in this sum is negligible, so that the lower limit of summation may be taken from

$n = 1$ instead of $n = 0$. The initial condition corresponding to $p(n,0) = \delta_{n,n_0}$ is represented by

$$G(z,0) = z^{n_0} \; . \tag{113}$$

The equation for the generating function is obtained if both sides of the master equation (99) are multiplied by z^n performing the summation over n afterwards. This yields

$$\frac{\partial}{\partial t} G(z,t) = \frac{1}{\tau}\left(\frac{1}{z} - 1\right) G(z,t) \; . \tag{114}$$

The solution of partial differential equation (114) with respect to the initial condition (113) is given by

$$G(z,t) = z^{n_0} \; \exp\left[\frac{t}{\tau}\left(\frac{1}{z} - 1\right)\right] \; . \tag{115}$$

The previous result for $p(n,t)$ at $n \geq 1$ (101) is obtained from this equation after substitution by (112) and expansion of the exponent in z. Starting from (115)

$$G(z,t) = z^{n_0} \, e^{-t/\tau} \; \exp\left(\frac{t}{\tau}\frac{1}{z}\right) \tag{116}$$

the power series is written as follows

$$G(z,t) = \sum_n z^n p(n,t) = z^{n_0} \, e^{-t/\tau} \sum_m \frac{1}{m!}\left(\frac{t}{\tau \, z}\right)^m \tag{117}$$

$$= e^{-t/\tau} \sum_m \frac{1}{m!}\left(\frac{t}{\tau}\right)^m \; z^{n_0 - m} \tag{118}$$

$$= e^{-t/\tau} \sum_n \frac{1}{(n_0 - n)!}\left(\frac{t}{\tau}\right)^{n_0 - n} \; z^n \tag{119}$$

and therefore we get by comparison of same order terms the Poisson distribution (101)

$$p(n,t) = \frac{(t/\tau)^{n_0 - n}}{(n_0 - n)!} \, e^{-t/\tau} \; . \tag{120}$$

The above discussed simple model can be improved to describe the dissolution of a vehicle queue at a signalized road intersection taking into account the car dynamics of the starting behavior when red traffic light is switched to green. The quantity we are interested in is a modified detachment probability (97) which now depends on the cluster size n. For a long queue the detachment rate $w_-(n)$ has constant value $1/\tau$ consistent with (97). However, due to the time spent for acceleration of the first cars and movement toward the stop line, the detachment rate is changed for smaller queues.

1.7 Traffic Jam Formation on a Circular Road

In the following we consider the attachment of a vehicle to the car cluster and the detachment from it as elementary stochastic events. The traffic thus is treated as a one–step Markov process described by the general master equation (83)

$$\frac{\partial}{\partial t} p(n,t) = w_+(n-1)\, p(n-1,t) + w_-(n+1)\, p(n+1,t) \\ - [w_+(n) + w_-(n)]\, p(n,t) \; . \qquad (121)$$

Now the basic problem is to find an appropriate ansatz for both transition probabilities $w_+(n)$ and $w_-(n)$. Note that physical boundary conditions ($0 \leq n \leq N$) for master equation (121) are ensured by formally setting $P(-1,t) = P(N+1,t) = 0$ and $w_+(N) = w_-(0) = 0$. The latter two transitions are impossible physically and they are not included in our further analysis. As before (97), we assume a constant value for the escape rate $w_-(n)$, i. e.,

$$w_-(n) = w_- = \frac{1}{\tau} \; . \qquad (122)$$

The probability per time unit $w_+(n)$ that a vehicle is added to a car cluster of size n is estimated based on the following physical model. The total number of cars is N. They are moving along a circular one–lane road of length L. If a road is crowded by cars, each car requires some minimal space or length which, obviously, is larger than the real length of a car. We call this the effective length ℓ of a car. The distance between the front bumpers of two neighboring cars, in general, is $\ell + \Delta x$. The distance Δx can be understood as the headway between two "effective" cars which, according to our definition, is always smaller than the real bumper–to–bumper distance. The maximal velocity of each car is $v_{\max}$. The desired (optimal) velocity v_{opt}, depending on the distance between two cars Δx, is given by the formula

$$v_{\text{opt}}(\Delta x) = v_{\max} \frac{(\Delta x)^2}{D^2 + (\Delta x)^2} \; , \qquad (123)$$

where the parameter D, called the interaction distance, corresponds to the velocity value $v_{\max}/2$. According to the ansatz (123) the optimal velocity is represented by a sigmoidal function with values ranging from 0, corresponding to zero distance between cars, to $v_{\max}$, corresponding to an infinitely large distance or absence of interaction between cars. Our assumption is that a vehicle changes its velocity from $v_{\text{opt}}(\Delta x_{\text{free}})$ in free flow to $v_{\text{opt}}(\Delta x_{\text{clust}})$ in jam and approaches the cluster as soon as the distance to the next car (the last car in the cluster) reduces from $\Delta x_{\rm free}$ to $\Delta x_{\rm clust}$. This assumption allows one to calculate the average number of cars joining the cluster per time unit or the attachment frequency $w_+(n)$ to an existing car cluster. Thus, we have the ansatz valid for $1 \leq n < N$

$$w_+(n) = \frac{v_{\rm opt}(\Delta x_{\rm free}(n)) - v_{\rm opt}(\Delta x_{\rm clust})}{\Delta x_{\rm free}(n) - \Delta x_{\rm clust}} \; . \tag{124}$$

This equation (124) requires the knowledge of $\Delta x_{\rm free}$ and $\Delta x_{\rm clust}$ as a function of the cluster size n. Measurements on highways have shown that the density of cars in congested traffic is independent of the size of the dense congested phase (jam). As a consequence, the distance between jammed cars, the spacing $\Delta x_{\rm clust}$, has a constant value which has to be treated as a given measured quantity or known control parameter. We have defined the length of the car cluster or jam size depending on the number of congested cars n by

$$L_{\rm clust} = \ell\, n + \Delta x_{\rm clust}\, S(n) \; , \tag{125}$$

where

$$S(n) = \begin{cases} 0 & : \quad n = 0 \\ n - 1 & : \quad n \geq 1 \end{cases} \tag{126}$$

is the number of spacings of size $\Delta x_{\rm clust}$. In such a way, we have for the total length of road

$$L = \underbrace{\ell\, n + \Delta x_{\rm clust}\, S(n)}_{L_{\rm clust}} \; + \; \underbrace{\ell(N-n) + \Delta x_{\rm free}(N - S(n))}_{L_{\rm free}} \; , \tag{127}$$

where

$$L_{\rm free} = L - L_{\rm clust} = L - \{\ell\, n + \Delta x_{\rm clust}\, S(n)\} \tag{128}$$

denotes the length of the non–congested or free road. For $L_{\rm free}$ we can write according to (127) also

$$L_{\rm free} = \ell(N-n) + \Delta x_{\rm free}(N - S(n)) \; . \tag{129}$$

Comparing these two equations we obtain for the distance in free flow depending on cluster size

$$\Delta x_{\rm free}(n) = \frac{L - \ell\, N - \Delta x_{\rm clust}\, S(n)}{N - S(n)} \; . \tag{130}$$

By this all the transition probabilities (124) are defined except the transition from the state without any cluster $n = 0$ to the smallest cluster size

$n = 1$. This transition and the meaning of the state with a single congested car ($n = 1$) called *precluster* requires some explanation. Some stochastic event or perturbation of the free traffic flow, which is represented by $n = 0$, is necessary to initiate the formation of a cluster. Such stochastic events are simulated assuming that one of the free cars can reduce its velocity to $v_{\rm opt}(\Delta x_{\rm clust})$, i. e., become a single congested car or a cluster of size $n = 1$. This process is characterized by the transition frequency $w_+(0)$ which cannot be calculated from the ansatz (124), but have to be considered as one of the control parameters of the model. A cluster of size one appears also when a two–car cluster is reduced by one car. In this consideration the vehicular cluster with size $n = 1$ is a car which still have not accelerated after this event. In any case, a precluster is defined as a single car moving with the velocity $v_{\rm opt}(\Delta x_{\rm clust})$. Since at $n = 0$ any of the N free cars has an opportunity to become a single congested car, an appropriate ansatz for the transition frequency $w_+(0)$ is

$$w_+(0) = \frac{p}{\tau}\, N \,, \tag{131}$$

where $p > 0$ is a dimensionless constant called the stochastic perturbation parameter or stochasticity.

In natural sciences and especially in physics it is usually accepted to write all the basic equations in dimensionless variables. It is suitable to introduce the dimensionless time T via $T = t/\tau$ and the dimensionless distances normalized to ℓ, i. e., $\Delta y = \Delta x/\ell$, $d = D/\ell$, $\Delta y_{\rm clust} = \Delta x_{\rm clust}/\ell$ and $\Delta y_{\rm free} = \Delta x_{\rm free}/\ell$, as well as the dimensionless optimal velocity $w_{\rm opt} = v_{\rm opt}/v_{\rm max}$.

Then the basic equations of this section can be rewritten as follows. The master equation for the scaled probability distribution $P(n, T)$ instead of $p(n, t)$:

$$\begin{aligned}\frac{1}{\tau}\frac{\partial}{\partial T}P(n,T) &= w_+(n-1)\; P(n-1,T) + w_-(n+1)\; P(n+1,T) \\ &\quad - [w_+(n) + w_-(n)]\; P(n,T)\;; \end{aligned} \tag{132}$$

the optimal velocity definition:

$$w_{\rm opt}(\Delta y) = \frac{(\Delta y)^2}{d^2 + (\Delta y)^2}\;; \tag{133}$$

the transition frequencies:

$$w_-(n) = w_- = \frac{1}{\tau} \; , \qquad 1 \le n \le N \; , \tag{134}$$

$$w_+(0) = \frac{1}{\tau} \, p \, N \; , \tag{135}$$

$$\begin{aligned} w_+(n) &= \frac{v_{\max}}{\ell} \frac{\left[v_{\text{opt}}(\Delta x_{\text{free}}) - v_{\text{opt}}(\Delta x_{\text{clust}}) \right] / v_{\max}}{\left[\Delta x_{\text{free}} - \Delta x_{\text{clust}} \right] / \ell} \\ &= \frac{1}{\tau} \, b \, \frac{w_{\text{opt}}(\Delta y_{\text{free}}(n)) - w_{\text{opt}}(\Delta y_{\text{clust}})}{\Delta y_{\text{free}}(n) - \Delta y_{\text{clust}}} \; , \quad 1 \le n \le N-1 \end{aligned} \tag{136}$$

with dimensionless parameter

$$b = v_{\max} \tau / \ell \; ; \tag{137}$$

and the ansatz for the cluster length and related quantities:

$$\frac{L_{\text{clust}}}{\ell} = n + \Delta y_{\text{clust}} \, S(n) = c_{\text{clust}}^{-1} \, n \; , \tag{138}$$

$$\frac{L_{\text{free}}}{\ell} = N - n + \Delta y_{\text{free}}(N - S(n)) = c_{\text{free}}^{-1} \, (N-n) \; , \tag{139}$$

$$\Delta y_{\text{free}}(n) = \frac{L/\ell - N - \Delta y_{\text{clust}} \, S(n)}{N - S(n)} \; . \tag{140}$$

According to the definitions, $c = \ell N / L = \ell \varrho$ is the total density of cars, $c_{\text{clust}} = n \ell / L_{\text{clust}}$ and $c_{\text{free}} = (N-n)\ell / L_{\text{free}}$ are the densities in jam and in the free flow, respectively.

