UNIVERSITÄT ROSTOCK

Institut für Physik

Lecture Notes

Stochastic Processes

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Contents

1 Random walks and diffusion

1.1 Introduction

- stochastic processes describe the temporal evolution of random events by probability distributions
- examples:
  - Brownian motion (Wiener process, diffusion, see Fig. 1)
    $\Rightarrow$ irregular motion of pollutes in a liquid
  - diffusion (note: this process is asymmetric in time)
  - Galton board
  - random walker: an object which steps either to the left or to the right (1dim walk on a line), generally asymmetric discrete random path

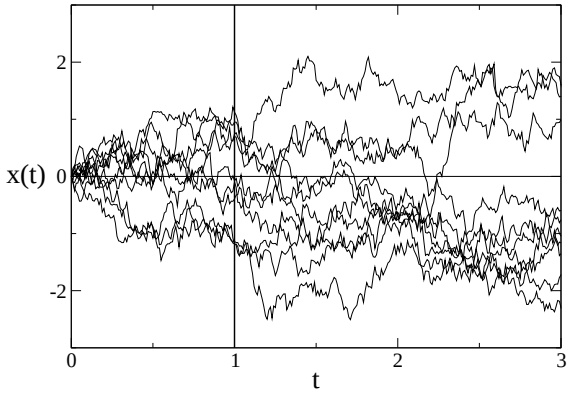

Figure 1: Ten stochastic trajectories with the same initial condition $x(t=0)=0$.

1.2 Markovian equations

1.2.1 Markov chain

discrete time and space

- $P(m,n)$ describes the probability of being at position m after n steps
- p and q are the probabilities for a step $m \to m+1$ and $m \to m-1$ respectively

$\Rightarrow$ equation of motion:

$$P(m,n+1) = pP(m-1,n) + qP(m+1,n)$$

- in case of $p \neq q$ the Markov chain describes an asymmetric walk (walk with drift)

- the solution for this equation with an initial point $(n_0, m_0) = (0, 0)$ is given by

$$P(m,n) = \frac{n!}{\left(\frac{n+m}{2}\right)!\left(\frac{n-m}{2}\right)!} p^{\frac{n+m}{2}} q^{\frac{n-m}{2}}$$

- substituting $r = \frac{n+m}{2}$ we get the well-known binomial distribution

$$P(m,n) = \frac{n!}{r!(n-r)!} p^r q^{n-r} = B(r,n)$$

$\Rightarrow$ mean value: $\langle m \rangle = 2n(p - \frac{1}{2})$, variance: $\sigma^2 = 4npq$

- the mean value describes the tendency for a preferred direction (drift)
- the variance describes the diffusion
- the relative variance tends to zero for great n: $\frac{\sigma}{\langle m \rangle} \propto \frac{1}{\sqrt{n}} \to 0$

1.2.2 Computing moments by generating functions

- the kth moment is defined as the mean value of r^k:

$$\langle r^k \rangle = \sum_r P(r) r^k$$

- for demonstration we compute the moments of the symmetric binomial distribution $P(m,n) = B(r,n) = \binom{n}{r} \frac{1}{2^n}$
- the left-hand side of the following equation is called the generating function:

$$(1+\omega)^n = \sum_{r=0}^{n} \binom{n}{r} \omega^r$$

- we substitute $\omega = e^y$ and write $(1+e^y)^n = \sum_{r=0}^{n} \binom{n}{r} e^{ry}$
- it is easy to see that the kth derivative of the right-hand side at $y = 0$ corresponds to the kth moment:

$$\frac{\mathrm{d}^k}{\mathrm{d}y^k} \sum_{r=0}^{n} \binom{n}{r} e^{ry}\Big|_{y=0} = \sum_r \binom{n}{r} r^k e^{ry}\Big|_{y=0}$$
$$= 2^n \sum_r \binom{n}{r} \frac{1}{2^n} r^k = 2^n \sum_r B(r,n) r^k = 2^n \langle r^k \rangle$$

- thus we can compute the kth moment as

$$\langle r^k \rangle = \frac{1}{2^n} \frac{\mathrm{d}^k}{\mathrm{d}y^k} \left[(1+e^y)^n\right]_{y=0}$$

- the first moments are $\langle r^0 \rangle = 1$, $\langle r \rangle = \frac{n}{2}$, $\langle r^2 \rangle = \frac{n(n+1)}{4}$

- we can further compute the moments of m by calculation of the moments of r and using the relation $r = \frac{n+m}{2}$

- the results are equivalent to the results of the Markov chain for the special case $p = q = \frac{1}{2}$

1.3 Master equation

continuous time, but discrete space

- we replace $t = n\Delta t$ with Δt as a fixed time step and compute the limit $\Delta t \to 0$

- the result is the Master equation:

$$\frac{\partial P(m,t)}{\partial t} = \frac{p}{\Delta t}P(m-1,t) + \frac{q}{\Delta t}P(m+1,t) - \frac{p+q}{\Delta t}P(m,t)$$

- therefore we can define transition rates as $w_+ = p/\Delta t$ and $w_- = q/\Delta t$

1.4 Drift-diffusion equation

continuous space and time
special case of Fokker-Planck equation

- we replace $x = m\Delta x$ with Δx as a fixed spatial distance and compute the limit $\Delta x \to 0$

- since all variables have a continuous domain, we describe probabilities with the density function: $P(m,t) \to p(x,t)\mathrm{d}x$

- the result is the Fokker-Planck equation:

$$\frac{\partial p(x,t)}{\partial t} = -v\frac{\partial p(x,t)}{\partial x} + D\frac{\partial^2 p(x,t)}{\partial x^2}$$

1.5 From symmetric binomial distribution to Gaussian distribution

- the symmetric Markov chain is defined by
$P(m,n+1) = \frac{1}{2}P(m-1,n) + \frac{1}{2}P(m+1,n)$

$\Rightarrow$ solution: binomial distribution

$$P(m,n) = \frac{n!}{\left(\frac{n+m}{2}\right)!\left(\frac{n-m}{2}\right)!}\frac{1}{2^n}$$

- continuous approximation: $x_m = m\,a$, $t_n = n\,\tau$ with a and τ as a characteristic spatial or temporal distance respectively

$\Rightarrow$ inserting in the definition of the binomial coefficients

$$P(x_m, t_n) = \frac{\left(\frac{t_n}{\tau}\right)!}{\left(\frac{t_n}{2\tau} + \frac{x_m}{2a}\right)!\left(\frac{t_n}{2\tau} - \frac{x_m}{2a}\right)!}\frac{1}{2^n}$$

- we now use the Stirling formula to approximate the factorial for great numbers:

$$n! \simeq e^{-n}n^n\sqrt{2\pi n} \quad ; \quad \ln n! \simeq n\ln n - n + \frac{1}{2}\ln(2\pi n)$$

- introduction of abbreviations: $r = \frac{t_n}{2\tau}(1+\delta)$, $n-r = \frac{t_n}{2\tau}(1-\delta)$ with $\delta = \frac{m}{n} = \frac{x_m}{a}\frac{\tau}{t_n}$

  $\Rightarrow$ δ tends to zero for $n \to \infty$

- from $P(r,n) = \binom{n}{r}\frac{1}{2^n}$ we can approximate

$$P(x_m, t_n) \approx \frac{2}{\sqrt{2\pi t_n}\sqrt{1-\delta^2}}\sqrt{\tau}\exp\Big(-\frac{x_m^2\tau}{2a^2t_n}\Big) \longrightarrow \frac{2}{\sqrt{2\pi t_n}}\sqrt{\tau}\exp\Big(-\frac{x_m^2\tau}{2a^2t_n}\Big)$$

- we can define the diffusion constant $D = \frac{1}{2}\frac{a^2}{\tau}$

- dividing the equation by $2a$ we get:

$$\frac{P(x_m, t_n)}{2a} \approx \frac{1}{\sqrt{4\pi t_n}}\sqrt{\frac{2\tau}{a^2}}\exp\Big(-\frac{x_m^2}{4Dt_n}\Big)$$

- this quantity describes the probability per length of the interval $[x_m - a, x_m + a]$ $\Rightarrow$ probability density

$\Rightarrow$ taking the limit $\tau \to 0$ for $t_n \to t$ and $a \to 0$ for $x_m \to x$ we receive

$$p(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\Big(-\frac{x^2}{4Dt}\Big)$$

  $\Rightarrow$ Gaussian distribution: solution of diffusion equation $\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2}$

- spatial limits: $\lim_{x\to\pm\infty} p(x,t) = 0$

- the probability density is defined for a continuous position $x \in (-\infty, \infty)$ (natural boundaries)

- comparison with the standard normal distribution (see Fig. 2)

$$P_{normal} = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\Big(-\frac{(x-\mu)^2}{2\sigma^2}\Big)$$

  $\Rightarrow$ mean value: $\mu = 0$ or $\mu = x_0$ with x_0 as the starting point

  $\Rightarrow$ standard deviation: $\sigma^2 = 2Dt$

  $\Rightarrow$ the mean square displacement grows with the square root of time: $\sigma \propto \sqrt{t}$

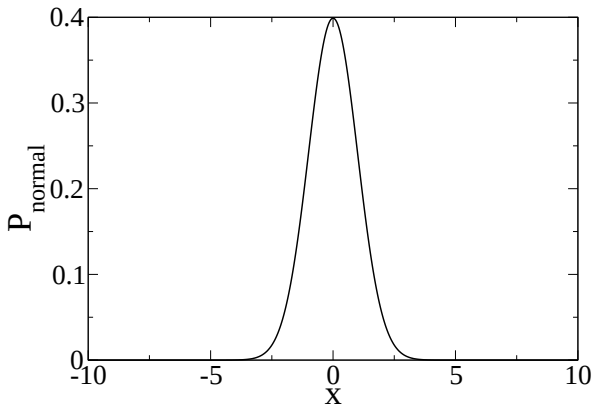

Figure 2: Gaussian distribution P_{normal} with $\mu = 0$ m and $\sigma = 1$ m^2/s for $t = 1$ s.

