Stochastik II
für Lehrämter und Physiker

PD Dr. Reinhard Mahnke

Lehrveranstaltung Nr. 11572
(2 SWS V + 2 SWS Ü)

Montag 15.00 bis 16.30 Uhr, Seminarraum R306
Mittwoch 7.30 bis 9.00 Uhr, Seminarraum R306
Institut für Physik, Universitätsplatz 1
Sommersemester 2009

About the contents:

1. **Basic concepts of deterministic dynamics**
(06.04.2009, R. Mahnke)
Defining dynamical system by n-dimensional state space (or phase space) and a mapping including set of control parameters as causal relationship. Time-discrete dynamics as iterated maps; time-continuous dynamics as coupled set of ordinary differential equations, always together with initial conditions. Dynamical system has unique solution called trajectory. Topological consequences like expanding/contracting or conservative dynamics are investigated within the so-called *qualitative theory of dynamical system*. Important classes are: Gradient system, canonical-dissipative system. Stability of regular or irregular (chaotic) motion measured by Ljapunov exponents.

2. **Qualitative theory of dynamical systems** (08.04.2009, R. Mahnke)
Recalling the definition of a dynamical system (x, T) consisting of an n–dimensional state space x and a nonlinear discrete or continuous

mapping T together with initial conditions. Examples are iterations, Newtonian dynamics, Hamiltonian canonical equations, overdamped motion in a potential field, etc. Key words in the *qualitative theory* (in distinction to the exact trajectory solution) are: stationary or steady state solutions (fixed point, periodic orbit), separatrix, saddle point, region of attraction, linear stability analysis (with respect to small changes), Ljapunov exponents, chaotic attractor, ...

3. **Double well potential** (15.04.2009, R. Mahnke)
The following examples of low–dimensional dynamical systems are discussed with respect to the motion of a particle in a single or double well potential. Without noise the motion is deterministic starting from given initial condition and evolving in time regular (periodic or quasi–periodic) or irregular (chaotic).

    (a) Mathematical pendulum

$$\frac{d}{dt}\alpha = \frac{p_\alpha}{ml^2} \tag{1}$$
$$\frac{d}{dt}p_\alpha = -mgl\sin\alpha \tag{2}$$

    (b) Chairoplane

$$\frac{d}{dt}\alpha = \frac{p_\alpha}{ml^2} \tag{3}$$
$$\frac{d}{dt}p_\alpha = ml^2\omega_0^2[-\sin\alpha + \Omega(A+\sin\alpha)\cos\alpha] \tag{4}$$

    (c) Van der Pol oscillator

$$\frac{d}{dt}x = x - y - x(x^2+y^2) \tag{5}$$
$$\frac{d}{dt}y = x + y - y(x^2+y^2) \tag{6}$$

    (d) Predator–prey dynamics, Lotka–Volterra system

$$\frac{d}{dt}x = k_1Ax - k_{12}xy \tag{7}$$
$$\frac{d}{dt}y = k_{21}xy - k_2y \tag{8}$$

4. **Stochastic Markovian process** (20.04.2009, R. Mahnke)
A stochastic process describes the temporal evolution of random events by probability distributions. A stochastic trajectory as a time series (sequence of states and times) is called a realization. After introduction of joint probability densities (jpd) and conditional probability densities (cpd) and their relationship the two time moments correlated Markov process has been discussed. In contract to factorization of temporally uncorrelated processes the Markovian dynamics is given by the *Chapman–Kolmogorov integral equation* which can be written in the short time limit as differential equation named *master equation*.

5. **Stochastic master equation I** (22.04.2009, R. Mahnke)
Doing a short time series expansion for the conditional probability and introducing the transition rates as new quantities the master equation as differential equation is derived out of the Chapman–Kolmogorov equation. The master equation as general, fundamental or basic equation has the meaning of a balance equation for the probability density.

6. **Stochastic master equation II** (27.04.2009, R. Mahnke)
Discussion of master equation for continuous and for discrete stochastic variables including its stationary and equilibrium solution. Representation of master equation in matrix form and its formal solution, finding the solution as a superposition of eigenfunctions. As an example the one–step master equation with given transition rates is stated.

7. **Examples of deterministic and stochastic models** (29.04.2009, R. Mahnke)
The following home works (please make at least two choices) should be performed (till 06.05.2009):

   (a) Consider the very important example of nonlinear physics: The Mathematical Pendulum (see above). Investigate the phase space portrait $p_\alpha = p_\alpha(\alpha)$ in general and the motion on the separatrix (border between bounded and unbounded motion) in detail.

   (b) What is a limit cycle? Investigate the given Van der Pol oscillator (see above) analytically. Explain the flow in state space by showing several trajectories. Hint: Transformation to polar coordinates.

   (c) Recall the discrete one–step master equation. Consider the decay process with a backward transition rate $w_-(n)$ only, at first given by a constant escape rate $1/\tau$ independent of the size n. This sometimes called Poisson process starts at n_0 and ends at $n = 0$.

Solve the set of master equations including boundaries and initial condition.

(d) By analogy with the Poisson process, solve the master equation for the (radioactive) decay process with $w_-(n) = 1/\tau(n) = n/\tau_0$. With the given initial condition $p(n, t = 0) = \delta_{n,n_0}$ find the analytical time–dependent solution $p(n, t)$ for $n \geq 0$.

8. **Home work** (04.05.2009)

9. **Seminar about home works** (06.05.2009, R. Mahnke)
The following exercises have been discussed:

(a) Task: Mathematical pendulum
Consider the very important example of nonlinear physics called mathematical pendulum. Investigate the phase space portrait $p_\alpha = p_\alpha(\alpha)$ in general and the motion on the separatrix (border between bounded and unbounded motion) in detail.
Solution:
Nonlinear regular dynamics of mathematical pendulum (see 1, 2) is given by

$$H(\alpha, p_\alpha) = \frac{p_\alpha^2}{2ml^2} + mgl(1 - \cos\alpha) = E \tag{9}$$

$$\dot{\alpha} = \frac{p_\alpha}{ml^2} \tag{10}$$

$$\dot{p}_\alpha = -mgl\sin\alpha \tag{11}$$

together with initial conditions. Use: $\omega_0^2 = g/l$; $a^2 = E/(2ml^2\omega_0^2)$ and $\sin^2\beta = (1 - \cos 2\beta)/2$.
Result: Trajectory (depending on parameter energy a)

$$p_\alpha(\alpha; a) = \pm 2ml^2\omega_0 a\sqrt{1 - \frac{1}{a^2}\sin^2\frac{\alpha}{2}} \tag{12}$$

Discussion of phase space portrait; dynamics of different types (vibration, rotation); integrable motion on separatrix (sx) as function of coordinate over time $\alpha_{sx} = \alpha_{sx}(t)$ with
$\alpha_{sx}(t) = 4\arctan[\exp(\pm\omega t)] - \pi$.
See also: Result by Martin Lahrz

(b) Task: Limit cycle behavior

(c) Task: Vehicular car cluster decay

Recall the discrete one–step master equation. Consider the decay process with a backward transition rate $w_-(n)$ only, at first given by a constant escape rate $1/\tau$ independent of the size n. This sometimes called Poisson process starts at n_0 and ends at $n = 0$. Solve the set of master equations including boundaries and initial condition.