In the stochastic approach an equation can be obtained for the average cluster size $\langle n \rangle$. Based on the master equation (83), we get a deterministic equation for the mean value

$$\frac{d}{dt} \langle n \rangle = \frac{d}{dt} \sum_n n p(n,t) = \langle w^+(n) \rangle - \langle w^-(n) \rangle \; , \tag{141}$$

which can be written in a certain approximation as follows

$$\frac{d}{dt} \langle n \rangle \approx w^+(\langle n \rangle) - w^-(\langle n \rangle) \; , \tag{142}$$

describing the time evolution of the average cluster size $\langle n \rangle$. The stationary cluster size $\langle n \rangle_{st}$ can be calculated from the condition $d\langle n \rangle / dt = 0$.

2 Fokker–Planck Equation

2.1 From Random Walk to Diffusion

The stochastic motion by discrete probabilistic jumps on an (asymmetrically) Galton board is called random walk. The random walk proceeds by discrete steps and is described by the diffusion equation in the continuum limit. The concept of the random walk, also called drunkard's walk, was introduced into science by Karl Pearson in a letter to Nature in 1905:

> A man starts from a point 0 and walks l yards in a straight line: he then turns through any angle whatever and walks another l yards in a straight line. He repeats this process n times. I require the probability that after these n stretches he is at a distance between r and $r + \delta r$ from the starting point 0.

The random walk on a line is much simpler. The positions are spaced regularly along a line. The walker has two possibilities: either one step to right $(+1)$ with probability p or one step to left (-1) with probability $q = 1 - p$. Symmetric case (pure diffusion) means $p = q = 1/2$.

The probability $P(m, n+1)$ that the walker is at position m after $n+1$ steps is given by the set of probabilities $P(m \pm 1, n)$ after n steps in accordance with the Markov chain equation (difference equation)

$$P(m, n+1) = p\, P(m-1, n) + q\, P(m+1, n)\ . \qquad (143)$$

The solution of (143) is the binomial distribution

$$P(m, n) = \frac{n!}{[(n+m)/2]!\,[(n-m)/2]!}\, p^{(n+m)/2}\, q^{(n-m)/2}\ . \qquad (144)$$

The first moment of this probability distribution is

$$\langle m\rangle(n) = \sum_{m=-n}^{n} mP(m, n) = 2n\left(p - \frac{1}{2}\right) \qquad (145)$$

and the second moment is

$$\langle m^2\rangle(n) = \sum_{m=-n}^{n} m^2 P(m, n) = 4npq + 4n^2\left(p - \frac{1}{2}\right)^2\ . \qquad (146)$$

Hence, the root–mean–square is given by

$$\sigma(n) = \sqrt{\left\langle (m - \langle m \rangle)^2 \right\rangle} = \sqrt{\langle m^2 \rangle - \langle m \rangle^2} = \sqrt{4npq} \ , \tag{147}$$

and the relative width (error)

$$\frac{\sigma}{\langle m \rangle} = \frac{\sqrt{4np(1-p)}}{2n(p-1/2)} = \sqrt{\frac{p(1-p)}{(p-1/2)^2}} \frac{1}{\sqrt{n}} \simeq n^{-1/2} \tag{148}$$

tends to zero when n goes to infinity.

After a series of n steps of equal length the particle (called drunken sailor as random walker) could be find at any of the following points

$$m = \{-n, -n+1, \ldots, -1, 0, +1, \ldots, n-1, n\} \ . \tag{149}$$

Position m consists of k steps in one direction (success) and $n-k$ in opposite direction (failure)

$$m = k - (n-k) = 2k - n \ . \tag{150}$$

For the k successes we get

$$k = \frac{1}{2}(n+m) \ . \tag{151}$$

Starting with the well–known binomial distribution for discrete probabilities

$$P(m,n) \equiv B(k,n) = \binom{n}{k} p^k (1-p)^{n-k} \tag{152}$$

we reduce to the symmetric case ($p = 1/2$)

$$P(m,n) = \frac{n!}{k!(n-k)!} \left(\frac{1}{2}\right)^n = \frac{n!}{[(n+m)/2]!\,[(n-m)/2]!} \left(\frac{1}{2}\right)^n \ . \tag{153}$$

Further on we introduce (still discrete) coordinate $x_m = d\,m$ and time $t_n = \tau\, n$, where d is the hopping distance (a length unit) and τ is the time step (a time unit) and rewrite the binomial distribution (153) as $P(x_m, t_n)$.

After introducing a new control parameter

$$D = \frac{d^2}{\tau} \ , \tag{154}$$

called diffusion coefficient, we consider the continuum limit where length unit d and time unit τ both tend to zero in such a way that D remains constant. In this case the physically interesting quantity is the probability density $p(x,t)$, i. e., the probability $p(x,t)dx$ to find a particle within $[x, x+dx]$ multiplied by the interval length dx, which equals to $2d$.

Taking into account the definition (154), we finally obtain the Gaussian distribution

$$p(x,t) = \frac{1}{\sqrt{2\pi Dt}} \exp\left(-\frac{x^2}{2Dt}\right) . \tag{155}$$

The dynamics of probability density $p(x,t)$ (155) for a one–dimensional random walk is given by the one–dimensional diffusion equation (partial differential equation)

$$\frac{\partial p(x,t)}{\partial t} = \frac{D}{2} \frac{\partial^2 p(x,t)}{\partial x^2} . \tag{156}$$

To obtain certain solution, the diffusion equation (156) has to be completed by initial and boundary conditions. We consider the initial condition $p(x, t = 0) = \delta(x - 0)$ given by the delta function (a sharp peak at $x = 0$), which physically means that the random walk starts at $x = 0$, as well as natural boundary conditions $\lim_{x\to\pm\infty} p(x,t) = 0$.

2.2 Derivation of Fokker–Planck Equation

The master equation as well as the Fokker–Planck equation are useful to describe the time development of the probability density function $p(x,t)$ for a continuous variable x.

In the following we want to discuss the one–dimensional case in detail. The Fokker–Planck equation follows from the master equation (65)

$$\frac{\partial p(x,t)}{\partial t} = \int\limits_{-\infty}^{+\infty} \left\{ w(x, x', t) p(x', t) - w(x', x, t) p(x, t) \right\} dx' \tag{157}$$

due to the Kramers–Moyal expansion where only the first two leading terms are retained. In distinction to (65), here we allow as a more general case that the transition frequencies depend on time t. The derivation can be found in many textbooks.

By introducing the quantity $f(y, x, t) = w(x + y, x, t)$, the master equation (157) can be written as

$$\frac{\partial p(x,t)}{\partial t} = \int\limits_{-\infty}^{+\infty} \{f(y, x-y, t)p(x-y, t) - f(y, x, t)p(x, t)\}\, dy \; . \tag{158}$$

It is assumed that $f(y, x-y, t)$ is a smooth function with respect to y. The basic idea is to expand the quantity $f(y, x-y, t)p(x-y, t)$ in a Taylor series around $y = 0$, which yields the Kramers–Moyal expansion

$$\frac{\partial p(x,t)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n} \left[\alpha_n(x,t)\, p(x,t)\right] \; , \tag{159}$$

where

$$\alpha_n(x,t) = \int\limits_{-\infty}^{+\infty} y^n f(y, x, t)\, dy = \int\limits_{-\infty}^{+\infty} (x' - x)^n w(x', x, t)\, dx' \tag{160}$$

are the nth order moments of the transition frequencies $w(x', x, t)$. Retaining only the first two expansion terms in (159) one obtains the well–known Fokker–Planck equation in forward notation

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left[\alpha_1(x,t)\, p(x,t)\right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[\alpha_2(x,t)\, p(x,t)\right] \; . \tag{161}$$

The first term in (161) is called the drift term and the second one – the diffusion or fluctuation term. This is due to the analogy with a drift–diffusion equation where the first derivative describes the drift of the probability profile without changing its form, whereas the second one describes the pure diffusion effect. In fact, (161) is a drift–diffusion equation for the probability $p(x,t)$. The diffusion or effluence of the probability distribution profile occurs due to the stochastic fluctuations, therefore the second term in (161) is also called the fluctuation term. More explicitly Eq. (161) is called the *forward Fokker–Planck equation* to distinguish from the *backward Fokker–Planck equation* which describes the evolution of the conditional probability $p(x, t \mid x', t')$ with respect to the initial time t'.

2.3 How to Solve the Fokker–Planck Equation?

Equation of motion

Study of Fokker–Planck dynamics $p(x,t)$ with known drift $f(x)$ given by

$$\boxed{\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[f(x)p(x,t)\right] + \frac{\sigma^2}{2}\frac{\partial^2 p(x,t)}{\partial x^2} \quad ; \quad p(x,t=0) = \delta(x-x_0)} \tag{162}$$

with natural boundary conditions.

Relationship between drift "force" $f(x)$ (in $\mathrm{m\,s^{-1}}$) and "potential" $V(x)$ (in $\mathrm{m^2s^{-1}}$):

$$\boxed{V(x) = -\int f(x)\,dx \qquad \Longleftrightarrow \qquad f(x) = -\frac{dV(x)}{dx}} \tag{163}$$

$$f(x) = -\alpha x - \beta x^3 \quad \Longleftrightarrow \quad V(x) = \frac{\alpha}{2}x^2 + \frac{\beta}{4}x^4 + C \tag{164}$$

Identity: Stochasticity $\sigma = \sqrt{2D}$ or diffusion coefficient $D = \sigma^2/2$.

First case: The free particle solution ($\alpha = 0, \beta = 0$) is called pure diffusion.

Second case: The linear force system ($\alpha > 0, \beta = 0$) has an analytical solution.

Third case: The nonlinear system with cubic force ($\beta > 0$) has numerical solution only.

Stationary solution

The stationary solution $p_{st}(x)$ is the long time limit of $p(x,t)$ for $t \to \infty$ and follows from

$$\boxed{0 = \frac{d}{dx}\left[f(x)p_{st}(x)\right] - \frac{\sigma^2}{2}\frac{d^2 p_{st}(x)}{dx^2} \;.} \tag{165}$$

Rearrangement gives

$$0 = -\frac{d}{dx}\left[\frac{dV(x)}{dx}p_{st}(x) + D\frac{dp_{st}(x)}{dx}\right] \;. \tag{166}$$

Due to natural boundary conditions we have zero flux

$$j_{st}(x) \equiv -\frac{dV(x)}{dx}p_{st}(x) - D\frac{dp_{st}(x)}{dx} = C \quad \text{with} \quad C = 0\ . \tag{167}$$

We get

$$\frac{dp_{st}(x)}{dx} = -\frac{1}{D}\frac{dV(x)}{dx}p_{st}(x) \tag{168}$$

$$\frac{dp_{st}(x)}{p_{st}(x)} = -\frac{1}{D}dV(x) \tag{169}$$

as stationary solution

$$p_{st}(x) = \mathcal{N}^{-1}\exp\left[-\frac{1}{D}V(x)\right] \tag{170}$$

with normalization constant

$$\mathcal{N} = \int_{-\infty}^{+\infty} dx \exp\left[-\frac{1}{D}V(x)\right]\ . \tag{171}$$

Time dependent solution

We start with the <u>transformation</u> $p(x,t) \to q(x,t)$ given by

$$p(x,t) = p_{st}(x)^{1/2}\, q(x,t) \equiv \mathcal{N}^{-1/2}\exp\left[-\frac{1}{D}\frac{V(x)}{2}\right] q(x,t)\ . \tag{172}$$