1.6 Diffusion equation

1.6.1 Fick's laws

- normalisation of the Gaussian distribution:

$$\int_{-\infty}^{\infty} p(x,t)\mathrm{d}x = 1 \quad \text{(global conservation law)}$$

- continuity equation for certain position x: change of probability at a fixed position in time equals to the spatial derivative of the propability flux

$$\frac{\partial p(x,t)}{\partial t} + \frac{\partial}{\partial x} j_{diff}(x,t) = 0 \quad \text{(local continuity equation)}$$

- phenomenological ansatz for diffusion flux: $j_{diff}(x,t) = -D\frac{\partial p(x,t)}{\partial x}$

  $\Rightarrow$ the flux is caused by spatial differences in probability

$\Rightarrow$ inserting the flux into the continuity equation we receive the diffusion equation

1.6.2 Einstein's derivation

- the position of a particle at the next moment depends on the present position $x(t)$ and a random step $l(t)$:

$$x(t+\tau) = x(t) + l(t)$$

- starting position: $x(t=0) = x_0$ ($= 0$ for reasons of simplity)

- we need the probability distribution of the stochastic events $l(t)$

  - therefore we assume that the continuous distribution $\xi(z)$ of $l(t)$ satisfies some equations for its moments:

- normalisation: $\int \xi(z)\mathrm{d}z = 1$
- no tendency for a special direction: $\langle z \rangle = \int \xi(z) z \mathrm{d}z = 0$
- finite second moment: $\langle z^2 \rangle = \int \xi(z) z^2 \mathrm{d}z = a^2$

- now we do the step from (x', t) to $(x, t+\tau)$:

- the probability of being at position x at time $t+\tau$ depends on the probability of being at position x' at time t and the probability $\xi(x-x')$ for doing the step from x' to x

- integrating over all possible positions we get

$$p(x, t+\tau) = \int_{-\infty}^{\infty} p(x', t)\xi(x-x')\mathrm{d}x'$$

- we replace $x - x' = z, \mathrm{d}x' = -\mathrm{d}z$

$$\begin{aligned}
\Rightarrow p(x, t+\tau) &= \int_{-\infty}^{\infty} p(x-z, t)\xi(z)\mathrm{d}z \\
&\approx \int_{-\infty}^{\infty} \Big[p(x,t) - z\frac{\partial p}{\partial x} + \frac{1}{2}z^2\frac{\partial^2 p}{\partial x^2}\Big]\xi(z)\mathrm{d}z \quad \text{(Taylor expansion)} \\
&= p(x,t)\underbrace{\int_{-\infty}^{\infty}\xi(z)\mathrm{d}z}_{1} - \frac{\partial p}{\partial x}\underbrace{\int_{-\infty}^{\infty} z\xi(z)\mathrm{d}z}_{0} + \frac{1}{2}\frac{\partial^2 p}{\partial x^2}\underbrace{\int_{-\infty}^{\infty} z^2\xi(z)\mathrm{d}z}_{a^2} \\
&= p(x,t) + \frac{1}{2}a^2\frac{\partial^2 p}{\partial x^2}
\end{aligned}$$

- we expand the left side of the equation with respect to time: $p(x, t+\tau) = p(x,t) + \tau\frac{\partial p}{\partial t}$

$\Rightarrow$ thus we end up with the diffusion equation:

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

1.7 Diffusion in a finite intervall

1.7.1 Semi-open boundaries

- before: natural boundaries $-\infty < x < \infty$

- now semi-open boundaries: $a \le x \le b$

1. equation of motion: $\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2}$
2. initial condition $p(x, t=0) = \delta(x - x_0) \quad (a \le x_0 \le b)$; (See notes in Sect. 1.7.2)
3. reflecting left boundary (particles reaching $x = a$ are reflected into the system)

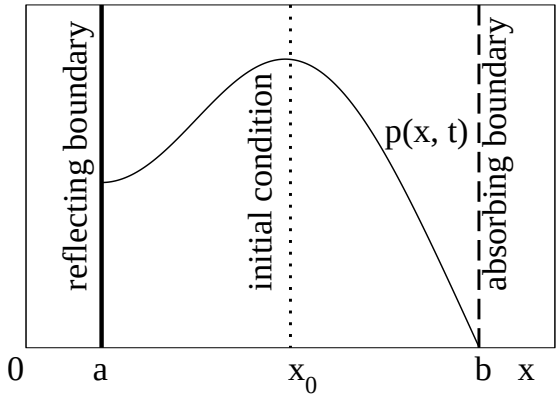

Figure 3: Schematic picture of the boundary–value problem showing the probability density $p(x\,,t)$ in the interval $a \leq x \leq b$.

$\Rightarrow$ the probability flux through the left border equals to zero:
$\left.\frac{\partial p(x,t)}{\partial x}\right|_{x=a} = 0$

4. absorbing right boundary (particles reaching $x = b$ leave the system)

   $\Rightarrow$ the probability of being at position $x = b$ vanishes to zero:
   $p(x,t)\big|_{x=b} = 0$

$\Rightarrow$ initial boundary value problem (see Fig. 3)

a) transforming into the unit interval $[a, b] \rightarrow [0, 1]$: $y = \frac{x-a}{b-a}$, $p(x,t) \rightarrow \tilde{p}(y,t)$

b) dimensionless time $t \rightarrow T$ by use of the diffusion constant D:
$T = \frac{D}{(b-a)^2}t \Rightarrow \tilde{p}(y,t) \rightarrow P(y,T)$

$\Rightarrow$ we are interested in the transformed diffusion equation

- conservation of the probability of being in an interval $[x, x + \mathrm{d}x]$:
  $p(x,t)\mathrm{d}x = P(y,T)\mathrm{d}y$

  $\Rightarrow$ we receive $P(y,T) = p(x,t)\frac{\mathrm{d}x}{\mathrm{d}y} = p(x,t)(b-a)$

- we further transform the derivatives:

$$\frac{\partial}{\partial t} = \frac{\partial T}{\partial t}\frac{\partial}{\partial T} = \frac{D}{(b-a)^2}\frac{\partial}{\partial T}$$
$$\frac{\partial}{\partial x} = \frac{\partial y}{\partial x}\frac{\partial}{\partial y} = \frac{1}{(b-a)}\frac{\partial}{\partial y} \quad \Rightarrow \quad \frac{\partial^2}{\partial x^2} = \frac{1}{(b-a)^2}\frac{\partial^2}{\partial y^2}$$

- inserting the results on both sides of the diffusion equation we receive

$$\frac{\partial p(x,t)}{\partial t} = \frac{D}{(b-a)^2}\frac{\partial}{\partial T}\frac{P(y,T)}{b-a} \stackrel{!}{=} D\frac{1}{(b-a)^2}\frac{\partial}{\partial y^2}\frac{P(y,T)}{b-a} = \frac{\partial^2 p(x,t)}{\partial x^2}$$

$\Rightarrow$ new dimensionless diffusion equation for $P(y,T)$:

$$\frac{\partial}{\partial T}P(y,T) = \frac{\partial^2}{\partial y^2}P(y,T)$$

$\Rightarrow$ new initial condition: $P(y, T=0) = \delta(y - y_0)$ with $y_0 = \frac{x_0 - a}{b-a}$

$\Rightarrow$ boundary conditions: $\frac{\partial}{\partial y}P(y,T)\Big|_{y=0} = 0,\ P(y=1,T)\big|_{y=1} = 0$

c) separation ansatz $P(y,t) = \chi(T)f(y)$ to solve the new equation

$\Rightarrow$ inserting the ansatz into the diffusion equation: $f(y)\frac{\partial \chi(T)}{\partial T} = \chi(T)\frac{\partial^2 f(y)}{\partial y^2}$

$\Rightarrow$ we divide by $P(y,T) = \chi(T)f(y)$ and receive $\frac{1}{\chi(T)}\frac{\partial \chi(T)}{\partial T} = \frac{1}{f(y)}\frac{\partial^2 f(y)}{\partial y^2}$

$\Rightarrow$ the left-hand side depends on T, the right-hand side depends on y

$\Rightarrow$ since the equation shall be satisfied for arbitrary y and T, both sides have to be constant

$$\Rightarrow \frac{1}{\chi(T)}\frac{\partial \chi(T)}{\partial T} = -\lambda\ , \quad \frac{1}{f(y)}\frac{\partial^2 f(y)}{\partial y^2} = -\lambda, \qquad \lambda - \text{separation constant}$$

- solution of the first equation: $\frac{\partial \chi(T)}{\partial T} = -\lambda\chi(T) \ \Rightarrow\ \chi(T) = \chi_0 e^{-\lambda T}$

d) second equation: wave equation $\frac{\partial^2 f(y)}{\partial y^2} + \lambda f(y) = 0$ with special boundary conditions

- real value ansatz $f(y) = A\sin(ky) + B\cos(ky)$ with $k^2 = \lambda$ (k being the wave number)
- boundary and initial conditions determine the constants $A,\ B$ and k
  - right boundary: $f(y=1) = 0 \ \Rightarrow\ A\sin k + B\cos k = 0$
  - left boundary: $\frac{\partial f(y)}{\partial y}\Big|_{y=0} = 0 \ \Rightarrow\ \{Ak\cos(ky) - Bk\sin(ky)\}\big|_{y=0} = Ak = 0$
  - since we are looking for nontrivial solutions, k should be different from zero $\Rightarrow A = 0$
  - then the first boundary condition reads as $B\cos k = 0$
  - since B has to be different from zero, we receive $\cos k = 0$ (otherwise we would receive $f(y) \equiv 0$)

  $\Rightarrow$ k has a discrete spectrum: $k_m = \pi(m + \frac{1}{2}) \quad (m = 0, 1, 2, \ldots)$

  $\Rightarrow$ the case $m = 0$ is referred as the ground state: $k_0 = \frac{\pi}{2}, \lambda_0 = k_0^2 = \frac{\pi^2}{4}$

  $\Rightarrow$ first excited state: $k_1 = \frac{3}{2}\pi,\ \lambda_1 = \frac{9\pi^2}{4}$

$\Rightarrow$ elementary solutions:

$$P_m(y,T) = B_m\chi_0 e^{-\lambda_m T}\cos(k_m y)$$

- without loss of generality we set $\chi_0 = 1$

$\Rightarrow$ general solution by superposition:

$$P(y,T) = \sum_{m=0}^{\infty} P_m(y,T) = \sum_{m=0}^{\infty} B_m e^{-\lambda_m T} \cos(k_m y)$$

e) the B_m are defined by the initial condition $P(y, T=0) = \sum_m B_m \cos(k_m y) \stackrel{!}{=} \delta(y - y_0)$

- Fourier expansion: we multiply both sides with $\cos(k_n y)$ and integrate over the unit interval $[0, 1]$ (expansion by orthogonal eigenfunctions)
- on the left-hand side $\int_0^1 \cos(k_m y)\cos(k_n y)dy = \frac{1}{2}\delta_{nm}$
- the right-hand side reads as $\int_0^1 \cos(k_n y)\delta(y - y_0)\mathrm{d}y = \cos(k_n y_0)$

$\Rightarrow$ we find the solution for the coefficients: $B_m = 2\cos(k_m y_0)$

$\Rightarrow$ we end up with the solution for our initial boundary value problem (see Fig. 4)

$$P(y,T) = 2\sum_{m=0}^{\infty} e^{-\lambda_m T} \cos(k_m y_0)\cos(k_m y)$$

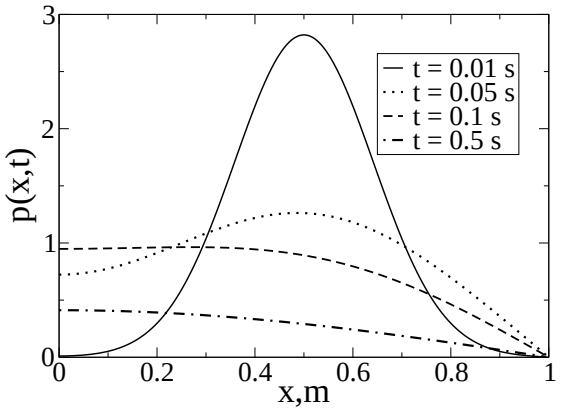

Figure 4: Time dependent solution $p(x,t)$ in m^{-1} of diffusion equation in finite interval $x \in [0,1]$ with reflecting boundary at $a = 0$ and absorbing boundary at $b = 1$ m. Parameters are initial condition $x_0 = 0.5$ m and diffusion constant $D = 1\ \mathrm{m}^2/\mathrm{s}$.