Solution:

Stochastic dynamics of dissolution of traffic jam is given by

$$\frac{\partial}{\partial t} p(n_0, t) = -\frac{1}{\tau}\, p(n_0, t) \ , \tag{13}$$

$$\frac{\partial}{\partial t} p(n, t) = \frac{1}{\tau}\, [p(n+1, t) - p(n, t)] \ , \qquad n_0 - 1 \geq n > 0 \ , \tag{14}$$

$$\frac{\partial}{\partial t} p(0, t) = \frac{1}{\tau}\, p(1, t) \tag{15}$$

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.

The general solution of the probability $p(n, t)$ to observe a car cluster of size n at time t is

$$p(n, t) = \frac{(t/\tau)^{n_0 - n}}{(n_0 - n)!}\, e^{-t/\tau} \ , \qquad 0 < n \leq n_0 \ , \tag{16}$$

$$p(0, t) = 1 - \sum_{m=0}^{n_0 - 1} \frac{(t/\tau)^m}{m!}\, e^{-t/\tau} \ . \tag{17}$$

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

$$\langle n \rangle(t) \equiv \sum_{n=0}^{n_0} n\, p(n, t) = \sum_{n=1}^{n_0} n\, p(n, t) \tag{18}$$

and can be calculated using the known probabilities (16) to get the exact result

$$\langle n \rangle(t) = n_0\, Q(n_0 - 1, t) - \frac{t}{\tau}\, Q(n_0 - 2, t) \tag{19}$$

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

$$Q(n, t) \stackrel{\text{def}}{=} e^{-t/\tau} \sum_{m=0}^{n} \frac{(t/\tau)^m}{m!} \ . \tag{20}$$

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

$$\langle\langle n \rangle\rangle = \langle (n - \langle n \rangle)^2 \rangle = \langle n^2 \rangle - \langle n \rangle^2 \tag{21}$$

and can be also calculated as follows

$$\begin{aligned}\langle\langle n \rangle\rangle(t) = n_0 \left[n_0 \, Q(n_0 - 1, t) - \frac{2t}{\tau} Q(n_0 - 2, t) \right] (1 - Q(n_0 - 1, t)) \\ + \left(\frac{t}{\tau} \right)^2 \left[Q(n_0 - 3, t) - Q^2(n_0 - 2, t) \right] + \frac{t}{\tau} Q(n_0 - 2, t) \ .\end{aligned} \tag{22}$$

In some approximation, where we set $Q(n,t)$ (20) to one, the mean value (19) reduces to a linearly decreasing function in time

$$\langle n \rangle(t) \approx n_0 - t/\tau \ , \tag{23}$$

whereas the variance (22) to a linearly increasing behavior

$$\langle\langle n \rangle\rangle(t) \approx t/\tau \ . \tag{24}$$

In the case of linear mean value approximation (23) the time required, that the jam dissolves totally, is given by

$$t_{\text{end}} = n_0 \tau \ . \tag{25}$$

See also: Result by Martin Lahrz

(d) Task: Molecular cluster decay (or radioactive decay)

10. **Car cluster formation on roads** (11.05.2009, R. Mahnke)
Starting to explain the deterministic car–following theory in general and the optimal velocity model (OVM) in detail. Discussing the steady state solution called free flow with homogeneous distribution of headways and velocities. After reaching a critical vehicular density the steady state solution (fixed point) becomes unstable and a limit cycle appears called congested or stop–and–go traffic. Having OVM in mind the stochastic cluster formation on roads is discussed as a one–step process (only one car is reaching or leaving the jam). Using a well–explained ansatz for the optimal velocity function the transition rates for the master equation are formulated.

11. **Traffic breakdown** (13.05.2009, R. Mahnke)
Defining a particular size of congestion (escape value) and using a particular initial situation (no jam) the time necessary to reach the escape value for the first time gives the breakdown event from free flow to congested traffic. How to calculate the traffic breakdown probability? Based on master equation dynamics the initial and boundary value problem in a finite interval with one reflecting and one absorbing (or open) boundary is introduced schematically. The outflow distribution at open boundary has to be calculated. Discussion of outflow function (probability per time) at absorbing boundary as well as the cumulative function within an given observation time interval.

12. **Fokker–Planck equation I** (18.05.2009, R. Mahnke)
One of the fundamental dynamical expressions for Markovian processes is the Fokker–Planck equation (FPE) in its forward and backward notation. Discussing the multi–dimensional forward FPE written as continuity equation and the corresponding backward FPE together with the same delta–like initial condition in both cases. Taking into account borders we consider the one–dimensional bounded drift–diffusion problem in a finite interval with a reflecting (left) and an absorbing (right) wall and state that both Fokker–Planck dynamics with the corresponding boundary conditions are equivalent and give the same result.

13. **Fokker–Planck equation II** (20.05.2009, R. Mahnke)
We consider the typical one–dimensional exit problem of a Brownian particle (drift–diffusion dynamics) from a bounded domain, whose boundary is usually reflecting except for an absorbing window. The escape problem and its solution is given by the outflow function as first passage time probability density. The first moment is called mean first passage time (MFPT) whereas the inverse is known as escape or breakdown rate. The MFPT tells us how long does it take in the average to move from the initial value inside the interval to the right open boundary taking into account the left reflecting wall. The result for the dynamics with constant drift as well as constant diffusion is shown graphically.

    The following home work should be performed (till 27.05.2009):

    (e) Calculate the time dependent outflow probabilty density $\mathcal{P}(t)$ at the right border $x = b$ as first–passage time problem for a pure diffusion process starting at x_0.
    Hint: See Chapter 6 (One–dimensional diffusion) in R. Mahnke et al, Physics of Stochastic Processes, Wiley, 2009.