This transformation removes the first derivative in the original Fokker–Planck equation and generates the following Schrödinger–like equation for the function $q(x,t)$

$$\frac{\partial q(x,t)}{\partial t} = -V_S(x)q(x,t) + D\frac{\partial^2 q(x,t)}{\partial x^2} \tag{173}$$

with the so–called Schrödinger potential

$$V_S(x) = -\left[\frac{1}{2}\frac{d^2V(x)}{dx^2} - \frac{1}{D}\left(\frac{1}{2}\frac{dV(x)}{dx}\right)^2\right]\ . \tag{174}$$

Using double–well potential

$$V(x) = \frac{\alpha}{2}x^2 + \frac{\beta}{4}x^4 \tag{175}$$

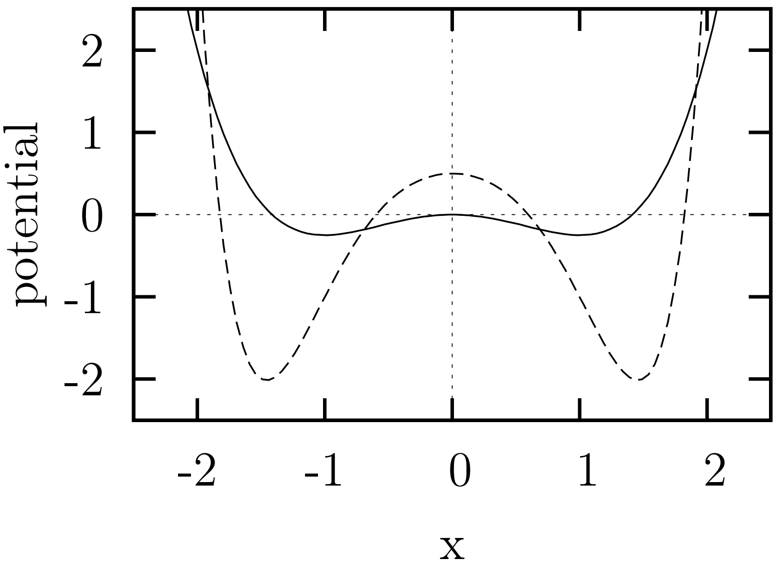

Fig. 27: *The solid line shows the potential $V(x)$, the dashed line shows the Schrödinger potential $V_S(x)$. The parameters of both curves are $\alpha = -1.0\ s^{-1}$, $\beta = 1.0\ s^{-1}m^{-2}$ and $D = 1.0\ m^2s^{-1}$.*

we get for the Schrödinger "potential" (in s^{-1})

$$V_S(x) = -\frac{\alpha}{2} + \left(\frac{1}{D}\frac{\alpha^2}{4} - \frac{3}{2}\beta\right)x^2 + \frac{1}{D}\frac{\alpha\beta}{2}x^4 + \frac{1}{D}\frac{\beta^2}{4}x^6 \ . \tag{176}$$

See Fig. 27 for double well potential.

Next step is superposition ansatz given by

$$q(x,t) = \sum_{n=0}^{\infty} a_n(t)\psi_n(x) \tag{177}$$

which can be written as

$$q(x,t) = p_{st}(x)^{1/2} + \sum_{n=1}^{\infty} a_n(t)\psi_n(x) \tag{178}$$

showing $a_0 = 1$ and $\psi_0(x) = p_{st}(x)^{1/2}$.

After inserting ansatz (177) into (173) we get the eigenvalue problem with eigenfunction $\psi_n(x)$ and eigenvalue $\lambda_n \geq 0$

$$D\,\frac{d^2\psi_n(x)}{dx^2} - V_S(x)\psi_n(x) = -\lambda_n\psi_n(x) \tag{179}$$

and the time dependent coefficients as

$$a_n(t) = a_n(0) \exp\left(-\lambda_n t\right) \ . \tag{180}$$

Up to now we have received

$$q(x,t) = \sum_{n=0}^{\infty} a_n(0) e^{-\lambda_n t} \psi_n(x) \tag{181}$$

where normalized orthogonal (or orthonormal) eigenfunctions $\psi_n(x)$ with

$$\int_{-\infty}^{+\infty} \psi_n(x)\psi_m(x) dx = \delta_{nm} \tag{182}$$

from Schrödinger–like eigenvalue equation (Hermitian operator $\mathcal{H}$)

$$\mathcal{H}\psi_n(x) = \lambda_n \psi_n(x) \quad \text{with} \quad \mathcal{H} = -D\frac{d^2}{dx^2} + V_S(x) \tag{183}$$

and eigenvalue spectrum $\lambda_0 = 0$ matching the eigenfunction $\psi_0(x) = p_{st}^{1/2}$ and all other $\lambda_n > 0$ for $n \geq 1$.

Taking into account closure condition (completeness relation)

$$\sum_{n=0}^{\infty} \psi_n(x')\psi_n(x) = \delta(x - x') \tag{184}$$

and using the given initial condition

$$p(x, t=0) = p_{st}(x)^{1/2} q(x, t=0) = \delta(x - x_0) \tag{185}$$

we get from

$$\delta(x - x_0) = p_{st}(x)^{1/2} \sum_{n=0}^{\infty} a_n(0)\psi_n(x) = \sum_{n=0}^{\infty} \psi_n(x_0)\psi_n(x) \tag{186}$$

the up to now unknown coefficients

$$a_n(0) = p_{st}(x_0)^{-1/2} \psi_n(x_0) \ . \tag{187}$$

Finally the result reads

$$p(x,t) = p_{st}(x)^{1/2} p_{st}(x_0)^{-1/2} \sum_{n=0}^{\infty} e^{-\lambda_n t} \psi_n(x_0)\psi_n(x) \tag{188}$$

or

$$p(x,t) = p_{st}(x) + \sqrt{\frac{p_{st}(x)}{p_{st}(x_0)}} \sum_{n=1}^{\infty} e^{-\lambda_n t} \psi_n(x_0)\psi_n(x) \ . \tag{189}$$

Summary: task and its result

The task is to solve the one–dimensional Fokker–Planck equation

$$\boxed{\frac{\partial p(x,t)}{\partial t} + \frac{\partial}{\partial x} j(x,t) = 0} \tag{190}$$

with flux $j(x,t)$ including given drift $f(x) = -dV(x)/dx$ and constant diffusion coefficient D

$$\boxed{j(x,t) = -\frac{dV(x)}{dx} p(x,t) - D\frac{\partial p(x,t)}{\partial x}} \tag{191}$$

getting the probability density $p(x,t)$ taking into account initial condition $p(x,t=0) = \delta(x-x_0)$ and natural boundary conditions $\lim_{x\to\pm\infty} j(x,t) = 0$.

The result is

$$\boxed{p(x,t) = \frac{\psi_0(x)}{\psi_0(x_0)} \sum_{n=0}^{\infty} e^{-\lambda_n t} \psi_n(x_0)\psi_n(x)} \tag{192}$$

where the eigenfunctions $\psi_n(x)$ and eigenvalues λ_n are determined from the eigenvalue equation

$$\boxed{\left(-D\frac{d^2}{dx^2} + V_S(x)\right) \psi_n(x) = \lambda_n \, \psi_n(x)} \tag{193}$$

with Schrödinger potential

$$\boxed{V_S(x) = -\left[\frac{1}{2}\frac{d^2V(x)}{dx^2} - \frac{1}{D}\left(\frac{1}{2}\frac{dV(x)}{dx}\right)^2\right]} \tag{194}$$

The lowest eigenvalue is always zero ($\lambda_0 = 0$) and the corresponding eigenfunction is related to the stationary solution via

$$\boxed{p_{st}(x) = \psi_0(x)^2 = \frac{\exp\left(-V(x)/D\right)}{\int_{-\infty}^{+\infty} dx \exp\left(-V(x)/D\right)}} \tag{195}$$

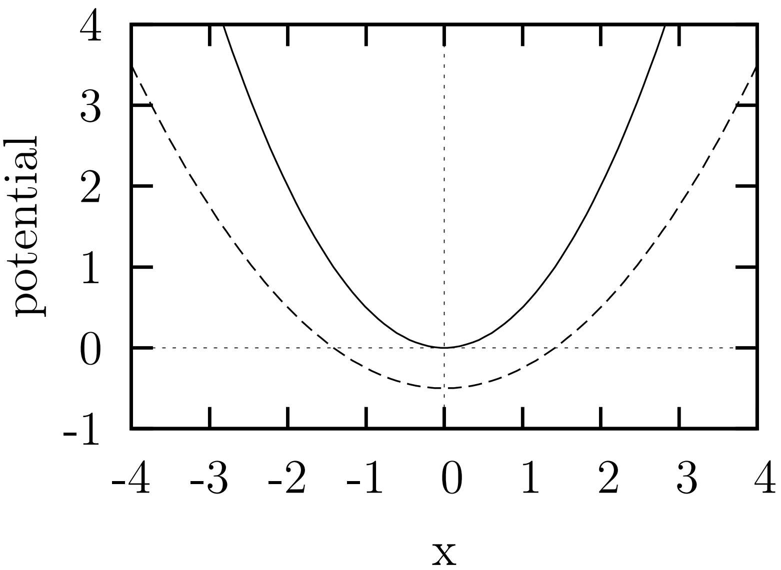

Fig. 28: *The solid line shows the potential $V(x)$, the dashed line shows the Schrödinger potential $V_S(x)$. The parameters of both curves are $\alpha = 1.0\ s^{-1}$ and $D = 1.0\ m^2 s^{-1}$.*

2.4 The Textbook Example: Linear Drift

The problem of drift under linear force has a well known analytical solution.

Starting with the drift ansatz given by

$$f(x) = -\alpha\, x \qquad (\alpha > 0)\ , \tag{196}$$

the potential (normalized to $V(x=0)=0$) reads

$$V(x) = \frac{\alpha}{2} x^2\ , \tag{197}$$

and the Schrödinger potential is also harmonic (quadratic)

$$V_S(x) = -\frac{\alpha}{2} + \frac{1}{D}\frac{\alpha^2}{4} x^2\ . \tag{198}$$

See Fig. 28 for single well potential.

The eigenvalue equation

$$-D\frac{d^2\psi_n(x)}{dx^2} + \left(-\frac{\alpha}{2} + \frac{1}{D}\frac{\alpha^2}{4}x^2\right)\psi_n(x) = \lambda_n\,\psi_n(x) \tag{199}$$

is related to the Hermite polynomial differential equation known as

$$\frac{d^2\psi_n(y)}{dy^2} + \left(2n+1-y^2\right)\psi_n(y) = 0\ , \tag{200}$$

with solution

$$\psi_n(y) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}}\, e^{-y^2/2} H_n(y)\ , \tag{201}$$

where functions $H_n(y)$ with $n = 0, 1, 2, \ldots$ are called Hermite polynomials.

Rewriting the 2nd order differential eigenvalue equation (199) we have to solve

$$\frac{d^2\psi_n(x)}{dx^2} + \frac{1}{D}\left(\lambda_n + \frac{\alpha}{2} - \frac{1}{D}\frac{\alpha^2}{4}x^2\right)\psi_n(x) = 0\ . \tag{202}$$

Change of variable x to a new dimensionless variable ξ via

$$\sqrt{\left(\frac{1}{D}\right)^2 \frac{\alpha^2}{4}} x^2 = \xi^2 \quad \text{or} \quad \xi^2 = \frac{1}{D}\frac{\alpha}{2}x^2 \tag{203}$$

gives the following second order differential equation

$$\frac{d^2\psi(\xi)}{d\xi^2} + \left(\frac{2}{\alpha}\lambda + 1 - \xi^2\right)\psi(\xi) = 0\ , \tag{204}$$

which is related to the Hermite polynomial differential equation (200).