1.7.2 Some notes on the δ-distribution

- in the last section we used the δ-distribution as the initial spatial probability density
- the δ-distribution can be described by the following properties:

$$(1) \quad \delta(x) = \begin{cases} \infty & x = 0 \\ 0 & x \neq 0 \end{cases} \qquad (2) \quad \int_{-\infty}^{\infty} \delta(x)\mathrm{d}x = 1$$

- we can interprete it as a probability distribution describing the secure event $x = 0$, any other event will not occur

- it is easy to compute integrals containing the δ-distribution:

$$\int_{-\infty}^{\infty} f(x)\delta(x-x_0)\mathrm{d}x \overset{(1)}{=} \int_{-\infty}^{\infty} f(x_0)\delta(x-x_0)\mathrm{d}x = f(x_0)\underbrace{\int_{-\infty}^{\infty}\delta(x-x_0)\mathrm{d}x}_{=1} \overset{(2)}{=} f(x_0)$$

1.7.3 Continuation: Diffusion in a finite intervall

- the solution for our initial boundary value problem was

$$P(y,T) = 2\sum_{m=0}^{\infty} e^{-\lambda_m T}\cos(k_m y_0)\cos(k_m y) \text{ with } k_m = \frac{\pi}{2}(2m+1) \text{ and } \lambda_m = k_m^2$$

- the inverse transformation to $p(x,t)$ leads to the solution of the diffusion equation:

$$p(x,t) = \frac{2}{b-a}\sum_{m=0}^{\infty} e^{-\lambda_m t}\cos(k_m(x_0-a))\cos(k_m(x-a))$$

$$\text{with} \quad k_m = \frac{\pi}{b-a}\Big(\frac{1}{2}+m\Big) \quad \text{and} \quad \lambda_m = Dk_m^2$$

- the probability to encounter a particle in the whole system is $\int_{-\infty}^{\infty} p(x,t)\mathrm{d}x = 1 \quad \forall t \in \Re^+$

- the probability to encounter a particle in the subsystem (on the intervall) $]a,b]$ equals to

$$P_{in} = \int_a^b p(x,t)\mathrm{d}x$$

- now we analyse the probability flux J_{out} at $x = b$

$$\frac{\mathrm{d}}{\mathrm{d}t}P_{in}(t) + J_{out}(t) = 0 \quad \longrightarrow \quad J_{out} = -\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b p(x,t)\mathrm{d}x$$

- integrating the diffusion equation we receive

$$J_{out} = -\int_b^a D\frac{\partial^2}{\partial x^2}p(x,t)\mathrm{d}x = -D\frac{\partial}{\partial x}p(x,t)\Big|_{x=b} + \underbrace{D\frac{\partial}{\partial x}p(x,t)\Big|_{x=a}}_{=0}$$

  $\Rightarrow$ it leads to the solution

$$J_{out} = \frac{2\pi D}{(b-a)^2}\sum_{m=0}^{\infty}(-1)^m\Big(\frac{1}{2}+m\Big)e^{-Dk_m^2 t}\cos(k_m(x_0-a))$$

- it is clear that $\int_0^{\infty} J_{out}(x,t)\mathrm{d}t = 1$, but what is the average time $\langle t\rangle = \int_0^{\infty} tP_{out}(x,t)\mathrm{d}t$

  - we compute the limit: $a \to -\infty$ (see Fig. 5)

$$\Rightarrow \qquad J_{out}(t, x=b) = \frac{b-x_0}{\sqrt{4\pi Dt^3}}e^{-\frac{(b-x_0)^2}{4Dt}} \Rightarrow \langle t\rangle \to \infty$$

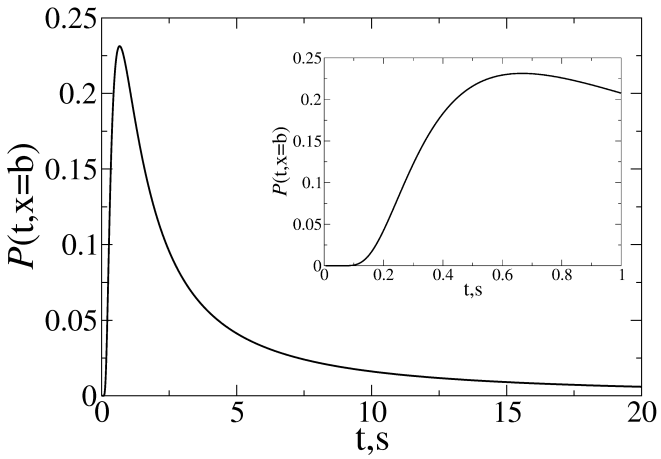

Figure 5: The first passage time probability density distribution $\mathcal{P}(t, x = b)$ in 1/s when $a \to -\infty$ with $b = 2$ m, initial condition $x_0 = 0$ and diffusion constant $D = 1$ m^2/s. Internal plot is a scaled picture of the time lag.

1.7.4 Exercise:
Properties of diffusion equation and Gaussian distribution

- applying the Fourier transformation $p(x,t) \Leftrightarrow \tilde{p}(k,t)$ to get $p(x,t)$

$$p(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \tilde{p}(k,t) \mathrm{d}k$$

$$\Rightarrow \qquad \frac{\partial p}{\partial t} = \frac{1}{\sqrt{2\pi}} \int e^{ikx} \frac{\partial \tilde{p}(k,t)}{\partial t} \mathrm{d}k$$
$$\frac{\partial^2 p}{\partial x^2} = \frac{i^2}{\sqrt{2\pi}} \int k^2 e^{ikx} \tilde{p}(k,t) \mathrm{d}k$$

- using the equation of motion

$$\frac{1}{\sqrt{2\pi}} \int e^{ikx} \frac{\partial \tilde{p}(k,t)}{\partial t} \mathrm{d}k = -\frac{D}{\sqrt{2\pi}} \int k^2 e^{ikx} \tilde{p}(k,t) \mathrm{d}k$$
$$\int e^{ikx} \frac{\partial \tilde{p}(k,t)}{\partial t} \mathrm{d}k = -\int Dk^2 e^{ikx} \tilde{p}(k,t) \mathrm{d}k$$
$$\Rightarrow \frac{\partial \tilde{p}(k,t)}{\partial t} = -Dk^2 \tilde{p}(k,t)$$
$$\int \frac{\mathrm{d}\tilde{p}(k,t)}{\tilde{p}(k,t)} \mathrm{d}k = -\int Dk^2 \mathrm{d}t$$
$$\ln p(\tilde{k},t) = -Dk^2 t + c_1$$
$$\tilde{p}(k,t) = c_2 e^{-Dk^2 t}$$

- initial condition: $\tilde{p}(k, t = 0) = c_2 e^0 = c_2 \Rightarrow \tilde{p}(k,t) = \tilde{p}(k, t = 0) e^{-Dk^2 t} = e^{-Dk^2 t}$

- spatial initial condition: $p(x, t = 0) = \delta(x - x_0)$

$\Rightarrow$ transformed initial condition: $\tilde{p}(k, t = 0) = \frac{1}{\sqrt{2\pi}} \int e^{-ikx} \delta(x - x_0) \mathrm{d}x = \frac{1}{\sqrt{2\pi}} e^{-ikx_0}$

- now the solution in Fourier space is known: $\tilde{p}(k, t) = \frac{1}{\sqrt{2\pi}} e^{-ikx_0} e^{-Dk^2 t}$

- we get $p(x, t)$ by the inverse transform

$$
\begin{aligned}
p(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \tilde{p}(k,t) \mathrm{d}k \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \frac{1}{\sqrt{2\pi}} e^{-ikx_0} e^{-Dk^2 t} \mathrm{d}k \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} e^{-ikx_0} e^{-Dk^2 t} \mathrm{d}k \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left\{ -Dt \left(k - \frac{i(x - x_0)}{2Dt} \right)^2 + Dt \left(\frac{i(x - x_0)}{2Dt} \right)^2 \right\} \mathrm{d}k \\
&= \frac{1}{2\pi} \exp\left\{ -\frac{(x - x_0)^2}{4Dt} \right\} \int_{-\infty}^{\infty} \exp\left\{ -Dt \left(k - \frac{i(x - x_0)}{2Dt} \right)^2 \right\} \mathrm{d}k \\
&= \frac{1}{2\pi} \exp\left\{ -\frac{(x - x_0)^2}{4Dt} \right\} \int_{-\infty}^{\infty} \exp\left\{ -Dtv^2 \right\} \mathrm{d}v \qquad \left(v = k - \frac{i(x - x_0)}{2Dt} \right) \\
&= \frac{1}{2\pi} \exp\left\{ -\frac{(x - x_0)^2}{4Dt} \right\} \sqrt{\frac{\pi}{Dt}} \qquad \left(\int_{-\infty}^{\infty} e^{-\alpha x^2} \mathrm{d}x = \sqrt{\frac{\pi}{\alpha}} \right) \\
&= \underline{\underline{\frac{1}{\sqrt{4\pi Dt}} \exp\left\{ -\frac{(x - x_0)^2}{4Dt} \right\}}} \qquad \text{Gaussian distribution}
\end{aligned}
$$

Discussion of the moments

- the zeroth moment $\langle x^0 \rangle$ represents the normalisation condition:

$$
\begin{aligned}
\langle x^0 \rangle &= \int_{-\infty}^{\infty} p(x,t) \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi Dt}} \exp\left\{ -\frac{(x - x_0)^2}{4Dt} \right\} \mathrm{d}x \qquad \left(y = x - x_0,\ \alpha = \frac{1}{4Dt} \right) \\
&= \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} e^{-\alpha y^2} \mathrm{d}y \\
&= \frac{1}{\sqrt{4\pi Dt}} \sqrt{\frac{\pi}{\alpha}} = \frac{1}{\sqrt{4\pi Dt}} \sqrt{4Dt\pi} = 1
\end{aligned}
$$

- the first moment can be calculated by

$$\begin{aligned}
\langle x^1\rangle(t) &= \int_{-\infty}^{\infty} x \frac{1}{\sqrt{4\pi Dt}} \exp\left\{-\frac{(x-x_0)^2}{4Dt}\right\} \mathrm{d}x \\
&= \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} (y+x_0) \exp\left\{-\frac{y^2}{4Dt}\right\} \mathrm{d}y \\
&= \frac{1}{\sqrt{4\pi Dt}} \underbrace{\int_{-\infty}^{\infty} y \exp\left\{-\frac{y^2}{4Dt}\right\} \mathrm{d}y}_{=0 \quad \text{(symmetry)}} + x_0 \underbrace{\frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} \exp\left\{-\frac{y^2}{4Dt}\right\} \mathrm{d}y}_{=1 \quad \text{(normalization)}} \\
&= \underline{\underline{x_0}}
\end{aligned}$$

- the second moment reads as

$$\begin{aligned}
\langle x^2\rangle(t) &= \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{4\pi Dt}} \exp\left\{-\frac{(x-x_0)^2}{4Dt}\right\} \mathrm{d}x \\
&= \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} (y+x_0)^2 \exp\left\{-\frac{y^2}{4Dt}\right\} \mathrm{d}y \qquad \left(\alpha = \frac{1}{4Dt}\right) \\
&= \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} y^2 \exp\left\{-\alpha y^2\right\} \mathrm{d}y + 0 + x_0^2 \\
&= -\frac{1}{\sqrt{4\pi Dt}} \frac{\mathrm{d}}{\mathrm{d}\alpha} \left(\int_{-\infty}^{\infty} \exp\left\{-\alpha y^2\right\} \mathrm{d}y \right) + x_0^2 \\
&= -\frac{1}{\sqrt{4\pi Dt}} \frac{\mathrm{d}}{\mathrm{d}\alpha} \left(\sqrt{\frac{\pi}{\alpha}} \right) + x_0^2 \\
&= \frac{1}{2} \frac{1}{\sqrt{4\pi Dt}} \sqrt{\frac{\pi}{\alpha^3}} + x_0^2 \\
&= \frac{1}{2} \frac{1}{\sqrt{4\pi Dt}} \sqrt{(4Dt)^3 \pi} + x_0^2 \\
&= \underline{\underline{2Dt + x_0^2}}
\end{aligned}$$