14. **Ornstein–Uhlenbeck process I** (25.05.2009, R. Mahnke)
Stochastic process including friction in velocity space coupled to position space, based on stochastic differential equations the corresponding Fokker–Planck equation for two–dimensional probability density serves as starting point with delta–like initial distribution, solution by Fourier transformation, discussion of general solution (graphically, see below) as well as special cases (analytically), especially the well–known stationary Maxwell–Boltzmann velocity distribution of an ideal gas

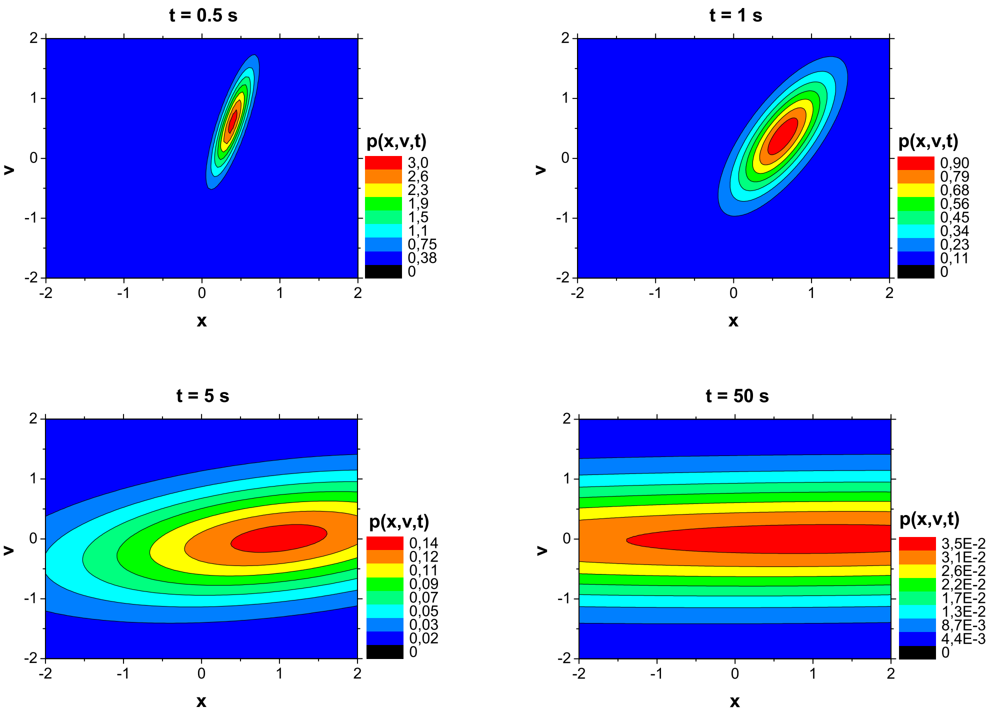

Abbildung 1: Darstellung der Wahrscheinlichkeitsdichteverteilung $p(x, v, t)$ aus der Lösung der Fokker–Planck Gleichung für vier verschiedene Zeitpunkte $t = 0.5\,s$ (links oben), $t = 1\,s$ (rechts oben), $t = 5\,s$ (links unten) und $t = 50\,s$ (rechts unten). Die gewählten Parameter sind $B = 0.5\,m^2/s^3$ und $\gamma = 1\,s^{-1}$. Die Anfangsbedingungen sind $x_0 = 0\,m$ und $v_0 = 1\,m/s$.

15. **Project works** (27.05.2009, R. Mahnke)
Given tasks to solve as project at home:

P1 **Deterministic vs molecular chaos** → Yeong Zen Chua
What is deterministic chaos? Compare regular and chaotic motion. Take a low–dimensional dynamical system as example (from literature, e.g. food chain or coupled resonators) to explain the chaotic attractor and its properties.
What is randomness? Are there true random (or stochastic) events in nature? Give examples for molecular chaos like heat and diffusion. Is quantum physics a probabilistic theory? Make a relationship to thermodynamics and the arrow of time as development into equilibrium (chaos) or out of equilibrium into nonequilibrium (selforganisation).
Please comment this paradox: Although a computer is a deterministic machine, it is possible to create good random numbers with it.

See e. g.: P. Coles, *From Cosmos to Chaos*, Oxford Univ. Press, 2006.

P2 **Jam or cluster dissolution: Breakdown rate** → Anna Wiktoria Oniszczuk
Take a one–step master equation with detachment terms only. Investigate this stochastic dissolution process analytically, starting from a given (large) size $n(t = 0) = n_0 > 0$, within two different models: (i) car cluster decay with constant transition rate $1/\tau$ and (ii) molecular or atomic decay process with linear transition rate αn. Define your system as open or closed depending on the property at the border $n = 0$ (absorbing or reflecting boundary).

P3 **Solution of Master equation by simulation technique** → Hannes Sobottka
Get knowledge about numerical method(s) how to solve the one–step master equation. Use the stochastic time step variant explained in literature.

Take the well–defined decay process and make a comparison between the analytical solution obtained by direct integration and your simulation results.

Show stochastic trajectories as well as probability distributions.

See: J. Honerkamp, *Stochastische Dynamische Systeme*, VCH, 1990 (Chap. 6)

P4 **Fokker–Planck equation with linear drift** → Lennart Seiffert
Study of Fokker–Planck dynamics $p(x,t)$ with known drift $f(x) = -\alpha x - \beta x^3$ given by

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[f(x)p(x,t)\right] + D\frac{\partial^2 p(x,t)}{\partial x^2} \; ; \; p(x,t=0) = \delta(x-x_0) \tag{26}$$

with natural boundary conditions.

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

$$V(x) = -\int f(x)\,dx \qquad \Longleftrightarrow \qquad f(x) = -\frac{dV(x)}{dx} \tag{27}$$

Only the case $\beta = 0$ has an analytical solution (similar, but different, to quantum harmonic oscillator). At first try to get the stationary solution, later the time–dependent result as superposition using a Schrödinger–like equation.

P5 **Vehicular motion and energy balance** → Martin Lahrz
Repeat the deterministic *optimal velocity model* (OVM) as particular follow–the–leader model with asymmetric interaction to the next car (particle) ahead. Use well–defined variables and control parameters (not dimensionless) and connect OVM to the stochastic description via one–step master equation. Make a relationship to a particle chain with symmetric interaction.

Investigate the energy balance in detail as precise as possible (e. g. perform numerical simulations).

Before considering the many–particle system start your energy flow analysis with the one–particle case. Having in mind (from textbooks) the one–particle Newton's equation

$$m\frac{dv}{dt} = F_{cons}(x) + F_{diss}(v) \qquad ; \qquad \frac{dx}{dt} = v \tag{28}$$

the energy balance out of the given dynamics (28) reads

$$\frac{d}{dt}\left(E_{kin} + E_{pot}\right) + \Phi = 0 \tag{29}$$

with $E_{kin} = mv^2/2$ as kinetic energy, $E_{pot} = -\int F_{cons}(x)\,dx$ as potential energy and flux term $\Phi = -v\,F_{diss}(v)$ as transformation rate (dissipation or creation) of mechanical energy.