Therefore comparing allows us to determine the eigenvalues

$$\frac{2}{\alpha}\lambda_n + 1 = 2n+1 \quad \Longrightarrow \quad \lambda_n = \alpha\, n \quad \text{for} \quad n = 0, 1, 2, \ldots\ . \tag{205}$$

Going back from variable ξ to x we know the set of orthonormal eigenfunctions as

$$\psi_n(x) = \sqrt[4]{\frac{1}{D}\frac{\alpha}{2}}\frac{1}{\sqrt{2^n n! \sqrt{\pi}}}\ \exp\left[-\left(\frac{1}{D}\frac{\alpha}{2}\right)\frac{x^2}{2}\right] H_n\left(\sqrt{\frac{1}{D}\frac{\alpha}{2}}\, x\right)\ , \tag{206}$$

where $H_n(y)$ are Hermite polynomials given by

$$H_n(y) = (-1)^n\, e^{y^2} \frac{d^n}{dy^n} e^{-y^2} \tag{207}$$

$$H_0(y) = 1 \quad ; \quad H_1(y) = 2y \quad ; \quad H_2(y) = 4y^2 - 2 \quad ; \quad \ldots \tag{208}$$

$$H_n(y) = 2yH_{n-1}(y) - 2(n-1)H_{n-2}(y) \qquad n = 2, 3, 4, \ldots\ . \tag{209}$$

The ground state $n = 0$ reflects zero eigenvalue $\lambda_0 = 0$ with

$$\psi_0(x) = \sqrt[4]{\frac{1}{D}\frac{\alpha}{2}}\frac{1}{\sqrt[4]{\pi}} \exp\left[-\left(\frac{1}{D}\frac{\alpha}{2}\right)\frac{x^2}{2}\right] H_0\left(\sqrt{\frac{1}{D}\frac{\alpha}{2}}\,x\right) \tag{210}$$

$$\text{where} \quad H_0\left(\sqrt{\frac{1}{D}\frac{\alpha}{2}}\,x\right) = 1 \ . \tag{211}$$

The first excited state $n = 1$ has eigenvalue $\lambda_1 = \alpha$ with

$$\psi_1(x) = \sqrt[4]{\frac{1}{D}\frac{\alpha}{2}}\frac{1}{\sqrt{2\sqrt{\pi}}} \exp\left[-\left(\frac{1}{D}\frac{\alpha}{2}\right)\frac{x^2}{2}\right] H_1\left(\sqrt{\frac{1}{D}\frac{\alpha}{2}}\,x\right) \tag{212}$$

$$\text{where} \quad H_1\left(\sqrt{\frac{1}{D}\frac{\alpha}{2}}\,x\right) = 2\sqrt{\frac{1}{D}\frac{\alpha}{2}}\,x \ . \tag{213}$$

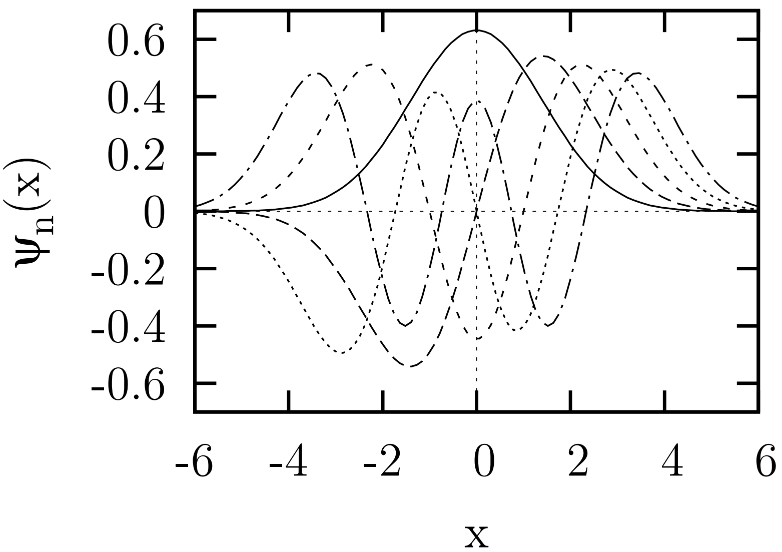

Fig. 29: *The picture shows the first five eigenfunctions $\psi_0(x)$ to $\psi_4(x)$. The order n is equal to the number of nodes. The parameters are $\alpha = 1.0\ s^{-1}$ and $D = 1.0\ m^2 s^{-1}$.*

Knowing all the eigenvalues λ_n and the complete set of eigenfunctions $\psi_n(x)$ for $n = 0, 1, \ldots$ we are able to write immediately the probability density (in agreement with (192)) as

$$p(x,t) = \frac{\psi_0(x)}{\psi_0(x_0)} \sum_{n=0}^{\infty} e^{-\lambda_n t} \psi_n(x_0)\psi_n(x) \ . \tag{214}$$

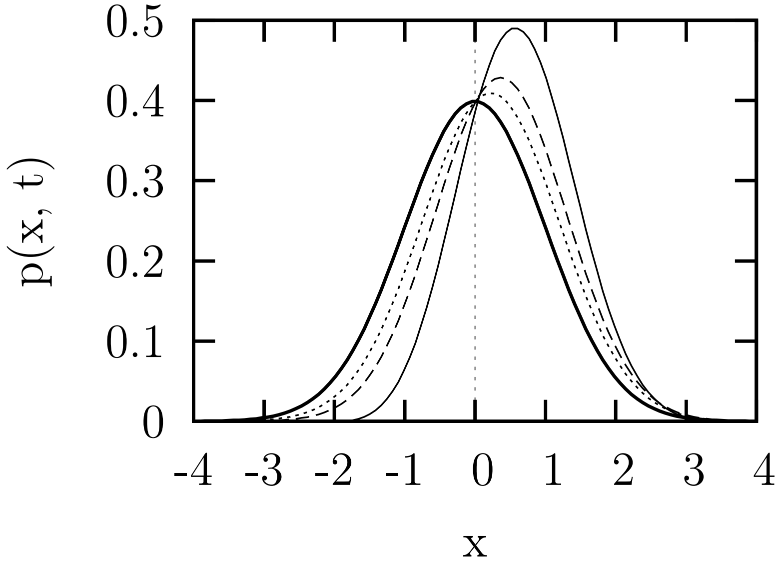

Fig. 30: *The picture shows the time dependent solution $p(x,t)$ taking into account the first five eigenfunctions only. The four time moments are $t = 0.5$ s, $t = 1.0$ s, $t = 1.5$ s and $t \to \infty$ (solid curve, stationary distribution). The parameters are $x_0 = 1.0$ m, $\alpha = 1.0$ s^{-1} and $D = 1.0$ $m^2 s^{-1}$.*

See Fig. 29 for eigenfunctions and Fig. 30 for time evolution.

Taking into account the stationary solution (compare (195)) we get

$$p_{st}(x) = \psi_0(x)^2 = \frac{\exp\left(-V(x)/D\right)}{\int_{-\infty}^{+\infty} dx \exp\left(-V(x)/D\right)} \tag{215}$$

$$= \sqrt{\frac{\alpha}{2\pi D}} \exp\left[-\left(\frac{\alpha}{2D}\right) x^2\right] . \tag{216}$$

Using the known probability density $p(x,t)$ we want to calculate overall quantities called moments of m-th order given by

$$\boxed{\langle x(t)^m \rangle = \int_{-\infty}^{+\infty} x^m \, p(x,t) \, dx \, .} \tag{217}$$

The zeroth moment is normalization. In general we are able to proof it as follows

$$\langle x(t)^0 \rangle = \langle 1 \rangle = \int_{-\infty}^{+\infty} p(x,t)\, dx \tag{218}$$

$$= \frac{1}{\psi_0(x_0)} \sum_{n=0}^{\infty} e^{-\lambda_n t} \psi_n(x_0) \int_{-\infty}^{+\infty} \psi_0(x)\psi_n(x)\, dx \tag{219}$$

$$= \int_{-\infty}^{+\infty} \psi_0(x)\psi_0(x)\, dx = \int_{-\infty}^{+\infty} p_{st}(x)\, dx = 1\ . \tag{220}$$

The <u>first moment</u> is variable x averaged over the distribution $p(x,t)$. We get

$$\langle x(t)^1 \rangle = \langle x(t) \rangle = \int_{-\infty}^{+\infty} x\, p(x,t)\, dx \tag{221}$$

$$= \frac{1}{\psi_0(x_0)} \sum_{n=0}^{\infty} e^{-\lambda_n t} \psi_n(x_0) \int_{-\infty}^{+\infty} x\, \psi_0(x)\psi_n(x)\, dx \tag{222}$$

and calculate the first two contributions in detail.
The term $n = 0$ with $\lambda_0 = 0$ gives zero

$$\frac{\psi_0(x_0)}{\psi_0(x_0)} \int_{-\infty}^{+\infty} x\, \psi_0(x)^2\, dx = \int_{-\infty}^{+\infty} x\, p_{st}(x)\, dx = 0 \tag{223}$$

due to asymmetry.
The term $n = 1$ with $\lambda_1 = \alpha$ gives

$$\frac{\psi_1(x_0)}{\psi_0(x_0)} e^{-\alpha t} \int_{-\infty}^{+\infty} x\, \psi_0(x)\psi_1(x)\, dx = x_0\, e^{-\alpha t} \tag{224}$$

as the only nonvanishing contribution.

Hint: Use

$$\int_{-\infty}^{+\infty} x^2 e^{-ax^2}\, dx = \frac{\sqrt{\pi}}{2\, a^{3/2}} \tag{225}$$

Hint: Use

$$\int_{-\infty}^{+\infty} x \frac{d^n}{dx^n} e^{-ax^2}\, dx = 0\ ; \qquad n = 2, 3, \ldots \tag{226}$$

Therefore, the time dependent first moment (mean) is calculated as

$$\boxed{\langle x(t) \rangle = x_0 \exp\left(-\alpha t\right) \to 0 \quad \text{if} \quad t \to \infty\ .} \tag{227}$$

The <u>second moment</u> is x^2 averaged over the distribution $p(x,t)$. We get

$$\langle x(t)^2 \rangle = \langle x(t) \rangle = \int_{-\infty}^{+\infty} x^2 \, p(x,t) \, dx \tag{228}$$

$$= \frac{1}{\psi_0(x_0)} \sum_{n=0}^{\infty} e^{-\lambda_n t} \psi_n(x_0) \int_{-\infty}^{+\infty} x^2 \psi_0(x) \psi_n(x) \, dx \tag{229}$$

and calculate the first three contributions in detail.
The term $n = 0$ with $\lambda_0 = 0$ gives a finite value

$$\frac{\psi_0(x_0)}{\psi_0(x_0)} \int_{-\infty}^{+\infty} x^2 \, \psi_0(x)^2 \, dx = \int_{-\infty}^{+\infty} x^2 p_{st}(x) \, dx = \frac{D}{\alpha} \, . \tag{230}$$

The term $n = 1$ with $\lambda_1 = \alpha$ gives zero due to asymmetry.
The term $n = 2$ with $\lambda_1 = 2\alpha$ gives

$$\frac{\psi_2(x_0)}{\psi_0(x_0)} e^{-2\alpha t} \int_{-\infty}^{+\infty} x^2 \psi_0(x) \psi_2(x) \, dx = \left(x_0^2 - \frac{D}{\alpha} \right) e^{-2\alpha t} \, . \tag{231}$$

All other terms do not contribute.