$\Rightarrow$ the average of the Gaussian distribution is independent from time

$\Rightarrow$ the standard deviation grows in time: $\sigma = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{2Dt} \sim \sqrt{t}$

$\Rightarrow$ every sharp initial distribution becomes broader

1.8 The drift-diffusion equation

- again we consider the probability density $p(x,t)$ in an interval $x \in [a,b]$
- we assume that a is a reflecting, b is an absorbing boundary
- the drift-diffusion equation is given by

$$\frac{\partial p}{\partial t} = \underbrace{-v\frac{\partial p}{\partial x}}_{\text{drift term}} + \underbrace{D\frac{\partial^2 p}{\partial x^2}}_{\text{diffusion term}}$$

$\Rightarrow$ v describes the velocity of the "motion" of the probability density $\Rightarrow$ tendency to move into a preferred direction

$\Rightarrow$ the diffusion equation is one special case ($v = 0$)

$\Rightarrow$ the opposite special case describes the deterministic drift ($D = 0$)

- the shape of the initial probability density is not changed
- the center of the probability density moves like a particle according to $x = vt + x_0$

$\Rightarrow$ we further assume $D > 0$ and search for solutions for arbitrary v

- the flux can be computed by the continuity equation $\frac{\partial p}{\partial t} + \frac{\partial j}{\partial x} = 0$

  $\Rightarrow$ according to the drift-diffusion equation the flux is given by $j(x,t) = vp(x,t) - D\frac{\partial p}{\partial x}$

  $\Rightarrow$ it can be proved easily that the probability flux obeying the drift-diffusion-equation also satisfies the continuity equation

  $\Rightarrow$ our boundary conditions can be written as:

$$\text{absorbing boundary:} \quad p(x = b, t) = 0$$

$$\text{reflecting boundary:} \quad j(x = a, t) = 0$$

  - we choose $p(x, t = 0) = \delta(x - x_0)$ as the initial condition

- initial condition: $p(x, t = 0) = \delta(x - x_0)$
- three steps to solve the problem:

1. dimensionless variables: $y = \frac{x-a}{b-a}$, $T = \frac{D}{(b-a)^2}t \qquad (y \in [0,1])$

   - transform of the probability density according to $p(x,t)\mathrm{d}x = P(y,T)\mathrm{d}y$

   $\Rightarrow$ we get a new drift-diffusion equation:

$$\frac{\partial P(y,T)}{\partial T} = -\Omega\frac{\partial P(y,T)}{\partial y} + \frac{\partial^2 P(y,T)}{\partial y^2} \quad \text{with} \quad \Omega = \frac{v}{D}(b-a)$$

$\Rightarrow$ new boundary conditions: $P(y=1,T)=0$
$J(y=0,T)=\left[\Omega P(y,T)-\frac{\partial P}{\partial y}\right]_{y=0}=0$

$\Rightarrow$ initial condition: $P(y,T=0)=\delta(y-y_0)$

2. transformation $Q(y,T)=e^{-\frac{\Omega}{2}y}P(y,T)$
   - drift-diffusion-equation:

$$\frac{\partial Q(y,T)}{\partial T}=-\frac{\Omega^2}{4}Q(y,T)+\frac{\partial^2 Q(y,T)}{\partial y^2}$$

   - boundary conditions: $Q(y=1,T)=0$, $\frac{\Omega}{2}Q(y=0,T)-\frac{\partial Q}{\partial y}\Big|_{y=0}=0$
   - initial condition: $Q(y,T=0)=e^{-\frac{\Omega}{2}y_0}\delta(y-y_0)$

3. method of separation of variables: $Q(y,T)=\chi(T)\psi(y)$
   - inserting the ansatz into the differential equation we receive:

$$\psi(y)\frac{\partial\chi(T)}{\partial T}=-\frac{\Omega^2}{4}\chi(T)\psi(y)+\chi(T)\frac{\partial^2\psi(y)}{\partial y^2}$$

   - dividing both sides of the equation by $Q(y,T)=\chi(T)\psi(y)$:

$$\frac{1}{\chi(T)}\frac{\partial\chi(T)}{\partial T}=-\frac{\Omega^2}{4}+\frac{1}{\psi(y)}\frac{\partial^2\psi(y)}{\partial y^2}$$

   - since the left side only depends on T whereas the other side only depends on y, both sides have to be constant (for instance equal to $-\lambda$)

$\Rightarrow$ we receive two ordinary differential equations:

$$\frac{1}{\chi(T)}\frac{\partial\chi(T)}{\partial T}=-\lambda,\qquad -\frac{\Omega^2}{4}+\frac{1}{\psi(y)}\frac{\partial^2\psi(y)}{\partial y^2}=-\lambda$$

$\Rightarrow$ we can rewrite them as

$$\frac{\partial\chi(T)}{\partial T}=-\lambda\,\chi(T),\qquad \frac{\partial^2\psi(y)}{\partial y^2}+\left(\lambda-\frac{\Omega^2}{4}\right)\psi(y)=0$$

$\Rightarrow$ the solution of both equations can be obtained easily as

$$\chi(T)=\chi_0 e^{-\lambda T},\quad \psi(y)=A\cos(ky)+B\sin(ky)\quad\left(k^2=\lambda-\frac{\Omega^2}{4}\right)$$

   - without loss of generality we set $\chi_0=1$
   - the parameter k is defined by the boundary conditions

$$\begin{aligned}\psi(y=1)=0 \quad &\Longrightarrow \quad A\,\cos(k)+B\,\sin(k)=0\\ \frac{\Omega}{2}\,\psi(y=0)-\frac{d\psi}{dy}\Big|_{y=0}=0 \quad &\Longrightarrow \quad A\,\frac{\Omega}{2}-B\,k=0\end{aligned}$$

- a nontrivial solution $(A, B) \neq (0, 0)$ exists if and only if

$$\begin{vmatrix} \cos(k) & \sin(k) \\ \frac{\Omega}{2} & -k \end{vmatrix} = 0 \quad \Longrightarrow k\,\cos(k) + \frac{\Omega}{2}\,\sin(k) = 0 \text{ or } \tan(k) = -\frac{2}{\Omega}\,k$$

  - unfortunately we cannot find an explicit expression for k_m as a solution of the transcendental equation $\tan k_m = -\frac{2}{\Omega} k_m$
  - nevertheless we get a discrete spectrum of eigenvalues k_m ($m = 0, 1, 2, \ldots$) since the left side is a periodic function whereas the right side is linear in k

- the constants A and B are connected to each other by

$$\frac{A}{B} = -\,\tan(k)$$

- that is why we can rewrite the formula for the eigenfunctions

$$\begin{aligned} \psi_m(y) &= A_m\,\cos(k_m\,y) + B_m\,\sin(k_m\,y) = B_m\,\left(\frac{A_m}{B_m}\,\cos(k_m\,y) + \sin(k_m\,y)\right) \\ &= B_m\,(-\,\tan(k_m)\,\cos(k_m\,y) + \sin(k_m\,y)) = R_m\,\sin(k_m\,(1-y)) \end{aligned}$$

  where $R_m = -\,\dfrac{B_m}{\cos(k_m)}$ is defined by orthonormalisation condition of the eigenfunctions $\psi_m(y)$ (see Fig. 6)

$$\int_0^1 \psi_m(y)\,\psi_n(y)\,dy = \delta_{mn}$$

$\Rightarrow$ the general solution can be written as an expansion of the eigenfunctions $\psi_m(y)$ according to the eigenvalues λ_m

$$Q(y,T) = \sum_{m=0}^{\infty} \chi_m(T)\psi_m(y) = \sum_{m=0}^{\infty} C_m\,e^{-\lambda_m T}\psi_m(y)$$

  with normalisation constants C_m which have to be found from δ–like initial condition

4. the final solution (see Fig. 7) reads as

$$P(y,T) = e^{\frac{\Omega}{2}(y-y_0)} \sum_{m=0}^{\infty} e^{-\lambda_m T}\psi_m(y_0)\psi_m(y)$$

- with eigenfunctions of the ground state ($m = 0$)

$$\psi_0(y) = \begin{cases} \sqrt{\dfrac{2}{1 + \frac{\Omega}{2}\,\frac{1}{\tilde{k}_0^2 + \Omega^2/4}}}\,\sin\left[\tilde{k}_0(1-y)\right], & \Omega > -2 \\ \sqrt{3}\,(1-y)\,, & \Omega = -2 \\ \sqrt{-\dfrac{2}{1 + \frac{\Omega}{2}\,\frac{1}{-\kappa_0^2 + \Omega^2/4}}}\,\sinh\left[\kappa_0(1-y)\right], & \Omega < -2 \end{cases}$$

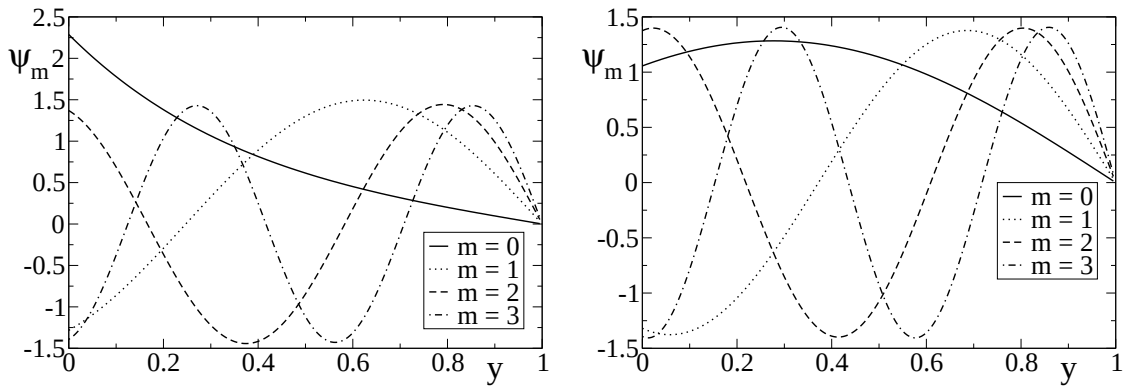

Figure 6: The eigenfunctions $\psi_m(y)$ for $m = 0, 1, 2, 3$ and for $\Omega = -5.0$ (left) and $\Omega = 3.0$ (right).

and all other eigenfunctions

$$\psi_m(y) = \sqrt{\frac{2}{1 + \frac{\Omega}{2}\frac{1}{\tilde{k}_m^2 + \Omega^2/4}}}\, \sin\left[\tilde{k}_m(1-y)\right] \qquad m = 1, 2, \ldots$$