See Chap. 10 (Vehicular Traffic) in *Physics of Stochastic Processes* by R. Mahnke et al., Wiley, 2009.

P6 **Vehicular motion and traffic breakdown** → Andreas Becker
Repeat the definition of a breakdown within a stochastic description as first–passage time phenomenon. Take the stochastic model of vehicular traffic with given attachment and detachment rates and explain the phase transition from free flow to congested traffic. Define the lower and upper boundary precisely. How to get (numerical) results for the outflow probability density and/or cumulative breakdown probability within a fixed observation time?

Make a comparison to laminar and tubulent flow in a pipe.

See Chap. 10 (Vehicular Traffic) in *Physics of Stochastic Processes* by R. Mahnke et al., Wiley, 2009.
See B. Hof et al.: Repeller or attractor? Selecting the dynamical model for the onset of turbulence in pipe flow, Phys. Rev. Lett. (PRL) 101, 214501 (2008)

P7 **Logistic mapping** → Markus Kersten
Consider the following iteration ($n = 0, 1, 2, \ldots$)

$$x_{n+1} = r x_n (1 - x_n) \tag{30}$$

starting at $x_0 \in (0, 1)$, including a control parameter r with $0 < r \leq 4$, in detail. Explain the Feigenbaum diagram.

P8 **Stochastic Brusselator** → Merten Siegfried
Start a project called stochastic Brusselator (named after city Brussels, where this model has been first discussed by Ilya Prigogine et al.). The model deals with certain idealized autocatalytic reactions. In general, these are chemical reactions in which at least one of the products is also a reactant. We consider the following example

$$R_1 \stackrel{k_1}{\to} X \ ; \ R_2 + X \stackrel{k_2}{\to} Y + F_1 \ ; \ 2X + Y \stackrel{k_3}{\to} 3X \ ; \ X \stackrel{k_4}{\to} F_2 \ ,$$

where k_1, k_2, k_3, k_4 are reaction constants; R_1 and R_2 are the raw substances; F_1 and F_2 are final products of the reaction; whereas X and Y are intermediate substances which are of particular interest. Let us denote the concentrations of R_1 and R_2 by r_1 and r_2, whereas those of X and Y — by x and y. In the following it is assumed that the concentrations of raw substances are so large that their depletion during a considered time of reaction can be neglected, i. e., r_1 and r_2 are constants. We thus are interested only in the temporal variation of the concentrations x and y, which are described by the system of two coupled differential equations

$$\frac{dx}{dt} = k_1 r_1 - k_2 r_2\, x + k_3\, x^2 y - k_4\, x \tag{31}$$
$$\frac{dy}{dt} = k_2 r_2\, x - k_3\, x^2 y\ . \tag{32}$$

One task is to find the fixed–point stationary solution of (31) – (32), determine the region of its stability depending on the parameters of the model, as well as analyze numerically the solution in the region, where the fixed point is unstable.

Another task is to construct the master equation for the corresponding stochastic model, where $p(N_x, N_y, t)$ is the probability to find the system in a state with N_x molecules of substance X and N_y molecules of substance Y at time t.

Hint: consider a finite volume V, where $x = N_x/V$ and $y = N_y/V$; estimate the transition rates using the mean–field concentration product ansatz multiplied with the reaction constant.

P9 **Drift and diffusion** → Alexander Schmidt

a.) Discrete Markov chain:

Study the stochastic motion by discrete probabilistic jumps on an (asymmetrically) Galton board named after *Sir Francis Galton.*

Entwickeln Sie die diskrete Beschreibung der Zufallsbewegung einer Kugel, die durch ein Galton–Brett fällt. Die elementaren Hüpfwahrscheinlickeiten p und $q = 1-p$ seien durch die Geometrie des Galtonschen Glückspielautomaten gegeben. Betrachen Sie auch die beiden Spezialfälle $p = q = 1/2$ (Symmetrie, reine Diffusion) und $p = 0$ bzw. $p = 1$ (totale Asymmetrie, reine Drift).

b.) From discrte hopping to continuous limit:

Lassen Sie sowohl die Hüpfzeit τ als auch die Sprungweite a gegen Null gehen. Führen Sie bei diesem Grenzprozess zwei neue endliche Parameter D (Diffusionskoeffizient) und v (Driftkoeffizient) ein. Berechnen Sie in dieser Kontinuumsgrenze den Drift–Diffusions–Prozess als Lösung einer partiellen Differentialgleichung (Fokker–Planck–Gleichung).

c.) Drift–Diffusion equation The motion named after *Robert Brown* shows the stochastic displacement of a particle by one–dimensional diffusion.

Study Einstein's concept of Brownian motion to derive the well–known diffusion equation by reading the original paper *Über die* *von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen* in Annalen der Physik 1905, pp. 549–560.

The solution of the diffusion equation is known as Gaussian distribution. Show its profile and discuss the properties, especially the moments.

See H. Haken: Synergetik, Springer–Verlag, Berlin, div. Auflagen ab 1977.
See: Chap 1–3 (pp. 131–163) in J. Vollmer: Chaos, spatial extension, transport, and non-equilibrium thermodynamics, Physics Reports 372, Dec. 2002, pp. 131–267.

16. **Project week** (01.–06.06.2009, R. Mahnke)
You should work with your project task.

17. **End of project week** (08.06.2009, R. Mahnke)
You should compile the presentation of your project work.

18. **Ornstein–Uhlenbeck process II** (10.06.2009, R. Mahnke)
After discussing all project works in general we recall the Ornstein–Uhlenbeck process. Based on the given Fokker–Planck equation the solution shown as graphical figure of isolines (see 1) has been interpreted.

19. **Ornstein–Uhlenbeck process III** (15.06.2009, R. Mahnke)
The following exercise should be performed

   (f) Use der Fokker–Planck equation of the Ornstein–Uhlenbeck process and calculate the stationary solution in velocity space
   $p_{st}(v) = \lim_{t\to\infty} \int p(x,v,t)dx$.
   Compare it with the Maxwellian distribution known from Statistical Physics. Get the so–called fluctuation–dissipation theorem valid under equilibrium condition. Discuss the relationship between stationarity and equilibrium.