Therefore, the time dependent second moment is given as

$$\boxed{\langle x(t)^2 \rangle = x_0^2 \exp\left(-2\alpha t\right) + \frac{D}{\alpha} \left(1 - \exp\left(-2\alpha t\right)\right) \, .} \tag{232}$$

We get for the variance

$$\langle x(t)^2 \rangle - \langle x(t) \rangle^2 = \frac{D}{\alpha} \left(1 - \exp\left(-2\alpha t\right)\right) \to \frac{D}{\alpha} \qquad \text{if} \qquad t \to \infty \, . \tag{233}$$

Remark:
If we want to treat the limit case called pure diffusion, we have to consider the situation that the control parameter α tends to zero ($\alpha \to 0$). For the moments we get easily $\langle x(t) \rangle = x_0$ and $\langle x(t)^2 \rangle \to \infty$.

But how to get the known probability density for the case $\alpha = 0$

$$p(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left[-\frac{(x - x_0)^2}{4Dt} \right] \tag{234}$$

from the calculated density $p(x,t)$ given by (214) with eigenvalues $\lambda_n = \alpha n$ and eigenfunctions $\psi_n(x)$ (206) including Hermite polynomials $H_n(x)$? The values $H_n(0)$ are called Hermite numbers.

Some more details who to solve the differential equation (204) named after Hermite

$$\frac{d^2\psi(\xi)}{d\xi^2} + \left(\frac{2}{\alpha}\lambda + 1 - \xi^2\right)\psi(\xi) = 0 \tag{235}$$

by power series expansion. We start with the ansatz

$$\psi(\xi) = h(\xi)e^{-\xi^2/2} \quad \text{with} \quad \psi(\xi \to \pm\infty) \to 0 \tag{236}$$

and after inserting we get the following differential equation

$$\frac{d^2h(\xi)}{d\xi^2} - 2\xi\frac{dh(\xi)}{d\xi} + \frac{2}{\alpha}\lambda h(\xi) = 0\ . \tag{237}$$

Here we try a power series for the unknown function

$$h(\xi) = \sum_{i=0}^{\infty} a_i\xi^i \tag{238}$$

using

$$\frac{dh(\xi)}{d\xi} = \sum_{i=1}^{\infty} a_i i\xi^{i-1} = \sum_{j=0}^{\infty} a_{j+1}(j+1)\xi^j \tag{239}$$

$$\frac{d^2h(\xi)}{d\xi^2} = \sum_{i=2}^{\infty} a_i i(i-1)\xi^{i-2} = \sum_{j=0}^{\infty} a_{j+2}(j+2)(j+1)\xi^j\ . \tag{240}$$

After inserting we get

$$\sum_{j=0}^{\infty} a_{j+2}(j+2)(j+1)\xi^j - 2\sum_{j=0}^{\infty} a_{j+1}(j+1)\xi^{j+1} + \frac{2}{\alpha}\lambda\sum_{j=0}^{\infty} a_j\xi^j = 0 \tag{241}$$

or

$$\sum_{i=0}^{\infty}\xi^i\left\{a_{i+2}(i+2)(i+1) - 2a_i i + \frac{2}{\alpha}\lambda a_i\right\} = 0\ . \tag{242}$$

To fulfill this equation we arrive at the mapping

$$a_{i+2} = \frac{2i - (2/\alpha)\lambda}{(i+2)(i+1)}a_i \tag{243}$$

which is a iteration of the following type:
If you know a_0, a_2 follows, a_4 follows, etc,
If you know a_1, a_3 follows, a_5 follows, etc.

Due to natural boundary conditions the power series has to be finite

$$h_n(\xi) = \sum_{i=0}^{n} a_i^{(n)} \xi^i \tag{244}$$

and the iteration will be truncated at $a_n^{(n)}$ by $a_{n+2}^{(n)} = 0$. From

$$0 = \frac{2n - (2/\alpha)\lambda}{(n+2)(n+1)} a_n^{(n)} \tag{245}$$

we find the condition for the eigenvalue λ with its spectrum

$$2n - \frac{2}{\alpha}\lambda = 0 \quad \Longrightarrow \quad \lambda_n = \alpha\, n\ . \tag{246}$$

Now we will explore the ground state $n = 0$ in detail. Since the ground state eigenvalue is zero $\lambda_0 = 0$, the solution $p(x,t)$ refers to the stationary situation $p_{st}(x) = p(x, t \to \infty)$ (216).
From $h_0(\xi) = \sum_{i=0}^{n=0} a_i^{(n)} \xi^i = a_0^{(0)} \xi^0 = a_0^{(0)}$ we get $\psi_0(\xi) = h_0(\xi) e^{-\xi^2/2} = a_0^{(0)} e^{-\xi^2/2}$. Doing inverse transformation from ξ to x we have so far

$$\psi_0(x) = a_0 \exp\left[- \left(\frac{1}{D} \frac{\alpha}{2} \right) \frac{x^2}{2} \right] . \tag{247}$$

The unknown coefficient $a_0^{(0)}$ can be calculated from orthonormality condition

$$\int_{-\infty}^{\infty} \psi_0(x) \psi_0(x)\; dx = 1 \quad \Longrightarrow \quad a_0^{(0)} = \sqrt[4]{\frac{1}{\pi} \frac{1}{D} \frac{\alpha}{2}}\ . \tag{248}$$

It gives the normalized ground state eigenfunction (see (210))

$$\psi_0(x) = \sqrt[4]{\frac{1}{\pi} \frac{1}{D} \frac{\alpha}{2}} \exp\left[- \left(\frac{1}{D} \frac{\alpha}{2} \right) \frac{x^2}{2} \right] . \tag{249}$$

Now we will explore the first excited state $n = 1$ with eigenvalue $\lambda_1 = \alpha$ in more detail.
From $h_1(\xi) = \sum_{i=0}^{n=1} a_i^{(n)} \xi^i = a_0^{(1)} \xi^0 + a_1^{(1)} \xi^1 = a_0^{(1)} + a_1^{(1)} \xi$ we get $\psi_1(\xi) = h_1(\xi) e^{-\xi^2/2} = a_0^{(1)} e^{-\xi^2/2} + a_1^{(1)} \xi\, e^{-\xi^2/2}$.
The unknown coefficients $a_0^{(1)}$ and $a_1^{(1)}$ should be determined from the orthonormalization condition. From

$$\int_{-\infty}^{\infty} \psi_0(x) \psi_1(x)\; dx = 0 \tag{250}$$

we find out via

$$\int_{-\infty}^{\infty} \left(\frac{1}{D}\frac{\alpha}{2}\right)^{-1/2} d\xi \left\{a_0^{(0)} e^{-\xi^2/2}\right\} \left\{a_0^{(1)} e^{-\xi^2/2} + a_1^{(1)} \xi e^{-\xi^2/2}\right\} = 0 \tag{251}$$

the result $a_0^{(1)} = 0$.

From

$$\int_{-\infty}^{\infty} \psi_1(x)\psi_1(x)\, dx = 1 \tag{252}$$

we find out via

$$a_1^{(1)2} \int_{-\infty}^{\infty} \left(\frac{1}{D}\frac{\alpha}{2}\right)^{-1/2} d\xi \left\{\xi e^{-\xi^2/2}\right\}^2 = 0 \tag{253}$$

the result $a_1^{(1)} = \sqrt[4]{\frac{1}{D}\frac{\alpha}{2}\frac{1}{\pi}}\sqrt{2}$.
The eigenfunction of first order reads

$$\psi_1(x) = \sqrt[4]{\frac{1}{D}\frac{\alpha}{2}\frac{1}{\pi}} \sqrt{\frac{1}{D}\frac{\alpha}{2}} \frac{1}{\sqrt{2}}\, 2x \exp\left[-\frac{1}{D}\frac{\alpha}{2}\frac{x^2}{2}\right] . \tag{254}$$

Now we will start to explore the second excited state $n = 2$ with eigenvalue $\lambda_2 = 2\alpha$ to some extend.
From $h_2(\xi) = \sum_{i=0}^{n=2} a_i^{(n)} \xi^i = a_0^{(2)} \xi^0 + a_1^{(2)} \xi^1 + a_2^{(2)} \xi^2$ we get
$\psi_2(\xi) = h_2(\xi) e^{-\xi^2/2} = a_0^{(2)} e^{-\xi^2/2} + a_1^{(2)} \xi\, e^{-\xi^2/2} + a_2^{(2)} \xi^2 e^{-\xi^2/2}$.
The coefficient $a_2^{(2)}$ is given by $a_0^{(2)}$ via recurrence formula

$$a_2^{(2)} = \frac{-2/\alpha \cdot 2\alpha}{2 \cdot 1} a_0^{(2)} = -2a_0^{(2)} . \tag{255}$$

So far we have

$$\begin{aligned}\psi_2(\xi) &= a_0^{(2)} e^{-\xi^2/2} + a_1^{(2)} \xi e^{-\xi^2/2} - 2a_0^{(2)} \xi^2 e^{-\xi^2/2} \\ &= a_0^{(2)} \left(1 - 2\xi^2\right) e^{-\xi^2/2} + a_1^{(2)} \xi e^{-\xi^2/2}\end{aligned} \tag{256}$$

and together with known eigenfunctions

$$\psi_1(\xi) = a_1^{(1)} \xi\, e^{-\xi^2/2} \tag{257}$$

$$\psi_0(\xi) = a_0^{(0)} e^{-\xi^2/2} \tag{258}$$

we get

$$\int_{-\infty}^{\infty} \psi_2(x)\psi_1(x)\, dx = 0 \quad \Longrightarrow \quad a_1^{(2)} = 0 \tag{259}$$

and since

$$\int_{-\infty}^{\infty} \psi_2(x)\psi_2(x)\,dx = 1 \quad \Longrightarrow \quad a_0^{(2)} = \ldots \neq 0 \tag{260}$$

finally

$$\psi_2(\xi) = a_0^{(2)}\left(1 - 2\xi^2\right)e^{-\xi^2/2}\,. \tag{261}$$

3 Langevin Equation

3.1 Traditional View on the Langevin Equation

Langevin equation describes the dynamics of a system in presence of an interaction with environment. For simplicity here we consider a one–dimensional case, where the state of the system is characterized by a scalar quantity $x(t)$ which depends on time t. The time evolution is described by the Langevin equation

$$\frac{dx}{dt} = f(x) + \psi(x)\,\xi(t) \tag{262}$$

together with the initial condition

$$x(t=0) = x_0 \; . \tag{263}$$

Here the dynamics of the system itself is given by the deterministic force $f(x)$, whereas the interaction with the environment is represented by the stochastic or Langevin force $\psi(x)\xi(t)$, where $\psi(x)$ is the noise intensity. If the latter one is constant then the Langevin force represents an additive noise. The intensity $\psi(x)$ may depend on x in general. In this case we deal with the so–called multiplicative noise. In the classical case $\xi(t)$ is the Gaussian white noise, representing random and normally distributed fluctuations, which are completely uncorrelated for different time moments.

It is important to notice, however, that other kind of noise $\xi(t)$ also may be of interest. For example, the Markovian dichotomous noise represents a stochastic process of switching between two discrete values. This type of noise is frequently used for modeling of various phenomena in biology, physics, and chemistry. States of the dichotomous process can be associated, e. g., with two different levels of external stimuli, presence or absence of an external perturbation, etc. It is interesting to mention that a combination of dichotomous and white noise can lead to a bimodal probability distribution even in a system with single–well potential $\phi(x) = \alpha x^2/2$ or linear force $f(x) = -d\phi/dx$. Thus, the noise can significantly change the behavior of a system. In this sense we can speak about noise–induced phase transitions.