- the eigenvalue of the ground state ($m = 0$) is given by

$$\lambda_0 = \begin{cases} \tilde{k}_0^2 + \Omega^2/4\,, & \Omega > -2 \\ 1\,, & \Omega = -2 \\ -\kappa_0^2 + \Omega^2/4\,, & \Omega < -2 \end{cases}$$

and all others are

$$\lambda_m = \tilde{k}_m^2 + \Omega^2/4 \qquad m = 1, 2, \ldots$$

where the wave numbers are calculated by a transcendental equation

$$\begin{aligned} \tilde{k}_0 \quad &: \quad \tan\tilde{k}_0 = -\frac{2}{\Omega}\,\tilde{k}_0 \qquad \Omega > -2 \\ \kappa_0 \quad &: \quad \tanh\kappa_0 = -\frac{2}{\Omega}\,\kappa_0 \qquad \Omega < -2 \\ \tilde{k}_m \quad &: \quad \tan\tilde{k}_m = -\frac{2}{\Omega}\,\tilde{k}_m \qquad m = 1, 2, \ldots \end{aligned}$$

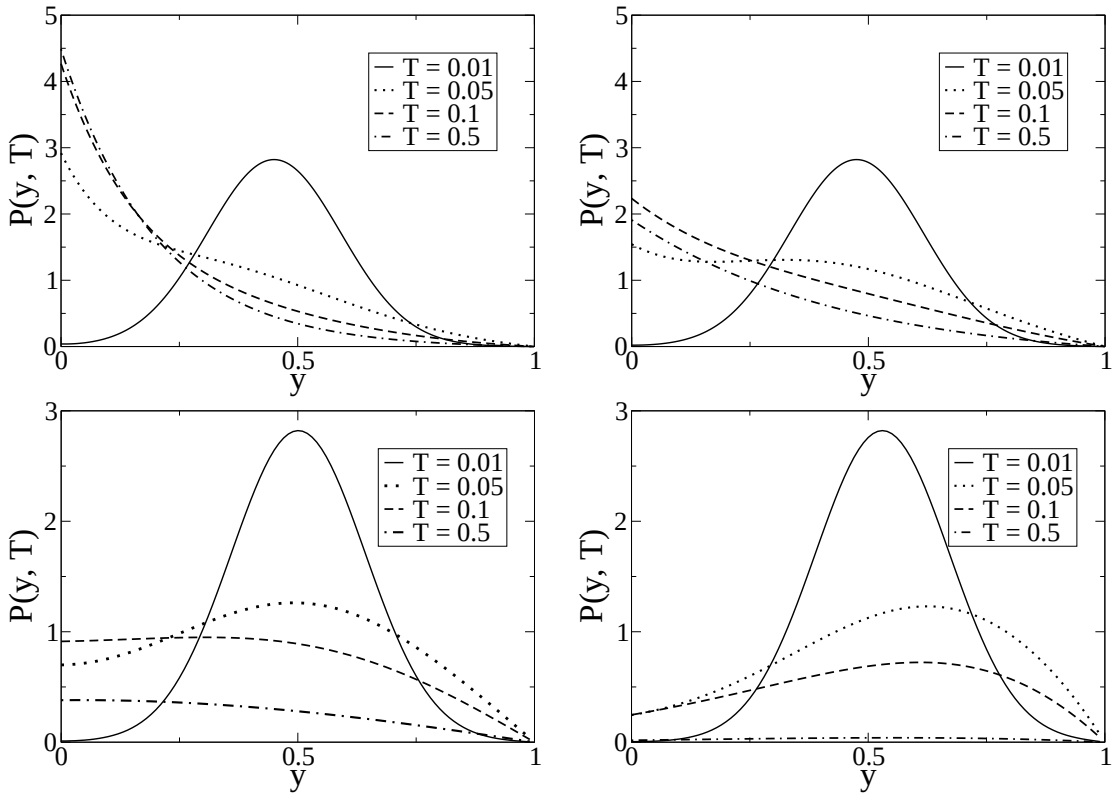

Figure 7: The solution of drift–diffusion Fokker–Planck equation with initial condition $y_0 = 0.5$ for different values of the control parameter Ω, i. e. $\Omega = -5.0$ (top left), $\Omega = -2.5$ (top right), $\Omega = 0.1$ (bottom left), $\Omega = 3.0$ (bottom right).

1.9 Homework on the drift–diffusion equation

1. Prove the orthogonality and normalisation of the set of eigenfunctions $\psi_m(y)$ as solutions for the drift–diffusion problem (dimensionless variables) in the simplest case of $\Omega = 0$ (pure diffusion) as well as for general Ω, i. e., prove the relation

$$\int_0^1 \psi_m(y)\psi_n(y)dy = \delta_{nm} \ .$$

2. Prove the completeness of the set of eigenfunctions $\psi_m(y)$ as solutions for the drift–diffusion problem (dimensionless variables) in the simplest case of $\Omega = 0$ (pure diffusion) as well as for general Ω, i. e., prove the relation

$$\sum_{m=0}^{\infty} \psi_m(y')\psi_m(y) = \delta(y - y') \ .$$

   Hint:

$$\lim_{N\to\infty} \sum_{m=0}^{N} \int_0^1 \psi_m(y')\psi_m(y)dy' = \int_0^1 \delta(y - y')dy' = 1 \ .$$

1.10 The Fokker-Planck Equation

- the Fokker-Planck equation is a generalisation of the drift-diffusion equation

$$\frac{\partial p(x,t)}{\partial t} = \underbrace{-\frac{\partial}{\partial x}\left[a(x)p(x,t)\right]}_{\text{drift term}} + \underbrace{\frac{1}{2}\frac{\partial^2}{\partial x^2}\left[b^2(x)p(x,t)\right]}_{\text{diffusion term}}$$

- the right side can be interpreted as the first leading terms of a Taylor expansion of the Master-equation
- this expansion is referred to as the Kramers-Moyal-expansion
- the drift-diffusion equation is equivalent to the special case $a(x) = v$, $\frac{1}{2}b^2(x) = D$
    - considering natural boundaries the solution is some kind of Gaussian function with moving and broadening profile:

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

    - for instance, this solution can describe an asymmetric (inclined) Galton board

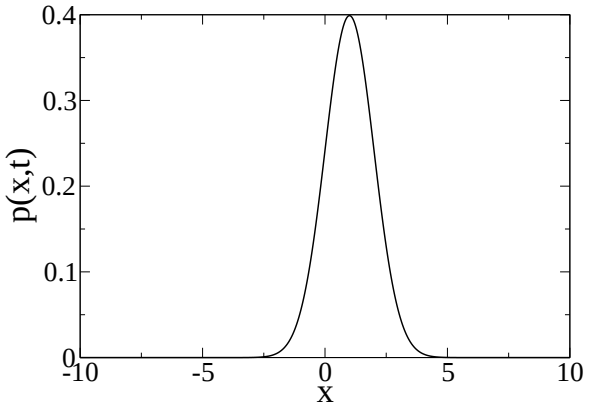

Figure 8: The solution $p(x,t)$ of drift–diffusion equation with constant drift $v = 1$ m/s and diffusion $D = 1$ m^2/s fo $t = 1$ s and $x_0 = 0$ m.

- the stochastic equation of motion is usually written in the form

$$\mathrm{d}x(t) = \underbrace{a(x(t))\mathrm{d}t}_{\text{drift}} + \underbrace{b(x(t))\mathrm{d}W(t)}_{\text{diffusion}}$$

    - the first term describes the deterministic part: $\frac{\mathrm{d}x(t)}{\mathrm{d}t} = a(x(t))$
    - the second term describes the stochastic part

- $x(t)$ describes a stochastic trajectory

$$x(t) - x_0 = \int_0^t a(x)\mathrm{d}t + \int_0^t b(x)\mathrm{d}W(t)$$

- for computing the probability for being at point x at time t we have to integrate over all trajectories which satisfy $x(t_0) = x_0$

- equation of motion for the Wiener process:
  $a = 0,\ b = 1 \Rightarrow \mathrm{d}x(t) = \mathrm{d}W(t)\ ,\ x(t = 0) = x_0 = 0$

  - the probability density equals to the Gaussian Normal distribution $N(0, 1)$
  - the first moments are then given by $\langle W(t)\rangle = 0,\ \langle W^2(t)\rangle = t$ (compare with diffusion process with $b = 2D = 1$)
  - increment of the Wiener process: $\mathrm{d}W(t) = W(t + \mathrm{d}t) - W(t)$
  - Wiener process (mathematically) is also referred to as white noise (in physics)
  - from $\sqrt{\langle W^2(t)\rangle} = \sqrt{t}$ we find $\mathrm{d}W(t) = Z\sqrt{\mathrm{d}t}$ with Z being a random number
  - for simulation we can use the following algorithm:
    1. generate initial state $x(t = 0) = x_0 = 0$
    2. Do-Loop $t \in [0, t_{max}]$:
       a) Generate random numbers $Z \propto N(0, 1)$ by the help of two uniformly distributed random numbers from $[0, 1]$ (Box-Müller-algorithm)
       b) Compute $\Delta W = Z\sqrt{\Delta t}$
       c) Calculate $\Delta x = \Delta W$
       d) Compute new point $x = x + \Delta x$ at new time $t = t + \Delta t$
  - in physics the equation of motion for the drift–diffusion process is often written in the following form:

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = a(x(t)) + b(x(t))\frac{\mathrm{d}W(t)}{\mathrm{d}t} \qquad \text{(Langevin equation)}$$

  - since the probability $W(t)$ is not always differentiable, its derivative does not exist
  - nevertheless we formally call $\xi(t) = \frac{\mathrm{d}W(t)}{\mathrm{d}t}$ the noise intensity or stochastic force (defined by the first and second moment)

1.11 The Ornstein-Uhlenbeck process

- up to now we only examined the spatial distribution in diffusion and drift processes

- in systems of physical interest the velocity distribution is also an important quantity

- we assume that the particles in a closed system are not disturbed by external forces but internal friction

- we describe the motion of a single particle by Newton's equation $m\frac{\mathrm{d}v}{\mathrm{d}t} = F(x, v, t)$

- the friction force is considered to be proportional to the velocity of a particle: $F_f(v) = -m\gamma v$

- since the particles do not stop after a period of time we assume that a second force keeps them moving: $F_s(t)\mathrm{d}t = m\sqrt{2B}\,\mathrm{d}W(t)$

    - this force can be understood as being caused by collisions between particles and is distributed stochastically
    - the average of all stochastic forces have to vanish: $\langle \mathrm{d}W(t)\rangle = 0$ (otherwise the particles would slow down or accelerate in average)
    - the correlation function shall be given by $\langle \mathrm{d}W(t)\mathrm{d}W(t')\rangle = \mathrm{d}t\delta(t - t')$

- the definition of the velocity can be written as

$$\mathrm{d}x = v\mathrm{d}t$$

- thus, the change of the velocity is given by

$$\mathrm{d}v = \underbrace{-\gamma v\mathrm{d}t}_{\text{friction}} + \underbrace{\sqrt{2B}\mathrm{d}W(t)}_{\text{stochastic part}}$$

- the corresponding Fokker-Planck-equation reads as

$$\frac{\partial p}{\partial t} = \underbrace{-\frac{\partial}{\partial x}(vp)}_{\text{spatial drift term}} - \underbrace{\frac{\partial}{\partial v}(-\gamma v p)}_{\text{velocity drift term}} + \underbrace{\frac{\partial^2}{\partial v^2}(Bp)}_{\text{velocity diffusion term}}$$

- we choose the initial condition: $p(x, v, t = 0) = \delta(x - x_0)\delta(v - v_0)$

- for solving this partial differential equation we introduce the Fourier transform with respect to x and v:

$$p(x, v, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}k_x\mathrm{d}k_v \exp\{ik_x x\}\exp\{ik_v v\}\,\tilde{p}(k_x, k_v, t)$$