20. **Presentation of projects** (17.06.2009, R. Mahnke)

   P7 **Logistic mapping** → Markus Kersten
   See: Results by Markus Kersten

   P1 **Deterministic vs molecular chaos** → Yeong Zen Chua
   See: Results by Yeong Zen Chua

21. **Again traffic flow: Empirical findings** (22.06.2009, Ch. Liebe)
Celebrating 75 years of the very first paper by Greenshield on speed–flow curves, the so–called *Fundamental Diagram* as steady state relationship of flux over density has its 75th anniversary in July 2008. The empirical traffic flow theory is described as phase transition between free flow and congested traffic. The concept of nucleation on roads is explained by forming of vehicular clusters in analogy to supersaturated vapours. The cluster size as number of bounded vehicles is introduced as stochastic variable. The breakdown probability density has to be calculated out of the given stochastic dynamics.
Greenshields started to create traffic data and extracted out of this data the first *Fundamental Diagram*. The technique to take pictures and extract the density and the velocity of the cars is also used to create the NGSIM–data (**N**ext **G**eneration **Sim**ulation Program). The recorded trajectories have to be smoothed. Otherwise the calculated velocities and accelerations are useless. It is possible to simulate the recorded data and compare different traffic models by comparing the fundamental diagrams. Out of the relationship between velocity and distance to the leading car, one can find at least two different driver states which occur in free flow and slightly dense traffic. The creation of an optimal velocity model out of forces leads to a physical picture of traffic with energies and energy flows. The model leads to a fundamental diagram, which is at least in the dense region similar to the one extracted from the NGSIM–data.

22. **Bistability** (24.06.2009, Ch. Liebe)
Out of the equation of motion

$$\begin{aligned}
\frac{\mathrm{d}x(t)}{\mathrm{d}t} &= F_{\mathrm{det}}(x) + F_{\mathrm{stoch}}(t) \\
\frac{\mathrm{d}x(t)}{\mathrm{d}t} &= -\alpha' x(t) - \beta x^3(t) + \sqrt{2D}\,\xi(t) \\
\mathrm{d}x(t) &= \left[-\alpha' x(t) - \beta x^3(t)\right]\mathrm{d}t + \sqrt{2D}\,\mathrm{d}W(t) \\
x(t=0) &= x_0
\end{aligned}$$

of a particle in a potential including white noise one can derive a Fokker–Planck equation (FPE) for the probability density. The equation is solvable in the special case of a harmonic potential only. Nevertheless every solution (numerical or analytical) of the FPE leads to an eigenvalue problem with a so–called Schrödinger–potential. A scaling of the equation of motion reduces the number of parameters from three to one (α). For the case of $\alpha \ll 0$ one can approximate the Schrödinger–potential with three harmonic potentials with its own eigenfunctions and eigenvalues. Due to the symmetry of the Schrödinger–potential the eigenfunctions have to be either summetric or antisymmetric. This leads to the possibility of the construction of eigenfunctions as solutions of the complete eigenvalue problem. The eigenvalues are degenerated. For the numerical solution of the eigenvalue problem the shooting Numerov method is used.

23. **Presentation of projects** (29.06.2009, R. Mahnke)

    P4 **Fokker–Planck equation with linear drift** → Lennart Seiffert
    See: Results by Lennart Seiffert
    See: Presentation by Lennart Seiffert

    P9 **Drift and diffusion** → Alexander Schmidt
    See: Results by Alexander Schmidt
    Compare: Results by Michael Brüdgam (2005)

24. **Presentation of projects** (01.07.2009, R. Mahnke)

    P5 **Vehicular motion and energy balance** → Martin Lahrz
    See: Results by Martin Lahrz
    See: Presentation by Martin Lahrz

    P6 **Vehicular motion and traffic breakdown** → Andreas Becker
    See: Results by Andreas Becker

    The following home work should be performed (till 08.07.2009):

    (f) Consider der ordinary diffusion equation with natural boundaries and initial condition as delta distribution. Calculate the solution analytically.

25. **Presentation of project work** (06.07.2009, R. Mahnke)

    P3 **Solution of Master equation by simulation technique** → Hannes Sobottka
    See: Results by Hannes Sobottka

    P2 **Jam or cluster dissolution: Breakdown rate** → Anna Wiktoria Oniszczuk
    See: Results by Anna Wiktoria Oniszczuk

26. **Thema** (08.07.2009, R. Mahnke)

    P8 **Stochastic Brusselator** → Merten Siegfried
    See: Results by Merten Siegfried

    Discussion of home work (f) to find the analytical solution $p(x,t)$ of the following diffusion equation

$$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2} \qquad (33)$$

    together with initial condition $p(x, t = 0) = \delta(x - x_0)$ and natural boundaries.

    See: Result by Markus Kersten

27. **Langevin equation I** (13.07.2009, R. Mahnke)
    Extension of a deterministic differential equation by a stochastic force (additive white noise) gives the Langevin equation. Important as equivalent description of stochastic trajectories is the Fokker–Planck equation, which shows the development of the probability density of a stochastic drift–diffusion process.
    The Brownian gas model as a system of many Brownian particles with interaction is considered. The dynamics of this many–body system is given as a set of Langevin equations. Usually thermal equilibrium is treated where the fluctuation–dissipation theorem (Einstein relation) is valid and the canonical distribution holds. The overdamped limit neglecting momenta is discussed.

28. **Langevin equation II** (15.07.2009, R. Mahnke)
    2dim linear extension (coordinate–velocity space) including special case $D = 0$ called Ornstein–Uhlenbeck process

$$dx = v\,dt + \sqrt{2D}\,dW(t) \qquad (34)$$

$$dv = -\gamma v\,dt + \sqrt{2B}\,dW(t) \qquad (35)$$

Results by Martin Lahrz

Examples of deterministic and stochastic models

Mathematical Pendulum

Die Berechnung des mathematischen Pendels ist wohlbekannt. Es sei daher an dieser Stelle nur eine kurze Herleitung in geeigneten (generalisierten) Koordinaten gegeben. Es gilt:

$$H = T + V = \frac{1}{2}\frac{p_x^2}{m} - mgx\,. \tag{36}$$

Unter Verwendung von $x = l\cos\alpha$ sowie $p_x = mv = ml\omega$ und $L = ml^2\omega \equiv p_\alpha$ lässt sich dies umschreiben zu:

$$H = \frac{1}{2}ml^2\omega^2 - mgl\cos\alpha = \frac{1}{2}\frac{p_\alpha^2}{ml^2} - mgl\cos\alpha \equiv E\,. \tag{37}$$