3.2 Additive White Noise

Historically, the Langevin equation has been designed to describe the Brownian motion, assuming $\psi(x) = \sigma$ in (262) as a constant. This is the usual case of the Langevin equation with the additive noise

$$\frac{dx}{dt} = f(x) + \sigma\xi(t) \; . \tag{264}$$

In general, $\xi(t)$ is a randomly fluctuating quantity. Traditionally it is the white noise, which has the following properties

$$\langle \xi(t) \rangle = 0 \; , \tag{265}$$

$$\langle \xi(t)\xi(t') \rangle = \delta(t - t') \; . \tag{266}$$

The equation (264) can be formulated as a stochastic differential equation with the initial condition (263). It is the conventional form of writing used in mathematical literature, i. e.,

$$dx(t) = f(x(t))dt + \sigma\, dW(t) \quad ; \quad x(t=0) = x_0 \; , \tag{267}$$

where $W(t)$ is the standard Wiener process with the following properties

$$\langle W(t) \rangle = 0 \; , \tag{268}$$

$$\langle W(t)W(t') \rangle = \min(t, t') \; . \tag{269}$$

For the increments of the Wiener process $dW(t) = W(t + dt) - W(t)$ at $dt \to 0$ we have

$$\langle dW(t) \rangle = 0 \; , \tag{270}$$

$$\langle dW(t)dW(t') \rangle = \begin{cases} dt \; , & t' = t \\ 0 \; , & t' \neq t \end{cases} \tag{271}$$

The formal relation between the Wiener process and the Langevin force is given by

$$\xi(t) = \frac{dW(t)}{dt} \qquad \Longleftrightarrow \qquad W(t) = \int_0^t \xi(s)ds \; . \tag{272}$$

Here we would like to mention that the formal solution of (267) is

$$x(t) = x_0 + \int_0^t f(x(s))ds + \sigma W(t) \; . \tag{273}$$

This, however, is only a different formulation of the problem by rewriting the stochastic differential equation (267) as an integral equation (273). Since the right hand side of (273) contains the unknown function $x(s)$, it cannot serve as a solution in practical applications.

The probability density distribution $p(x,t)$ for the variable x at time t is given by the following Fokker–Planck equation which corresponds to (264) or (267) respectively

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}\left[f(x)p(x,t)\right] + \frac{\sigma^2}{2}\frac{\partial^2 p(x,t)}{\partial x^2} \tag{274}$$

with the initial condition

$$p(x,t=0) = \delta(x-x_0) \ . \tag{275}$$

The averages over ensemble of stochastic realizations, like the mean value $\langle x(t)\rangle$ and the correlation function $\langle x(t)x(t')\rangle$, can be expressed in terms of the probability distribution functions as

$$\langle x(t)\rangle = \int\limits_{-\infty}^{\infty} xp(x,t)dx \ , \tag{276}$$

$$\langle x(t)x(t')\rangle = \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} xy\, p(x,t;y,t')\, dxdy \ . \tag{277}$$

Here $p(x,t;y,t')$ is the joint probability density for two time moments.

Returning to the Langevin equation (264), first let us consider the dynamics without fluctuations, which is given by the equation with $\sigma = 0$,

$$\frac{dx}{dt} = f(x) \ . \tag{278}$$

The force can be represented as

$$f(x) = -\frac{d\phi(x)}{dx} \ , \tag{279}$$

where $\phi(x)$ is the potential. A simple classical example is the double–well potential

$$\phi(x) = \frac{\alpha}{2}x^2 + \frac{\beta}{4}x^4 \ , \tag{280}$$

where $\beta > 0$. It has one minimum if $\alpha > 0$ and two minima if $\alpha < 0$. The corresponding force is

$$f(x) = -\alpha x - \beta x^3 \ . \tag{281}$$

The stationary solutions of (278) are the roots of the equation $f(x) = 0$ or the extremum points of the potential $\phi(x)$. They are given by

$$x(\alpha + \beta x^2) = 0 \, . \tag{282}$$

One root always is $x_0 = 0$. At $\alpha \geq 0$ this is the only real solution. At $\alpha < 0$, two other real solutions appear $x_{1,2} = \pm\sqrt{-\alpha/\beta}$ corresponding to two minima of the potential. The solution $x_0 = 0$ corresponds to the only minimum of the potential at $\alpha > 0$, which is changed to the maximum at $\alpha < 0$. Minimum of $\phi(x)$ always corresponds to a stable, whereas maximum to an unstable solution of (278), as it follows from the stability analysis considering small deviations from the extremum point. These solutions depending on the parameter α represent the so–called supercritical bifurcation diagram. It is called supercritical, since the stable branches merge continuously at the bifurcation point $\alpha = 0$.

A bifurcation diagram of an other kind emerges for the potential

$$\phi(x) = \frac{\alpha}{2} x^2 + \frac{\beta}{4} x^4 + \frac{\gamma}{6} x^6 \tag{283}$$

with $\beta < 0$ and $\gamma > 0$. It corresponds to

$$f(x) = -\alpha x - \beta x^3 - \gamma x^5 \, . \tag{284}$$

In this case the equation $f(x) = 0$ has five roots, some of which may be complex. One solution is $x_0 = 0$. The other four roots are given by

$$x_{1,2,3,4} = \pm \sqrt{-\frac{\beta}{2\gamma} \pm \sqrt{\left(\frac{\beta}{2\gamma}\right)^2 - \frac{\alpha}{\gamma}}} \, . \tag{285}$$

Only the real solutions have physical meaning. Besides, the solutions corresponding to the minima of the potential are stable, whereas those representing the maxima are unstable. At $\alpha > \beta^2/(4\gamma)$ the only real solution is $x_0 = 0$. All five solutions are real within $0 \leq \alpha \leq \beta^2/(4\gamma)$. Three of them, including $x_0 = 0$, are stable and correspond to three minima of $\phi(x)$. The other two roots represent two local maxima in between. At $\alpha = 0$, the minimum at $x = 0$ transforms into the maximum and two other maxima disappear. Thus, at $\alpha < 0$ there are two stable solutions and one unstable solution $x_0 = 0$. This is the corresponding so–called subcritical bifurcation diagram.

In distinction to the supercritical bifurcation diagram here the stable nonzero branches start at certain nonzero x values at $\alpha = \beta^2/(4\gamma)$, where the $x_0 = 0$ branch still is stable. Therefore the system cannot switch to these nonzero branches if the initial x value is near zero. In the deterministic dynamics it first happens with a jump only at $\alpha = 0$ if α is decreased. If α is increased, starting from negative values, then a jump from one of the nonzero stable solutions to the zero solution occurs at $\alpha = \beta^2/(4\gamma) > 0$. In other words, a hysteresis is observed.

The behavior of the dynamical system in the case of supercritical as well as subcritical bifurcation is essentially changed by the noise included in the Langevin equation (264). Due to the noise, the system with potential (280) can be randomly switched between two stable states $x_{1,2} = \pm\sqrt{-\alpha/\beta}$ at $\alpha < 0$, which is never possible in the deterministic dynamics. Similarly, in the system with potential (283), the noise enables a switching between three stable states within $0 \leq \alpha \leq \beta^2/(4\gamma)$, or between two stable branches of the bifurcation diagram at $\alpha < 0$. Considering an ensemble of different stochastic realizations of the process $\xi(t)$, the Langevin equation (264) allows to calculate the probability density $p(x,t)$ to have certain value of x at time t. The stationary probability density $p^{st}(x) = \lim_{t\to\infty} p(x,t)$ is given by the stationary solution of the corresponding Fokker–Planck equation (274), i. e.,

$$p^{st}(x) = \frac{e^{-2\phi(x)/\sigma^2}}{\int\limits_{-\infty}^{\infty} e^{-2\phi(x)/\sigma^2} dx} \, . \tag{286}$$

3.3 Brownian Motion in Three–Dimensional Velocity Space

Consider first a deterministic motion of a Brownian particle with initial velocity $\mathbf{v}(t=0) = \mathbf{v}_0$ in a medium (liquid) with friction. Here velocity is a three–dimensional vector. Its time evolution is described by the equation

$$\frac{d\mathbf{v}(t)}{dt} = -\gamma \mathbf{v}(t) \, , \tag{287}$$

where γ is the friction coefficient. The solution reads

$$\mathbf{v}(t) = \mathbf{v}_0 e^{-\gamma t} \, . \tag{288}$$

Thus, in this simple model the particle reduces asymptotically its velocity to zero due to the friction. This equation, however, does not completely describe the motion of a particle in liquid. One needs to take into account the randomness caused by stochastic collisions with liquid molecules, which never allow to relax the velocity to zero. This effect is described by the Langevin equation

$$\frac{d\mathbf{v}(t)}{dt} = -\gamma \mathbf{v}(t) + \sqrt{2B}\,\xi(t) \;, \tag{289}$$

where (287) is completed by a stochastic (Langevin) force $\sqrt{2B}\,\xi(t)$. Here B is the diffusion coefficient in the velocity space and $\xi(t)$ is a three–dimensional vector with components $\xi_i(t)$, representing a stochastic process. The actual Brownian motion in the space of velocity $\mathbf{v}$ and coordinate $\mathbf{x}$ is known as the Ornstein–Uhlenbeck process.

The stochastic force should have the following properties.

1. Each component of the stochastic force has zero mean value

   $$\langle \xi_i(t) \rangle_{\mathbf{v}_0} = 0 \;, \tag{290}$$

   where the symbol $\mathbf{v}_0$ indicates that only those stochastic realizations are considered for which $\mathbf{v}(t=0) = \mathbf{v}_0$ holds. It means that the stochastic force has no influence on the averaged motion.

2. The Langevin force is the Gaussian stochastic process, which means that all higher order correlation functions reduce to the two–time correlation function $\langle \xi_i(t_1)\xi_j(t_2) \rangle_{\mathbf{v}_0}$ according to

   $$\langle \xi(t_1)\xi(t_2)\cdots\xi(t_{2n}) \rangle_{\mathbf{v}_0} = \sum_{\text{all pairings}} \langle \xi(t_i)\xi(t_j) \rangle_{\mathbf{v}_0} \cdots \langle \xi(t_k)\xi(t_l) \rangle_{\mathbf{v}_0} \;. \tag{291}$$

   Like the first moment (290), all odd–order moments are zero.

3. The $\langle \xi_i(t)\xi_j(t') \rangle_{\mathbf{v}_0}$ function is δ–correlated in time

   $$\langle \xi_i(t)\xi_j(t') \rangle_{\mathbf{v}_0} = \delta_{ij}\delta(t-t') \;. \tag{292}$$

   Besides, this formula implies that different components are uncorrelated or statistically independent.

4. The stochastic process for the velocity $\mathbf{v}(t)$ of the Brownian particle is statistically independent of the stochastic force $\sqrt{2B}\,\xi(t')$ for $t' > t$, i. e., $\mathbf{v}(t)$ at a given time moment is independent of the stochastic force in future:

   $$\langle \mathbf{v}(t)\xi(t') \rangle_{\mathbf{v}_0} = 0 \qquad \text{for} \quad t' > t \;. \tag{293}$$

   The velocity $\mathbf{v}(t)$, naturally, will be affected by $\xi(t')$ at $t' < t$.