- we receive the following equation:

$$\frac{\partial}{\partial t}\tilde{p}(k_x, k_v, t) + [\gamma k_v - k_x]\frac{\partial}{\partial k_v}\tilde{p}(k_x, k_v, t) = -Bk_v^2\tilde{p}(k_x, k_v, t)$$

- we define $\bar{k}_v$ such that $\frac{\partial}{\partial\tau}\bar{k}_v = \gamma\bar{k}_v - x$

- applying this ansatz our original Fokker-Planck-equation reduces to an ordinary differential equation:

$$\frac{\partial}{\partial t}\tilde{p} = -B\bar{k}_v^2\tilde{p} \quad \text{for} \quad 0 \leq \tau \leq t \quad \bar{k}_v(\tau = t) = k_v$$

- the solution for $\bar{k}_v$ can be found easily as

$$\bar{k}_v(\tau) = \left[k_v - \frac{k_x}{\gamma}\right] \exp\left\{\gamma(\tau - t)\right\} + \frac{k_x}{\gamma}$$

- we can now insert this result into the differential equation $\frac{\partial}{\partial t}\tilde{p} = -B\bar{k}_v^2\tilde{p}$ and receive

$$\begin{aligned}
\tilde{p}(k_x, k_v, t) &= \frac{1}{2\pi} e^{-ik_x x_0} e^{-iv_0(A+C)} e^{-\Phi(t)} \\
\text{with } \Phi(t) &= B\left[\frac{A^2}{2\gamma}\left(e^{2\gamma t} - 1\right) + C^2 t + 2\frac{AC}{\gamma}\left(e^{\gamma t} - 1\right)\right] \\
A &= \left[k_v - \frac{k_x}{\gamma}\right] e^{-\gamma t} \\
C &= \frac{k_x}{\gamma}
\end{aligned}$$

- of course we are interested in the physical properties of the solutions

- if we examine the velocity distribution, we have to integrate $p(x, v, t)$ over space:

$$p_v(v, t) = \int_{-\infty}^{\infty} \mathrm{d}x\, p(x, v, t)$$

  - using the inverse Fourier transform with respect of x of our solution we receive

$$p_v(v, t) = \sqrt{2\pi}\left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\, p(x, v, t) e^{-ik_x x}\Big|_{k_x = 0}\right] = \sqrt{2\pi}\mathcal{F}\left\{\tilde{p}(k_x = 0, v, t)\right\}$$

  $\Rightarrow$ our result reads as

$$p_v(v, t) = \frac{1}{\sqrt{2\pi\sigma_v^2(t)}} \exp\left\{-\frac{\left(v - v_0 e^{-\gamma t}\right)^2}{2\sigma_v^2(t)}\right\} \quad \text{with} \quad \sigma_v^2(t) = \frac{B}{\gamma}\left(1 - e^{-2\gamma t}\right)$$

  $\Rightarrow$ the limit of time approaching infinity can be computed as

$$\lim_{t\to\infty} \sigma_v^2(t) = \frac{B}{\gamma}, \qquad \lim_{t\to\infty} p_v(v, t) = \frac{1}{\sqrt{2\pi\frac{B}{\gamma}}} \exp\left\{-\frac{v^2}{2\frac{B}{\gamma}}\right\}$$

  - the distribution does not depend on time anymore $\Rightarrow$ stationary solution

$\Rightarrow$ with defining $B = \gamma \frac{k_B T}{m}$ the result equals to the Maxwell-Boltzmann-velocity distribution of an ideal gas:

$$\lim_{t\to\infty} p_v(v,t) = \frac{1}{\sqrt{2\pi \frac{k_B T}{m}}} \exp\left\{ -\frac{v^2}{2\frac{k_B T}{m}} \right\}$$

- the second case $t \to 0$ can be found as

$$\lim_{t\to 0} \sigma_v^2(t) = 0, \quad \lim_{t\to 0} p_v(v,t) = \frac{1}{\sqrt{2\pi\sigma_v^2(0)}} \exp\left\{ -\frac{(v-v_0)^2}{2\sigma_v^2(0)} \right\} = \delta(v - v_0)$$

$\Rightarrow$ all particles start with the same velocity v_0

- considering the spatial distribution $p_x(x,t)$ the same method can be applied
  - in this case the variance reads as

$$\sigma_x^2(t) = \frac{2B}{\gamma^2} t - 3\frac{B}{\gamma^3} + 4\frac{B}{\gamma^3} e^{-\gamma t} - \frac{B}{\gamma^3} e^{-2\gamma t}$$

  - for $t \to \infty$ we receive the variance of the diffusion process: $\sigma_x(t \to \infty) \simeq \frac{2B}{\gamma^2} t = 2Dt$
  - since the variance depends on time, this solution cannot be stationary
  - this fact can be understand if we consider that the system should find an equilibrium state after some relaxation time

- the space-velocity-distribution $p(x,v,t)$ (see Fig. 9) can be found by the inverse transform of $\tilde{p}(k_x, k_v, t)$ resulting in

$$\begin{aligned}
p(x,v,t) &= \frac{1}{\sqrt{2\pi 2\sigma_v^2}} \exp\left[-\frac{1}{2} \frac{(v-\mu_v)^2}{2\sigma_v^2} \right] \frac{1}{\sqrt{2\pi 2\bar{\sigma}_x^2}} \exp\left[-\frac{1}{2} \frac{(x-\bar{\mu}_x)^2}{2\bar{\sigma}_x^2} \right] \\
\bar{\mu}_x &= \mu_x + \frac{(v-\mu_v)\sigma_{xv}^2}{2\sigma_v^2} \\
\bar{\sigma}_x^2 &= \sigma_x^2 - \frac{\sigma_{xv}^4}{4\sigma_v^2} \\
\mu_x &= x_0 + \frac{v_0}{\gamma} \left[1 - \exp(-\gamma t) \right] \\
\mu_v &= v_0 \exp(-\gamma t) \\
\sigma_x^2 &= \frac{B}{2\gamma^3} \left[1 - \exp(-2\gamma t) \right] + \frac{B}{\gamma^2} t - 2\frac{B}{\gamma^3} \left[1 - \exp(-\gamma t) \right] \\
\sigma_v^2 &= \frac{B}{2\gamma} \left[1 - \exp(-2\gamma t) \right] \\
\sigma_{xv}^2 &= -\frac{B}{\gamma^2} \left[1 - \exp(-2\gamma t) \right] + 2\frac{B}{\gamma^2} \left[1 - \exp(-\gamma t) \right]
\end{aligned}$$

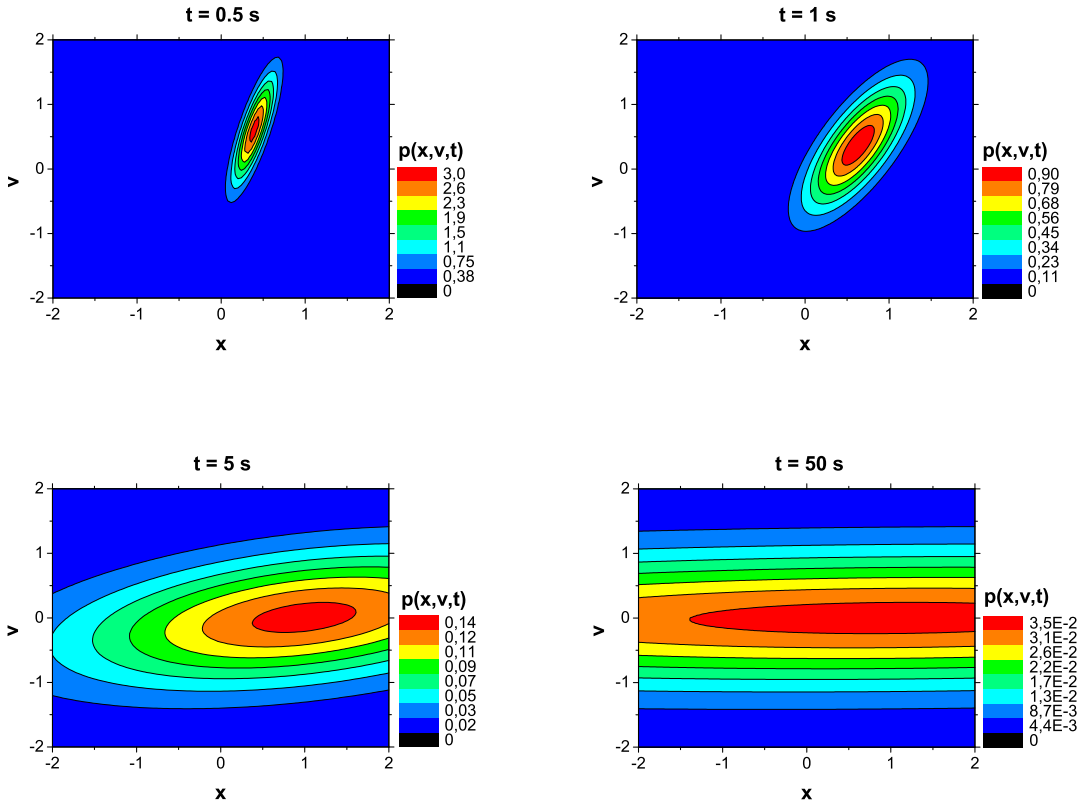

Figure 9: Snapshots of space–velocity–distribution of Ornstein–Uhlenbeck process at different time moments. Set of parameters: $B = 0.5\ \mathrm{m}^2/\mathrm{s}^3\,; \gamma = 1\ \mathrm{s}^{-1}$, initial conditions $x_0 = 0\ \mathrm{m}\,; v_0 = 1\ \mathrm{m/s}$.

2 The Master equation

2.1 Basic equation

- the Master equation describes continuous random walk processes
- the probability density of being at position x at time t can be composed of two terms
  - being at some position x' and doing a step from x' to x: $w(x,x')p(x',t)$
  - being at position x and walking to some different position x': $w(x',x)p(x,t)$
  - $w(x,x')$ describes the transition rate for a step from x' to x and is independent from time in our considerations

  $\Rightarrow$ the time derivative of the probability density $p(x,t)$ is the difference of both parts integrated over all positions x'

$$\Rightarrow \frac{\partial p(x,t)}{\partial t} = \int \{w(x,x')p(x',t) - w(x',x)p(x,t)\}\,\mathrm{d}x'$$

  - normalisation condition: $\int p(x,t)\mathrm{d}x = 1$
- in case of discrete states the Master equation reads as

$$\frac{\mathrm{d}P(n,t)}{\mathrm{d}t} = \sum_{n\neq n'} \Big\{ w(n,n')P(n',t) - w(n',n)P(n,t) \Big\} \qquad (0 \leq n \leq N)$$

- for closed systems $\left(\sum_n P(n,t) = 1\right)$ we can find a stationary solution:

$$\lim_{t\to\infty} P(n,t) = P^{St}(n) \quad \Leftrightarrow \quad \lim_{t\to\infty} \frac{\mathrm{d}P(n,t)}{\mathrm{d}t} = 0$$

- equilibrium states are special stationary states: $\frac{\mathrm{d}P(n,t)}{\mathrm{d}t} = 0,\ P(n,t) = P^{eq}(n)$