Die Nichtlinearität $\cos\alpha$ wird spätestens hier deutlich. Es sei weiterhin in Anbetracht der generalisierten Koordinaten $\alpha \equiv q$ und $p_\alpha \equiv p$. Für die Darstellung im Phasendiagramm lässt sich obige Gleichung nach dem generalisierten Impuls p auflösen. Es gilt:

$$p^2 = 2ml^2\left(E + mgl\cos q\right) \tag{38}$$

oder

$$p = \pm\sqrt{2ml^2\left(E + mgl\cos q\right)}\,. \tag{39}$$

Der Verlauf ist in Abbildung 2 für unterschiedliche Energien E dargestellt. Es ist gut zu erkennen, dass für geringe Energien $E < mgl$ nur abgeschlossene Intervalle $\alpha = \left[-\arccos\frac{E}{mgl}, \arccos\frac{E}{mgl}\right]$ möglich sind und sich mit der Periode 2π wiederholen. Dazwischen gibt es stets einen verbotenen Bereich. Das Pendel schwingt wie gewöhnlich. Für $E = mgl$ kann das System zwischen den einzelnen Intervallen hin- und herwechseln. Real bedeutet dies, dass die Energie gerade ausreicht, um das Pendel senkrecht nach oben zeigen zu lassen. Es kann dort (zufällig) in beide Richtungen fallen und entsprechend seine ursprüngliche Richtung und damit das Vorzeichen des Impulses ändern. Ist $E > mgl$, sind zwei voneinander getrennte Zustände zu beobachten, die symmetrisch um die q-Achse liegen. Das Pendel rotiert und kann ohne äußeren Einfluss nicht mehr seine Richtung ändern.

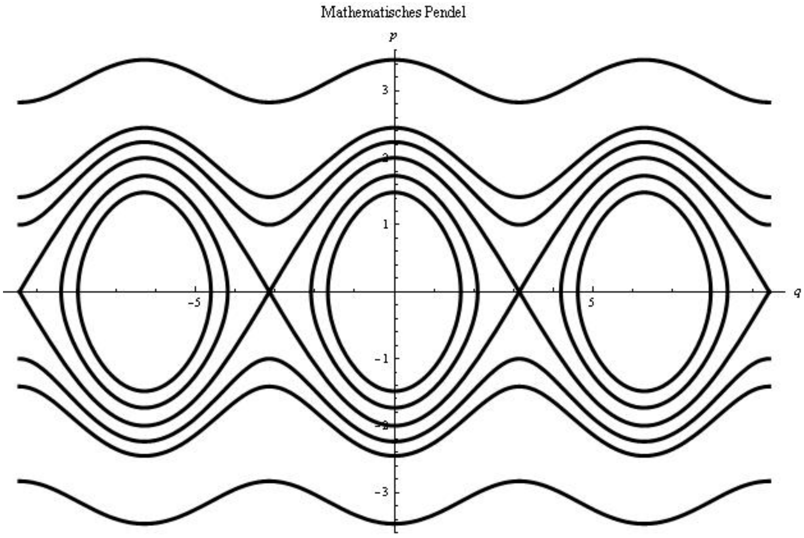

Abbildung 2: Phasendiagramm für das mathematische Pendel.

Poisson process

Beim Poisson-Prozess zerfällt der k-te Zustand in den $(k-1)$-ten Zustand mit einer von der Besetzung beider Zustände unabhängigen Rate $1/\tau$. Allgemein können wir damit die Einschritt–Mastergleichung (one–step master equation) dafür aufstellen:

$$\dot{p}(n,t) = -\frac{1}{\tau}p(n,t) + \frac{1}{\tau}p(n+1,t)\,. \tag{40}$$

Besondere Beachtung finden die Ränder dieser Verteilung, d.h. $p(n_0,t)$ sowie $p(0,t)$. Dabei ist n_0 der höchste (Anfangs-)Zustand. Die entsprechenden Gleichungen folgen direkt aus (40) unter Berücksichtigung, dass weder $n = n_0+1$ noch $n = -1$ existieren. Es gilt:

$$\dot{p}(0,t) = \frac{1}{\tau}p(1,t)\,, \tag{41}$$

$$\dot{p}(n_0,t) = -\frac{1}{\tau}p(n_0,t)\,. \tag{42}$$

Weiterhin ist die Anfangsbedingung

$$p(n,0) = \delta_{nn_0} \tag{43}$$

zu beachten. Zum Anfangszeitpunkt $t = 0$ ist die Wahrscheinlichkeit, ein Teilchen im Zustand n_0 anzufinden Eins, überall sonst Null. Direkt aus (42) kann, da nur von n_0 abhängig, bereits $p(n_0, t)$ bestimmt werden. Wie leicht nachzuprüfen ist, gilt:

$$p(n_0, t) = C_0 e^{-t/\tau} \,. \tag{44}$$

Mit der Anfangsbedingung (43) $p(n_0, 0) = C_0 \equiv 1$ lässt sich sogar schon schreiben:

$$p(n_0, t) = e^{-t/\tau} \,. \tag{45}$$

Alle weiteren Zustände lassen sich nun rekursiv nach (40) bestimmen. Für $n = n_0 - 1$ erhält man beispielsweise:

$$\dot{p}(n_0 - 1, t) = -\frac{1}{\tau} p(n_0 - 1, t) + \frac{1}{\tau} p(n_0, t) = -\frac{1}{\tau} p(n_0 - 1, t) + \frac{1}{\tau} e^{-t/\tau} \,. \tag{46}$$

Dies ist eine inhomogene Differentialgleichung erster Ordnung. Wir bestimmen die homogene Lösung wie oben sehr leicht und erhalten:

$$p(n_0 - 1, t)|_{hom} = C_1 e^{-t/\tau} \,. \tag{47}$$

Zum Beispiel durch die Methode "Variation der Konstanten" können wir nun eine partikuläre Lösung der inhomogenen Differentialgleichung ermitteln. Es gilt:

$$p(n_0 - 1, t) = C_1 e^{-t/\tau} + \frac{t}{\tau} e^{-t/\tau} \,. \tag{48}$$

Unter Verwendung der Anfangsbedingung (43) $p(n_0 - 1, 0) = C_1 \equiv 0$ erhalten wir endgültig:

$$p(n_0 - 1, t) = \frac{t}{\tau} e^{-t/\tau} \,. \tag{49}$$

Auf gleiche Weise lassen sich nun weitere Ordnungen bestimmen. Es sei nur soviel gesagt, dass die homogene Lösung stets verschwindet und die partikuläre Lösung bereits die Anfangsbedingung erfüllt. Ohne weitere Angaben gilt:

$$p(n_0 - 2, t) = \frac{1}{2} \left(\frac{t}{\tau} \right)^2 e^{-t/\tau} \,, \tag{50}$$

$$p(n_0 - 3, t) = \frac{1}{6} \left(\frac{t}{\tau} \right)^3 e^{-t/\tau} \,, \tag{51}$$

$$\vdots$$

Es lässt sich die folgende, allgemeine Form erkennen:

$$p(n_0 - k, t) = \frac{1}{k!}\left(\frac{t}{\tau}\right)^k e^{-t/\tau}\,, \tag{52}$$

die wir noch beweisen wollen. Auf Grund der Eindeutigkeit der Lösung einer linearen Differentialgleichung, reicht es zu zeigen, dass diese Lösung die Anfangsbedingung (43) und die Differentialgleichung (40) erfüllt. Dies tun wir mittels Induktion, d.h. die Lösung von $n = k + 1$ sei nach (52) bekannt. Behauptung:

$$p(n_0 - k, t) = \frac{1}{k!}\left(\frac{t}{\tau}\right)^k e^{-t/\tau}\,. \tag{53}$$