In the following we consider two different ways to get the solution of the Langevin equation (289) – by direct integration. The direct integration yields a formal solution for each specific realization of the stochastic process $\xi(t)$,

$$\mathbf{v}(t) = \mathbf{v}_0 e^{-\gamma t} + e^{-\gamma t} \int_0^t e^{\gamma t'} \sqrt{2B}\, \xi(t')\, dt' \ , \tag{294}$$

as it can be verified by inserting (294) into (289). This solution allows us to calculate moments of the velocity distribution for the ensemble of all stochastic realizations with given initial velocity $\mathbf{v}_0$. The first moment is

$$\langle \mathbf{v}(t) \rangle_{\mathbf{v}_0} = \mathbf{v}_0 e^{-\gamma t} + e^{-\gamma t} \int_0^t e^{\gamma t'} \sqrt{2B}\, \langle \xi(t') \rangle_{\mathbf{v}_0} dt' \ . \tag{295}$$

The last term vanishes, since the Langevin force has zero mean value, as discussed above. Thus we have

$$\langle \mathbf{v}(t) \rangle_{\mathbf{v}_0} = \mathbf{v}_0 e^{-\gamma t} \ . \tag{296}$$

The correlation function $\langle \mathbf{v}(t)\mathbf{v}(t') \rangle_{\mathbf{v}_0}$ for velocities at different time moments also can be calculated in this way. Alternatively, the correlation function can be defined for deviations from the mean values as $\langle (\mathbf{v}(t) - \langle \mathbf{v}(t) \rangle)(\mathbf{v}(t') - \langle \mathbf{v}(t') \rangle) \rangle_{\mathbf{v}_0}$. Both definitions are equivalent for long times, where the mean velocity $\langle \mathbf{v}(t) \rangle_{\mathbf{v}_0}$ tends to zero. For definiteness we assume that $t' > t$ holds. Then for any velocity component we have

$$\begin{aligned}
\langle v_i(t) v_i(t') \rangle_{\mathbf{v}_0} &= v_{i,0}^2\, e^{-\gamma(t'+t)} + 2B e^{-\gamma(t'+t)} \int_0^t \int_0^{t'} e^{+\gamma(s'+s)} \langle \xi_i(s) \xi_i(s') \rangle ds ds' \\
&= v_{i,0}^2\, e^{-\gamma(t'+t)} + 2B e^{-\gamma(t'+t)} \int_0^t e^{\gamma(s+s)} ds \\
&= v_{i,0}^2\, e^{-\gamma(t'+t)} + \frac{B}{\gamma} \left(e^{-\gamma(t'-t)} - e^{-\gamma(t'+t)} \right) \ .
\end{aligned} \tag{297}$$

By using the definition of scalar product, the correlation function $\langle \mathbf{v}(t)\mathbf{v}(t') \rangle_{\mathbf{v}_0}$ is easily calculated from (297) as

$$\langle \mathbf{v}(t)\mathbf{v}(t') \rangle_{\mathbf{v}_0} = \sum_i \langle v_i(t) v_i(t') \rangle_{\mathbf{v}_0} \ . \tag{298}$$

The second moment for each velocity component is obtained from (297) by setting $t' = t$, i. e.,

$$\langle v_i^2(t)\rangle_{\mathbf{v}_0} = v_{i,0}^2\, e^{-2\gamma t} + \frac{B}{\gamma}\left(1 - e^{-2\gamma t}\right) \ . \tag{299}$$

Apart from the mean values, the probability density $p(v_x, v_y, v_z, t)$ in the three–dimensional velocity space also is of interest. Taking into account that the velocity components in (289) are not coupled, their probability distributions are independent, and we have

$$p(v_x, v_y, v_z, t) = p(v_x, t)\, p(v_y, t)\, p(v_z, t) \ , \tag{300}$$

where $p(v_x, t)$, $p(v_y, t)$, and $p(v_z, t)$ are the probability densities for one component. The latter ones can be calculated by solving the corresponding Fokker–Planck equation for one–dimensional problem. Here we only report the result

$$p(v_i, t) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} \exp\left[-\frac{(v_i - v_{i,0}\exp[-\gamma t])^2}{2\sigma^2(t)}\right] \ , \tag{301}$$

where $i = x, y, z$ denotes the i-th component of vector $\mathbf{v}$ and

$$\sigma^2(t) = \langle v_i^2\rangle - \langle v_i\rangle^2 = \frac{B}{\gamma}(1 - \exp[-2\gamma t]) \tag{302}$$

is the variance consistent with (296) and (299).

For large times t the initial state (velocity $\mathbf{v}_0$) is forgotten and the final equilibrium state is given by

$$\lim_{t\to\infty} \langle v_i^2(t)\rangle_{\mathbf{v}_0} = B/\gamma \ . \tag{303}$$

On the other hand, it is well known that

$$\langle v_i^2\rangle = \frac{k_B T}{m} \tag{304}$$

holds in the equilibrium of a classical system. Comparing (303) and (304) we arrive to the relation

$$\frac{B}{\gamma} = \frac{k_B T}{m} \tag{305}$$

known as the Einstein formula. It relates the macroscopic quantity (friction coefficient) γ, which describes the dissipation of the momentum, to the microscopic quantity (diffusion coefficient) B, which describes the stochastic force.

3.4 Stochastic Differential Equations

As a starting point we consider the one–dimensional stochastic differential equation for the variable x, which can be, e. g., the coordinate of a particle performing random walk in one dimension. The motion of particle is described by the stochastic differential equation (SDE)

$$dx(t) = a(x)\,dt + b_\eta(x)\,dW(t)\ , \tag{306}$$

where $a(x)$ and $b_\eta(x)$ are given functions of x, $dx(t) = x(t+dt) - x(t)$ is the increment of x in the time interval from t to $t+dt$, whereas $dW(t) = W(t+dt) - W(t)$ is the increment of the standard Wiener process having the properties $\langle dW(t)\rangle = 0$ and $\langle (dW(t))^2\rangle = dt$. Later on, the Wiener process will be discussed in detail. This equation (306), written in the form (262)

$$\frac{dx}{dt} = a(x) + b_\eta(x)\,\xi(t)\ , \tag{307}$$

is known as Langevin equation. The Langevin force, formally $\xi(t) = dW(t)/dt$, has to be understood as a fluctuating quantity having the Gaussian distribution

$$p(\xi(t)) = \sqrt{\frac{dt}{2\pi}}\exp\left[-\frac{dt}{2}\xi^2\right] \tag{308}$$

with $\langle\xi(t)\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = \delta(t-t')$. According to the formal substitution $\xi(t) = dW(t)/dt$ we should have the variance which diverges like $\langle\xi(t)^2\rangle = 1/dt \to \infty$ at $dt \to 0$. The above incorrect substitution $dW(t) = \xi(t)dt$ however represents only a formal way of writing and has no rigorous mathematical meaning, since stochastic trajectories are not differentiable.

An important peculiarity of the stochastic differential equations (306) and of the Langevin equation (307) is that their solution essentially depends on that how the coefficient $b_\eta(x)$ at the noise term is defined. Namely, it is important whether this coefficient is determined at $x = x(t)$, $x = x(t+dt)$, or at x in some intermediate time moment. The parameter η is introduced to distinguish between these cases. Different possibilities can be chosen according to

$$b_\eta(x) = b(x(t+\eta\,dt))\ . \tag{309}$$

The case $\eta = 0$, when the coefficient b is determined at the left border of the integration interval $[t, t+dt]$, is called Ito stochastic process. In the case of Stratonovich process, where $\eta = 1/2$, it is determined in the middle of the interval. Finally, if $b_\eta(x)$ is determined at the right border $t+dt$, which corresponds to $\eta = 1$, then we deal with Hänggi–Klimontovich process.

Alternatively, one can define the coefficient $b_{\eta'}(x)$ as

$$b_{\eta'}(x) = b((1-\eta')x(t)) + \eta'\, x(t+dt)) \; . \tag{310}$$

The two definitions (309) and (310) are identical at $\eta = \eta' = 0$ and $\eta = \eta' = 1$. For arbitrary stochastic trajectory $x(t)$, however, the relation between η and η' is different if $0 < \eta < 1$.

The solution of the stochastic differential equation of Ito type (Ito–SDE)

$$dx(t) = a[x(t)]dt + b[x(t)]dW(t) \tag{311}$$

is represented by the Ito stochastic integral

$$x(t) = x(t_0) + \int\limits_{t_0}^{t} a[x(t')]dt' + \int\limits_{t_0}^{t} b[x(t')]dW(t') \; . \tag{312}$$

Eq. (311) thus has unique solution (312) which is a Markov process.

The probability density $p(x,t)$ for finding the particle at a position x at time moment t is given by the Fokker–Planck equation with general η

$$\frac{\partial}{\partial t} p = \frac{\partial}{\partial x}\left\{ -a(x)p + \frac{1}{2} b(x)^{2\eta} \frac{\partial}{\partial x}\left[b(x)^{2(1-\eta)} p \right] \right\} \; . \tag{313}$$

The stationary solution of (313) reads

$$p_{st}(x) = \frac{C}{b(x)^{2(1-\eta)}} \exp\left[2 \int^{x} dy \frac{a(y)}{b(y)^2} \right] \tag{314}$$

with integration constant C given by the normalization condition $\int p_{st}(x)dx = 1$.

In the case of Ito stochastic calculus (integration at left border), the stochastic differential equation (311) in typical notations is written as

$$dx(t) = a(x)\, dt + b(x)\, dW(t) \; , \tag{315}$$

and the corresponding Fokker–Planck equation reads

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left\{ -a(x)p + \frac{1}{2}\frac{\partial}{\partial x}\left[b(x)^2 p \right] \right\} \tag{316}$$

$$= -\frac{\partial}{\partial x}\left[a(x)p \right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[b(x)^2 p \right] \; . \tag{317}$$

To distinguish from Ito–SDE, the Stratonovich–SDE (integration at middle) in these notations is written using special symbol $\circ$

$$dx(t) = a(x)\,dt + b(x) \circ dW(t)\ . \tag{318}$$

The corresponding Fokker–Planck equation is

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left\{ -a(x)p + \frac{1}{2} b(x) \frac{\partial}{\partial x} \left[b(x)p \right] \right\}\ . \tag{319}$$

One has to take into account that deviations from the usual differentiation rules take place at $\eta \neq 1/2$. It is important when making a transformation of variable $y = g(x) \Longleftrightarrow x = g^{-1}(y)$. The transformed Langevin equation then reads

$$\frac{dy}{dt} = \tilde{a}(y) + \tilde{b}_\eta(y)\,\xi(t) \tag{320}$$

or

$$dy = \tilde{a}(y)\,dt + \tilde{b}_\eta(y)\,dW(t) \tag{321}$$

with coefficients

$$\tilde{a}(y) = g'(x)\,a(x) + \left(\frac{1}{2} - \eta \right) g''(x)\,b(x)^2\ , \tag{322}$$

$$\tilde{b}(y) = g'(x)\,b(x)\ , \tag{323}$$

where $g' = dg/dx$.

3.5 Arithmetic Brownian Motion

The standard Brownian motion is defined as constant drift function together with white noise already known from the Wiener process

$$dx(t) = a\,dt + b\,dW(t) \tag{324}$$

together with following initial conditions $x(t=0) = x_0$ and $W(t=0) = 0$.