$\Rightarrow$ a stronger condition is called the detailed balance: every summand of the sum vanishes

$$w(n,n')P^{eq}(n') - w(n',n)P^{eq}(n) = 0$$

2.2 General solution

- since the Master equation is a set of linear differential equations we can write it as a vectorial equation

$$\vec{P}(t) = \begin{pmatrix} P(0,t) \\ \vdots \\ P(N,t) \end{pmatrix}, \quad W(n,n') = \begin{cases} w(n,n') & n \neq n' \\ -\sum\limits_{m\neq n} w(m,n) & n = n' \end{cases}$$

$$\Rightarrow \frac{\mathrm{d}\vec{P}(t)}{\mathrm{d}t} = \hat{W}\vec{P}(t)$$

- properties of the matrix of coefficients: $W(n,n') \geq 0, \quad \sum_n W(n,n') = 0$

$\Rightarrow$ formal representation of the solution:

$$\vec{P}(t) = \vec{P}(0)e^{\hat{W}t} \quad \text{with } e^{\hat{W}t} := \sum_{m=0}^{\infty} \frac{1}{m!}(\hat{W}t)^m$$

$\Rightarrow$ in this case the time derivative of the exponential function reads as

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}e^{\hat{W}t} &= \sum_{m=0}^{\infty} \frac{1}{m!}\hat{W}^m m t^{m-1} \\ &= \hat{W}\sum_{m=1}^{\infty} \frac{1}{(m-1)!}\hat{W}^{m-1}t^{m-1} \\ &= \hat{W}\sum_{m=0}^{\infty} \frac{1}{m!}\hat{W}^m m t^m = \hat{W}e^{\hat{W}t} \end{aligned}$$

$\Rightarrow$ thus it is obvious that the formal solution obeys the Master equation

- for an explicit solution it is convenient to write the solution as a linear combination of eigenstates

$$\vec{P}(t) = \sum_{i=0}^{N} c_i \vec{u}_i e^{\lambda_i t} \qquad \text{with eigenvectors } \vec{u}_i : \ \hat{W}\vec{u}_i = \lambda_i \vec{u}_i$$

$\Rightarrow$ the vectors $\vec{u}_i$ $(0 \leq i \leq N)$ are eigenvectors of the matrix $\hat{W}$

- for finding the general solution we define $\tilde{W}(n,n')$ as follows:

$$\tilde{W}(n,n') := W(n,n')\sqrt{\frac{P^{eq}(n')}{P^{eq}(n)}}$$

- $P^{eq}(n)$ are the equilibrium states (see above)
- we want to solve its eigenvalue equation: $\hat{W}\vec{u}_i = \lambda_i \vec{u}_i$
  - explicitly written: $\sum_{n'} W(n,n')u_i(n') = \lambda_i u_i(n)$
  - in terms of $\tilde{W}(n,n')$ it reads as $\sum_{n'} \tilde{W}(n,n')\sqrt{\frac{P^{eq}(n)}{P^{eq}(n')}}u_i(n') = \lambda_i u_i(n)$

  $\Rightarrow$ we introduce new eigenvectors defined by $u_i(n) = \sqrt{P^{eq}(n)}\tilde{u}_i(n)$

  $\Rightarrow$ the probabilities have to be transformed as well: $P(n,t) = \sqrt{P^{eq}(n)}\tilde{P}(n,t)$

  $\Rightarrow$ our new eigenvalue equation reads as $\tilde{W}\tilde{\vec{u}}_i = \lambda_i \tilde{\vec{u}}_i$
- for equilibrium states the condition $W(n,n')P^{eq}(n') = W(n',n)P^{eq}(n)$ has to be fulfilled (see detailed balance equation)

$$\Rightarrow \tilde{W}(n,n') = W(n,n')\sqrt{\frac{P^{eq}(n')}{P^{eq}(n)}} = W(n',n)\sqrt{\frac{P^{eq}(n)}{P^{eq}(n')}} = \tilde{W}(n',n)$$

- since $\tilde{W}$ is a symmetric matrix, its eigenvalues are real and its eigenvectors are orthogonal

  $\Rightarrow$ we can normalise the eigenvectors such that $\tilde{\vec{u}}_i \cdot \tilde{\vec{u}}_j = \sum_n \tilde{u}_i(n)\tilde{u}_j(n) = \delta_{ij}$

$\Rightarrow$ the general solution of such a system of linear differential equations can be written as

$$\tilde{\vec{P}}(t) = \sum_{i=0}^{N} c_i \tilde{\vec{u}}_i e^{\lambda_i t} \quad \text{or} \quad \tilde{P}(n,t) = \sum_{i=0}^{N} c_i \tilde{u}_i(n) e^{\lambda_i t}$$

- the c_i are defined by the transformed initial condition $\tilde{\vec{P}}(0) = \sum_{i=0}^{N} c_i \tilde{\vec{u}}_i$ and can be computed by

$$c_i = \tilde{\vec{u}}_i \cdot \tilde{\vec{P}}(0) = \sum_{n=0}^{N} \tilde{u}_i(n)\tilde{P}(n,0) = \sum_{n=0}^{N} \frac{\tilde{u}_i(n)P(n,0)}{\sqrt{P^{eq}(n)}}$$

- inserting the result the general solution reads as:

$$P(n,t) = \sqrt{P^{eq}(n)}\tilde{P}(n,t) = \sqrt{P^{eq}(n)} \sum_{i=0}^{N} c_i \tilde{u}_i(n) e^{\lambda_i t}$$
$$= \sqrt{P^{eq}(n)} \sum_{i=0}^{N} \tilde{u}_i(n) e^{\lambda_i t} \sum_{m=0}^{N} \tilde{u}_i(m) \frac{P(m,0)}{\sqrt{P^{eq}(m)}}$$

- the equilibrium solution is described by the eigenvalue $\lambda_0 = 0$:

  $\Rightarrow$ since $\lim_{t\to\infty} e^{\lambda t} \to 0$ for all $\lambda \neq 0$, we compute

$$P^{eq}(n) = \lim_{t\to\infty} P(n,t) = \sqrt{P^{eq}(n)}\tilde{u}_0(n) \sum_{m=0}^{N} \tilde{u}_0(m) \frac{P(m,0)}{\sqrt{P^{eq}(m)}}$$

$\Rightarrow$ $P(n,t) = P^{eq}(n) + \sqrt{P^{eq}(n)} \sum_{i:\lambda_i \neq 0} \tilde{u}_i(n) e^{\lambda_i t} \sum_{m=0}^{N} \tilde{u}_i(m) \frac{P(m,0)}{\sqrt{P^{eq}(m)}}$

2.3 One-step master equation

- we now consider a system of n states $n = 0, 1, 2, \ldots, N$ with transitions $n \to n \pm 1$

$\Rightarrow$ Master equation (see Fig. 10):

$$\frac{\mathrm{d}P(n,t)}{\mathrm{d}t} = W_+(n-1)P(n-1,t) + W_-(n+1)P(n+1,t) - \big[W_+(n) + W_-(n)\big]P(n,t)$$

with $W_+(n-1) = w(n, n-1)$ and $W_-(n+1) = w(n, n+1)$

- considering closed boundaries: $P(-1) = W_-(0) = W_+(N) = P(N+1) = 0$

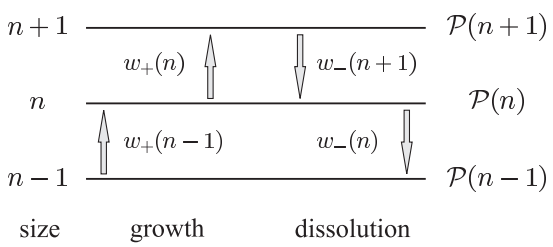

Figure 10: Schematic illustration of one-step master equation.

- left boundary $n = 0$: $\frac{\mathrm{d}P(0,t)}{\mathrm{d}t} = W_-(1)P(1,t) - W_+(0)P(0,t)$
- right boundary $n = N$: $\frac{\mathrm{d}P(N,t)}{\mathrm{d}t} = W_+(N-1)P(N-1,t) - W_-(N)P(N,t)$

- we are now looking for stationary solutions: $P(n,t) = P(n)$, $\frac{\mathrm{d}P(n,t)}{\mathrm{d}t} = 0$
- rewriting the equations with the flux:
  $J(n,t) = W_-(n)P(n,t) - W_+(n-1)P(n-1,t)$

  $\Rightarrow$ condition for stationarity: $\frac{\mathrm{d}P(n,t)}{\mathrm{d}t} = J(n+1,t) - J(n,t) \stackrel{!}{=} 0$

  $\Rightarrow$ starting at the left boundary we find $\frac{\mathrm{d}P(0,t)}{\mathrm{d}t} = J(1,t) = 0$

  $\Rightarrow$ we can directly conclude $\frac{\mathrm{d}P(1,t)}{\mathrm{d}t} = J(2,t) - J(1,t) = J(2,t) = 0$

  $\Rightarrow$ a solution is stationary if all $J(n,t) = W_-(n)P(n,t) - W_+(n-1)P(n-1,t)$ vanish to zero

$\Rightarrow$ from $W_+(n-1)P(n-1) = W_-(n)P(n)$ we can compute the probabilities step by step:

$$P^{st}(1) = P^{st}(0)\frac{W_+(0)}{W_-(1)}, \quad P^{st}(n+1) = P^{st}(n)\frac{W_+(n)}{W_-(n+1)}$$

$\Rightarrow$ for $n = 2$ the solution reads as $P^{st}(2) = P^{st}(1)\frac{W_+(1)}{W_-(2)} = P^{st}(0)\frac{W_+(1)}{W_-(2)}\frac{W_+(0)}{W_-(1)}$

$\Rightarrow$ the general stationary solution can be written as

$$P^{st}(n) = P^{st}(0)\prod_{m=1}^{n}\frac{W_+(m-1)}{W_-(m)}$$

$\Rightarrow$ the factor $P^{st}(0)$ can be found by the normalisation condition: $\sum_{n=0}^{N} P^{st}(n) = 1$

$$\Rightarrow P^{st}(0) = \frac{1}{1 + \sum_{n=1}^{N}\prod_{m=1}^{n}\frac{W_+(m-1)}{W_-(m)}}$$

2.4 Simple example: dissolution of traffic jam

- we now choose special transition rates: $W_+(n) = 0,\ W_-(n) = \frac{1}{\tau}$
- only transitions to lower states are possible
- e. g. queue of cars: observation of cars leaving the cluster
- let n_0 be the initial cluster length (number of cars in the cluster)

$\Rightarrow$ the Master equation reads as:

$$\begin{aligned}
\frac{\partial P(n,t)}{\partial t} &= \frac{1}{\tau}\big[P(n+1,t) - P(n,t)\big] \qquad (1 \le n \le n_0 - 1) \\
\frac{\partial P(n_0,t)}{\partial t} &= -\frac{1}{\tau}P(n_0,t) \\
\frac{\partial P(0,t)}{\partial t} &= \frac{1}{\tau}P(1,t)
\end{aligned}$$

- initial condition: $P(n, t = 0) = \delta_{n,n_0}$

2.4.1 Direct method

- to calculate the solution we start at $n = n_0$:
  - $\frac{\partial P(n_0,t)}{\partial t} = -\frac{1}{\tau}P(n_0,t) \Rightarrow P(n_0,t) = \exp\big\{-\frac{t}{\tau}\big\}$
  - equation for $n_0 - 1$: $\frac{\partial P(n_0-1,t)}{\partial t} = \frac{1}{\tau}\big[\exp\big\{-\frac{t}{\tau}\big\} - P(n_0-1,t)\big]$