Beweis:

$$p(n_0 - k, 0) = 0 \tag{54}$$

$$\dot{p}(n_0 - k, t) = -\frac{1}{\tau}p(n_0 - k, t) + \frac{1}{\tau}p(n_0 - k + 1, t) \tag{55}$$

$$\Leftrightarrow \frac{t^{k-1}}{(k-1)!\tau^k}e^{-t/\tau} - \frac{t^k}{k!\tau^{k+1}}e^{-t/\tau} = -\frac{1}{\tau}\frac{t^k}{k!\tau^k}e^{-t/\tau} + \frac{1}{\tau}\frac{t^{k-1}}{(k-1)!\tau^{k-1}}e^{-t/\tau}\,. \tag{56}$$

q.e.d.

Für $k = n_0$ muss gilt die Rekursion nicht mehr. Wir können jedoch den Zustand $n = 0$ sehr leicht durch die normierte Gesamtwahrscheinlichkeit von Eins minus die Summe aller anderen Wahrscheinlichkeiten bestimmen. In (52) substituieren wir der Übersicht halber $m = n_0 - k$ und erhalten als Gesamtlösung bei gegebenen n_0:

$$p(m, t) = \begin{cases} \frac{1}{(n_0-m)!}\left(\frac{t}{\tau}\right)^{n_0-m} e^{-t/\tau}\,, & m \geq 1 \\ 1 - e^{-t/\tau}\sum_{n=1}^{n_0}\frac{1}{n!}\left(\frac{t}{\tau}\right)^n\,, & m = 0 \end{cases} \tag{57}$$

Dies lässt sich für verschiedene Zeiten t auswerten, vgl. Abbildung 3. Die Verteilung läuft mit der Zeit von rechts nach links, wird dabei breiter und schmaler. Am Rand $m = 0$ sammeln sich alle Zustände und verweilen dort. Der Mittelwert nimmt, wie in Abbildung 4 zu erkennen, zunächst linear ab. Zum Ende schmiegt er sich jedoch an die Abszissenachse an, was besonders im Ausschnitt der Abbildung 5 zu sehen ist.

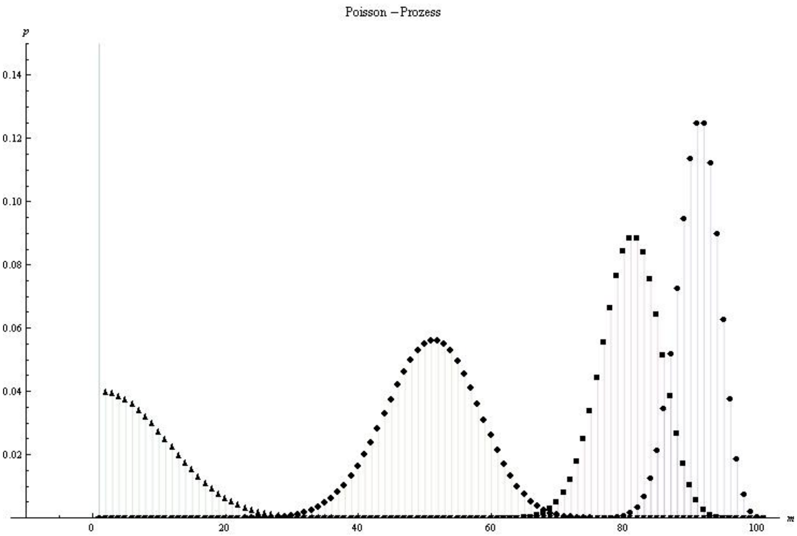

Abbildung 3: Wahrscheinlichkeitsverteilung $p(m, t)$ für verschiedene Zeiten t.

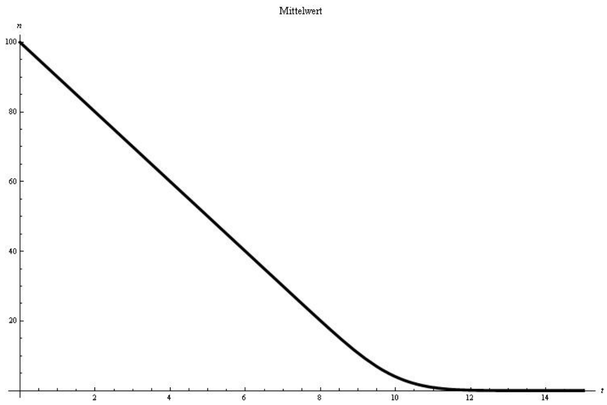

Abbildung 4: Mittelwert in zeitlicher Abhängigkeit.

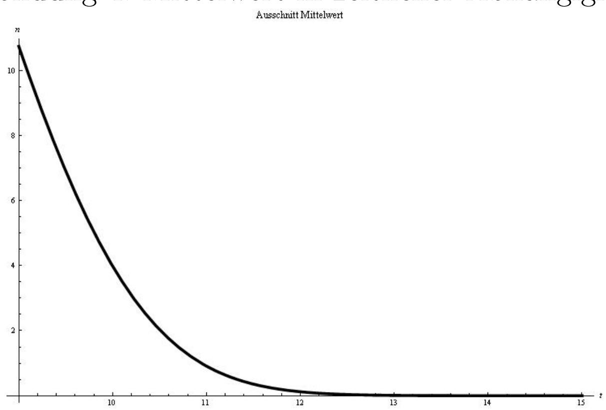

Abbildung 5: Mittelwert in zeitlicher Abhängigkeit (Ausschnitt).

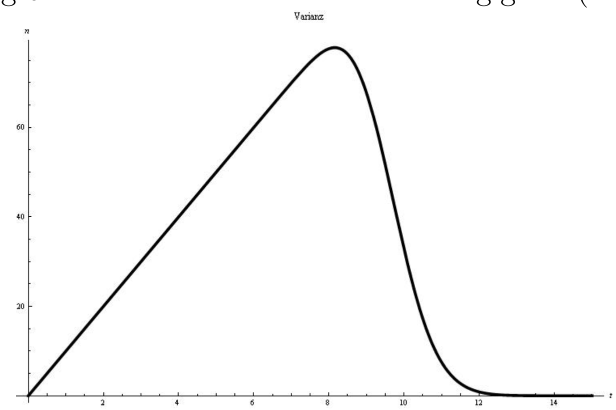

Abbildung 6: Varianz in zeitlicher Abhängigkeit.