Simple integration gives the solution

$$x(t) = x_0 + at + b\,W(t)\ . \tag{325}$$

The probability distribution function thus is Gaussian, i. e.,

$$p(x,t) = \frac{1}{\sqrt{2\pi b^2 t}} \exp\left(-\frac{(x - x_0 - at)^2}{2b^2 t} \right)\ . \tag{326}$$

It is a solution of the Fokker–Planck equation (313) with $\eta = 0$

$$\frac{\partial}{\partial t} p(x,t) = -a \frac{\partial}{\partial x} p(x,t) + \frac{b^2}{2} \frac{\partial^2}{\partial x^2} p(x,t) \; . \tag{327}$$

From (326) we obtain directly the first two moments

$$\langle x(t) \rangle = x_0 + at \tag{328}$$
$$\langle x(t)^2 \rangle = \langle x(t) \rangle^2 + b^2 t \; . \tag{329}$$

3.6 Geometric Brownian Motion

The stochastic differential equation with linear drift and multiplicative noise term is called geometric Brownian motion. It has a wide applicability in financial modelling and is given in Ito notation by

$$dx(t) = a\,x(t)\,dt + b\,x(t)\,dW(t) \tag{330}$$

with typical initial conditions $x(t=0) = x_0 > 0$ and $W(t=0) = 0$. It is a special case of the Ito–SDE (315) with $a(x) = ax$ and $b(x) = bx$.

In the following we will use the transformation

$$y(x) = \ln\left(\frac{x}{x_0}\right) \; , \tag{331}$$

where $x_0 = x(t=0)$. According to (321) we have

$$dy(t) = \tilde{a}(y)\,dt + \tilde{b}(y)\,dW \tag{332}$$

with

$$\tilde{a}(y) = \frac{dy}{dx}\,a(x) + \frac{1}{2}\frac{d^2y}{dx^2}\,b(x)^2 \tag{333}$$
$$\tilde{b}(y) = \frac{dy}{dx}\,b(x) \; . \tag{334}$$

Here

$$y' \equiv \frac{dy}{dx} = \frac{x_0}{x}\frac{1}{x_0} = \frac{1}{x} \; ; \quad y'' = -\frac{1}{x^2} \; ,$$

and hence we have $\tilde{a}(y) = a - b^2/2$ and $\tilde{b}(y) = b$. Consequently, the stochastic differential equation for the transformed variable $y(t)$ reads

$$dy(t) = d\ln x(t) = \left(a - \frac{b^2}{2}\right) dt + b\,dW(t) \; , \tag{335}$$

Integrating both sides the solution results in

$$x(t) = x_0 \exp\left\{\left(a - \frac{b^2}{2}\right) t + b\,W(t)\right\} \tag{336}$$

The probability density for the variable $y(t)$ is given by the Gaussian distribution

$$\tilde{p}(y,t) = \frac{1}{\sqrt{2\pi\, b^2 t}} \exp\left[-\frac{\left(y - (a - b^2/2)t\right)^2}{2b^2 t}\right] \; . \tag{337}$$

The probability distribution $p(x,t)$ for the original variable is easily calculated according to

$$p(x,t) = \tilde{p}(y,t)\,\frac{dy}{dx} = \frac{1}{x}\,\tilde{p}(\ln[x/x_0],t) \; . \tag{338}$$

It yields the log–normal distribution

$$p(x,t) = \frac{1}{\sqrt{2\pi\, b^2 t}}\,\frac{1}{x}\,\exp\left[-\frac{\left(\ln[x/x_0] - (a - b^2/2)t\right)^2}{2b^2 t}\right] \; . \tag{339}$$

This distribution is a solution of the following Fokker–Planck equation

$$\begin{aligned} \frac{\partial}{\partial t} p(x,t) &= -\frac{\partial}{\partial x}[ax\,p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[b^2 x^2\, p(x,t)\right] \\ &= \left(b^2 - a\right)\, p + \left(2b^2 - a\right) x \frac{\partial p}{\partial x} + \frac{1}{2}(bx)^2 \frac{\partial^2 p}{\partial x^2} \; . \end{aligned} \tag{340}$$

The mean value (first moment) of (339) is calculated as follows

$$\begin{aligned} \langle x(t)\rangle &= \int_0^\infty x p(x,t)\,dx = \int_0^\infty x\tilde{p}(y,t)\frac{dy}{dx}\,dx = x_0 \int_{-\infty}^{\infty} e^y \tilde{p}(y,t)dy \\ &= \frac{x_0}{\sqrt{2\pi b^2 t}} \int_{-\infty}^{\infty} \exp\left(y - \frac{\left(y - [a - b^2/2]\,t\right)^2}{2b^2 t}\right) dy \\ &= \frac{x_0 e^{at}}{\sqrt{2\pi b^2 t}} \int_{-\infty}^{\infty} \exp\left(-\frac{\left(y - [a + b^2/2]\,t\right)^2}{2b^2 t}\right) dy \\ &= x_0 e^{at} \frac{1}{\sqrt{2\pi b^2 t}} \int_{-\infty}^{\infty} \exp\left(-\frac{z^2}{2b^2 t}\right) dz = x_0 e^{at} \; . \end{aligned} \tag{341}$$

It increases exponentially

$$\langle x(t) \rangle = x_0 \, e^{a\,t} \; . \tag{342}$$

The mean square value (second moment) is calculated in a similar way

$$\begin{aligned}
\langle x(t)^2 \rangle &= \int\limits_0^\infty x^2 p(x,t)\,dx = \int\limits_0^\infty x^2 \tilde{p}(y,t)\frac{dy}{dx}\,dx = x_0^2 \int\limits_{-\infty}^\infty e^{2y}\tilde{p}(y,t)dy \\
&= \frac{x_0^2}{\sqrt{2\pi b^2 t}} \int\limits_{-\infty}^\infty \exp\left(2y - \frac{\left(y - [a - b^2/2]\,t\right)^2}{2b^2 t}\right) dy \\
&= \frac{x_0^2 e^{\left(2a+b^2\right)t}}{\sqrt{2\pi b^2 t}} \int\limits_{-\infty}^\infty \exp\left(-\frac{\left(y - [a + 3b^2/2]\,t\right)^2}{2b^2 t}\right) dy \\
&= \frac{x_0^2 e^{\left(2a+b^2\right)t}}{\sqrt{2\pi b^2 t}} \int\limits_{-\infty}^\infty \exp\left(-\frac{z^2}{2b^2 t}\right) dz = x_0^2 e^{\left(2a+b^2\right)t} \; .
\end{aligned} \tag{343}$$

Thus we have

$$\langle x(t)^2 \rangle = x_0^2 \, e^{2\left(a + b^2/2\right)\,t} \tag{344}$$

giving the variance .

$$\langle x(t)^2 \rangle - \langle x(t) \rangle^2 \; = x_0^2 \, e^{2a\,t} \left[e^{b^2 t} - 1 \right] \; . \tag{345}$$

Typical stochastic trajectories show exponential growth in time. It agrees with the formulas (342) and (345).

3.7 Fourier Analysis

The Fourier or spectral analysis is a powerful tool to analyze the solution of the Langevin equation.As an example, here we apply the spectral analysis to the time evolution of a vector $\mathbf{v}(t)$. In particular, $\mathbf{v}(t)$ can be the velocity of a Brownian particle moving in three–dimensional space. Its Fourier representation as infinite sum reads

$$\mathbf{v}(t) = \mathbf{v}(t+T) = \sum_{k=-\infty}^\infty \mathbf{a}_k \cos\left(\frac{2\pi k t}{T}\right) + \sum_{k=-\infty}^\infty \mathbf{b}_k \sin\left(\frac{2\pi k t}{T}\right) \; . \tag{346}$$

Here $\mathbf{a}_k$ and $\mathbf{b}_k$ are the Fourier coefficients given by

$$\mathbf{a}_k = \frac{1}{T}\int\limits_0^T \mathbf{v}(t)\cos\left(\frac{2\pi k t}{T}\right) dt \tag{347}$$

$$\mathbf{b}_k = \frac{1}{T}\int\limits_0^T \mathbf{v}(t)\sin\left(\frac{2\pi k t}{T}\right) dt \ . \tag{348}$$

Using the well known Euler formulas

$$e^{ix} = \cos(x) + i\sin(x) \ , \tag{349}$$

and

$$\cos(x) = \frac{e^{ix}+e^{-ix}}{2} \ , \qquad \sin(x) = \frac{e^{ix}-e^{-ix}}{2i} \ , \tag{350}$$

the transformation (346) can be represented by complex Fourier amplitudes $\tilde{\mathbf{v}}(\omega)$ as follows

$$\mathbf{v}(t) = \mathbf{v}(t+T) = \frac{1}{T}\sum_{\omega} \tilde{\mathbf{v}}(\omega) e^{i\omega t} \ , \tag{351}$$

where the summation runs over a set of discrete frequencies $\omega = 2\pi k/T$ with $k = 0, \pm1, \pm2, \ldots$. The inverse transformation reads

$$\tilde{\mathbf{v}}(\omega) = \int\limits_0^T \mathbf{v}(t) e^{-i\omega t} dt \ . \tag{352}$$

Eq. (351) can be viewed as an expansion in the basis of orthogonal wave functions $e^{i\omega t}$, which satisfy the periodic boundary conditions and has the orthogonality property

$$\frac{1}{T}\int\limits_0^T e^{i\omega t} e^{-i\omega' t} dt = \delta_{\omega,\omega'} \ . \tag{353}$$

Note that the term $\omega = 0$ in (351) represents the constant, i. e., time–independent contribution. If in general $\lim_{T\to\infty}\langle \mathbf{v}(t)\rangle$ is a constant, it is just $\tilde{\mathbf{v}}(0)/T$. In this case we have

$$\mathbf{v}(t) - \langle \mathbf{v} \rangle = \frac{1}{T}\sum_{\omega\neq 0} \tilde{\mathbf{v}}(\omega) e^{i\omega t} \ . \tag{354}$$

If the period T tends to infinity ($T \to \infty$), the discrete sum over $\omega \neq 0$ may be replaced by an integral. This substitution in (354) yields

$$\mathbf{v}(t) - \langle \mathbf{v} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\mathbf{v}}(\omega) e^{i\omega t} d\omega \; . \tag{355}$$

As a simple example, where the Fourier or spectral density $S(\omega)$ can be easily calculated, we consider an exponentially decaying function

$$\varphi(t) = A e^{-|t|/\tau} \; . \tag{356}$$

The spectral density is

$$\begin{aligned} S(\omega) &= \int_{-\infty}^{\infty} \varphi(t) e^{-i\omega t} dt = \int_{-\infty}^{\infty} A e^{-|t|/\tau} e^{-i\omega t} dt \\ &= A \left[\int_{-\infty}^{0} e^{(1-i\omega\tau)t/\tau} dt + \int_{0}^{\infty} e^{-(1+i\omega\tau)t/\tau} dt \right] \\ &= A \left[\frac{\tau}{1 - i\omega\tau} + \frac{\tau}{1 + i\omega\tau} \right] = \frac{2A\tau}{1 + (\omega\tau)^2} \end{aligned} \tag{357}$$

In the limit $\tau \to 0$ and $A \to \infty$ at a constant $A\tau$, the function (356) is proportional to the delta function. It corresponds to the white noise. According to (357), the Fourier spectrum of the white noise, obtained in this limit, is independent of the frequency ω. In other words, like the white light, it contains the whole uniform spectrum of frequencies. At a finite value of the parameter τ, which can be interpreted as a correlation time, the Fourier spectrum has a smooth cut-off at $\omega \approx 1/\tau$. Such a spectrum corresponds to colored noise.