Umsetzung in MATHEMATICA:

```
n0 = 100;
tau = 0.1;
p[m_, t_] =
  If [m <= 0, 1 - E^(-t/tau)*Sum[t^n/(n!*tau^n), {n, 1, n0}],
   t^(n0 - m)/((n0 - m)!*tau^(n0 - m))*E^(-t/tau)];
liste[t_] = Table[p[m, t], {m, 0, n0, 1}];
ListPlot[{liste[1], liste[2], liste[5], liste[10], liste[20]},
 PlotRange -> 0.15,
 AxesOrigin -> {-n0/10, 0},
 Filling -> Axis,
 PlotLabel -> Poisson - Prozess,
 AxesLabel -> {m, p},
 PlotMarkers -> Automatic,
 PlotStyle -> Black]
avg[t_] = Sum[p[m, t]*m, {m, 0, n0, 1}];
var[t_] = Sum[p[m, t]*m^2, {m, 0, n0, 1}] - avg[t]^2;
Plot[avg[t], {t, 0, 15},
 PlotRange -> Full,
 PlotLabel -> Mittelwert,
 AxesLabel -> {t, n},
 PlotStyle -> {{Thickness[0.005], Black}}]
Plot[avg[t], {t, 9, 15},
 PlotRange -> Full,
 PlotLabel -> Mittelwert Ausschnitt,
 AxesLabel -> {t, n},
 PlotStyle -> {{Thickness[0.005], Black}}]
Plot[var[t], {t, 0, 15},
 PlotRange -> Full,
 PlotLabel -> Varianz,
 AxesLabel -> {t, n},
 PlotStyle -> {{Thickness[0.005], Black}}]
Quit[];
```

Result by Markus Kersten

Method to solve the diffusion equation analytically

Wir haben zu lösen:

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2}; \qquad D = \text{const.} \tag{58}$$

mit natürlichen Rand- und folgenden Anfangsbedingungen:

$$p(x, t = 0) = f(x) = \delta(x - x_0)\ ; \qquad -\infty < x_0 < \infty$$

Wir beginnen mit einem Separationsansatz $p(x,t) = X(x) \cdot T(t)$. Damit hat die Diffusionsgleichung die folgende Gestalt:

$$\frac{X''}{X} = \frac{T'}{DT} = \lambda = \text{const.} \tag{59}$$

Dies führt auf die zwei Differentialgleichungen

$$\begin{aligned} &(1) \quad X'' - \lambda X = 0, \\ &(2) \quad T' - DT\lambda = 0. \end{aligned}$$

Wir beachten, dass die Funktion X keine Exponentialfunktion sein soll, da die Lösung für $x \to \pm\infty$ nicht unendlich werden soll. Daher wählen wir $\lambda = -k^2,\ k \in \mathbb{R}$ und erhalten folgende Ansätze:

$$X(x) = a_k \mathrm{e}^{ikx}, \qquad T(t) = c_k \mathrm{e}^{-k^2 Dt}.$$

Wir überlagern nun die beiden Lösungen, betrachten die Koeffizienten als Funktion $a(k)$ und integrieren

$$p(x,t) = \int_{-\infty}^{\infty} a(k) \mathrm{e}^{ikx - k^2 Dt} \mathrm{d}k. \tag{60}$$

Aus den allgemeinen Anfangsbedingungen ergibt sich nun $a(k)$:

$$p(x,0)=\int_{-\infty}^{\infty}a(k)\mathrm{e}^{ikx}\mathrm{d}k=f(x). \tag{61}$$

Dabei handelt es sich um eine Fourier-Transformation mit der Periode 2π, woraus folgt

$$a(k)=\frac{1}{2\pi}\int_{-\infty}^{\infty}f(y)\mathrm{e}^{-iky}\mathrm{d}y. \tag{62}$$

Einsetzen liefert dann

$$p(x,t)=\int_{-\infty}^{\infty}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}f(y)\mathrm{e}^{-iky}\mathrm{d}y\right]\mathrm{e}^{ikx-k^2Dt}\mathrm{d}k=\frac{1}{2\pi}\int_{-\infty}^{\infty}f(y)\mathrm{d}y\int_{-\infty}^{\infty}\mathrm{e}^{ik(x-y)-k^2Dt}\mathrm{d}k. \tag{63}$$

Jetzt wird das Argument der Exponentialfunktion vermittelst einer quadratischen Ergänzung umgeschrieben:

$$ik(x-y)-k^2Dt=-Dt\left[\left(k-\frac{i(x-y)}{2Dt}\right)^2+\left(\frac{x-y}{2Dt}\right)^2\right].$$

Also ergibt sich auf Grund der Summenstruktur für die Lösung

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}f(y)\mathrm{e}^{-\frac{(x-y)^2}{4Dt}}\mathrm{d}y\int_{-\infty}^{\infty}\mathrm{e}^{-Dt\left(k-\frac{i(x-y)}{2Dt}\right)^2}\mathrm{d}k. \tag{64}$$

Nun führen wir eine Variablensubstitution durch, so dass

$$z=\sqrt{Dt}\left(k-\frac{i(x-y)}{2Dt}\right),\qquad \frac{\mathrm{d}z}{\mathrm{d}k}=\sqrt{Dt}.$$

Das führt dazu, dass wir das zweite Integral als Standardintegral betrachten kïnen:

$$\frac{1}{\sqrt{Dt}}\int_{-\infty}^{\infty}\mathrm{e}^{-z^2}\mathrm{d}z=\frac{1}{\sqrt{Dt}}\sqrt{\pi}.$$

Damit haben wir jetzt also nur noch

$$p(x,t)=\frac{1}{2\sqrt{\pi Dt}}\int_{-\infty}^{\infty}f(y)\mathrm{e}^{-\frac{(x-y)^2}{4Dt}}\mathrm{d}y. \tag{65}$$

Unter genauerer Berücksichtigung der Anfangsbedingungen ergibt sich schließlich

$$p(x,t) = \frac{1}{2\sqrt{\pi D t}} \int_{-\infty}^{\infty} \delta(y - x_0) \mathrm{e}^{-\frac{(x-y)^2}{4Dt}} \mathrm{d}y \tag{66}$$

$$p(x,t) = \frac{1}{\sqrt{4\pi D t}} \mathrm{e}^{-\frac{(x-x_0)^2}{4Dt}}. \tag{67}$$

Damit führt die Lösung der gewöhnlichen Diffusionsgleichung gerade auf die Gaußsche Normalverteilung.

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