  $\Rightarrow$ this equation can be solved with standard methods of linear differential equations:
    - solution of the homogeneous equation: $P(n_0 - 1, t) = \exp\big\{-\frac{t}{\tau}\big\}$
    - inhomogeneous equation: variation of constants:

    $\Rightarrow$ we insert $P(n_0 - 1, t) = C(t)\exp\big\{-\frac{t}{\tau}\big\}$ into the differential equation and compute $C(t) = \frac{t}{\tau} + C_2$

    $\Rightarrow$ the constant C_2 is determined by the initial condition $P(n_0 - 1, t) = 0 \Rightarrow C_2 = 0$

    $\Rightarrow$ we receive $P(n_0 - 1, t) = \frac{t}{\tau}\exp\{-\frac{t}{\tau}\}$
  - these steps are repeated for $P(n_0 - 2, t), \ldots$

  $\Rightarrow$ it can be shown that the solution for $n \ge 1$ has the following form (see Fig. 11):

$$P(n,t) = \frac{1}{(n_0-n)!}\left(\frac{t}{\tau}\right)^{n_0-n} e^{-\frac{t}{\tau}} \quad \text{or} \quad P(n_0-m,t) = \frac{1}{m!}\left(\frac{t}{\tau}\right)^{m} e^{-\frac{t}{\tau}}$$

  $\Rightarrow$ for instance $P(n_0,t) = e^{-\frac{t}{\tau}}, P(n_0-1,t) = \big(\frac{t}{\tau}\big)\,e^{-\frac{t}{\tau}}$, $P(n_0-2,t) = \frac{1}{2!}\big(\frac{t}{\tau}\big)^2 e^{-\frac{t}{\tau}}, \ldots$

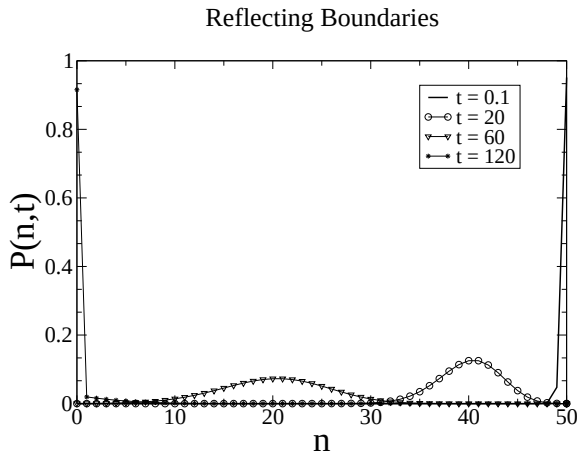

Figure 11: Probability $P(n,\, t)$ for the case of reflecting boundaries at $n = 0$ and $n = N$ with the initial condition $P(n,\, 0) = \delta_{n,\, N}$, $(\tau = 2)$.

$\Rightarrow$ the solution for $n = 0$ can be found be the normalisation condition:

$$\Rightarrow P(0,t) = 1 - \sum_{m=0}^{n_0-1} \frac{1}{m!} \left(\frac{t}{\tau}\right)^m e^{-\frac{t}{\tau}}$$

- for a better understanding it is often useful to compute moments:
  - first moment:

$$\begin{aligned}
\langle n \rangle(t) &= \sum_{n=0}^{n_0} nP(n,t) = \sum_{n=1}^{n_0} \frac{n}{(n_0-n)!} \left(\frac{t}{\tau}\right)^{n_0-n} e^{-\frac{t}{\tau}} \\
&= \sum_{n=1}^{n_0} \frac{n-n_0}{(n_0-n)!} \left(\frac{t}{\tau}\right)^{n_0-n} e^{-\frac{t}{\tau}} + \sum_{n=1}^{n_0} \frac{n_0}{(n_0-n)!} \left(\frac{t}{\tau}\right)^{n_0-n} e^{-\frac{t}{\tau}} \\
&= -\frac{t}{\tau} \sum_{n=1}^{n_0-1} \frac{1}{(n_0-n-1)!} \left(\frac{t}{\tau}\right)^{n_0-n-1} e^{-\frac{t}{\tau}} \\
&\quad + \sum_{n=1}^{n_0} \frac{n_0}{(n_0-n)!} \left(\frac{t}{\tau}\right)^{n_0-n} e^{-\frac{t}{\tau}}
\end{aligned}$$

  - substituting $m = n_0 - n - 1$ we receive

$$\langle n \rangle(t) = -\frac{t}{\tau} \sum_{m=0}^{n_0-2} \frac{1}{m!} \left(\frac{t}{\tau}\right)^m e^{-\frac{t}{\tau}} + \sum_{m=0}^{n_0-1} \frac{n_0}{m!} \left(\frac{t}{\tau}\right)^m e^{-\frac{t}{\tau}}$$

  - for reasons of convenience we define $Q(n,t) = e^{-\frac{t}{\tau}} \sum_{m=0}^{n} \frac{1}{m!} \left(\frac{t}{\tau}\right)^m$ and can write the first moment as

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

- in case of $n \gg 1,\ \frac{t}{\tau} \sim 1$ we compute $Q(n,t) \simeq 1$

  $\Rightarrow$ the average of n decreases linearly: $\langle n \rangle(t) \simeq n_0 - \frac{t}{\tau}$

  !! at the end of this process $n \gg 1,\ t \sim \tau$ is violated $\Rightarrow$ graph is not linear anymore

- variance

$$\begin{aligned}\langle n^2 \rangle - \langle n \rangle^2 = \ & n_0 \big[n_0 Q(n_0 - 1, t) - \tfrac{2t}{\tau} Q(n_0 - 2, t) \big] \times \big(1 - Q(n_0 - 1, t) \big) \\ & + \big(\tfrac{t}{\tau} \big)^2 \big[Q(n_0 - 3, t) - Q^2(n_0 - 2, t) \big] + \tfrac{t}{\tau} Q(n_0 - 2, t)\end{aligned}$$

- special cases: $n \gg 1,\ \frac{t}{\tau} \sim 1 \Rightarrow Q(n,t) \simeq 1$
  - variance increases linearly at the beginning of the process: $\langle n^2 \rangle - \langle n \rangle^2 \simeq \frac{t}{\tau}$
  - at the end of the process the number of cars reaches zero

  $\Rightarrow$ the variance has to tend to zero, too

2.4.2 Method using generating functions

- definition of the generating function:

$$G(z,t) := \sum_{n=0}^{\infty} z^n P(n,t) \simeq \sum_{n=1}^{\infty} z^n P(n,t)$$

- we have chosen well-known initial conditions: $P(n_0, t=0) = \delta_{n,n_0}$
  $\Rightarrow G(z,0) = z^{n_0}$

- in case of $W_+(n) = 0,\ W_-(n) = \frac{1}{\tau}$ we can sum the Master equation for each n:

$$\frac{\partial}{\partial t} \sum_{n=1}^{n_0} P(n,t) z^n \simeq \frac{1}{\tau} \Big(\frac{1}{z} \sum_{n=0}^{n_0 - 1} z^{n+1} P(n+1,t) - \sum_{n=1}^{n_0} z^n P(n,t) \Big)$$

$\Rightarrow$ inserting the generating function we get

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

$\Rightarrow$ the solution of this equation reads as

$$G(z,t) = C \exp \left\{ \frac{t}{\tau} \left(\frac{1}{z} - 1 \right) \right\}$$

$\Rightarrow$ the constant can be derived by the initial condition $G(z,0) = z^{n_0}$

$$\Rightarrow G(z,t) = z^{n_0} \exp \left\{ \frac{t}{\tau} \left(\frac{1}{z} - 1 \right) \right\}$$

$\Rightarrow$ to find the probabilities $P(n,t)$ we can expand the generating function into a power series:

$$\begin{aligned} G(z,t) = z^{n_0} e^{-\frac{t}{\tau}} e^{\frac{t}{\tau z}} &= z^{n_0} e^{-\frac{t}{\tau}} \sum_m \frac{1}{m!} \left(\frac{t}{\tau z}\right)^m \\ &= \sum_m \frac{1}{m!} z^{n_0-m} \left(\frac{t}{\tau}\right)^m e^{-\frac{t}{\tau}} \\ &= \sum_n \frac{1}{(n_0-n)!} z^n \left(\frac{t}{\tau}\right)^{n_0-n} e^{-\frac{t}{\tau}} \end{aligned}$$

- comparing the coefficients of this result with the definition of the generation function we receive

$$P(n,t) = \frac{1}{(n_0-n)!} \left(\frac{t}{\tau}\right)^{n_0-n} e^{-\frac{t}{\tau}} \qquad (0 < n \leq n_0)$$

2.5 Second example: Jam formation and dissolution

- we are now considering N cars on a circular road of length L
- the stochastic variable n describes the number of cars in a cluster
- we choose the same ansatz for the dissolution rate as above:

$$W_-(t) = \frac{1}{\tau}$$

- the inflow rate W_+ has to be described more complicated
  - we choose the following ansatz:

$$W_+ = \frac{v_{opt}\left(\Delta x_{free}\right)}{\Delta x_{free}}$$

  - the length Δx_{free} describes the free head way of a car in free traffic flow
    - we distinguish free cars and cars bounded in jam : $N = N_{free} + N_{jam} = (N-n) + n$
    - the total length of the road can be composed of the free road and the cluster length: $L = L_{free} + L_{cluster}$

    $\Rightarrow$ assuming that our cars are described by points and therefore the cluster length is small, we can compute the average free head way as $\Delta x_{free} = \frac{L_{free}}{N_{free}} \approx \frac{L}{N-n}$
  - the optimal velocity of a car should be connected to realistic situations:
    - if the free head way is long, the cars drive with maximum speed: $v_{opt} \to v_{max}$ for $\Delta x_{free} \to \infty$
    - in case of no free head way, the car has to stop: $v_{opt} \to 0$ for $\Delta x_{free} \to 0$

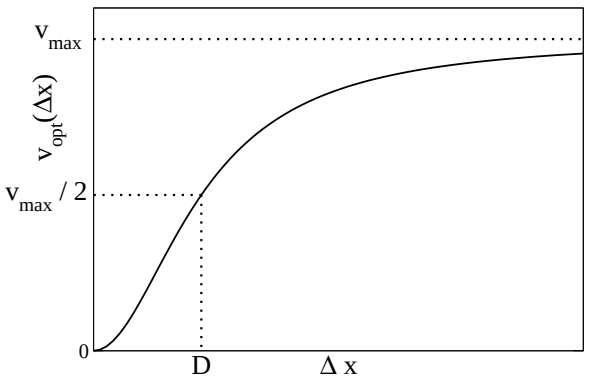

Figure 12: Optimal velocity function.

- the following ansatz satisfies both conditions (see Fig. 12):

$$v_{opt}(\Delta x) = v_{max}\frac{(\Delta x)^2}{D^2 + (\Delta x)^2}$$

$\Rightarrow$ the inflow rate is high for small free head way

$\Rightarrow$ the corresponding master equation can be composed of these parameters according to

$$\frac{\mathrm{d}P(n,t)}{\mathrm{d}t} = W_+(n-1)P(n-1,t)+W_-(n+1)P(n+1,t)-\big[W_+(n)+W_-(n)\big]P(n,t)$$

- we can now consider the car density $c = \frac{N}{L}$
  - for small densities $0 < c \leq c_{cr}$ we observe a dilute system with free flow
  - for systems with a density greater than some critical density $c > c_{cr}$ we observe car clusters
  - this behaviour is quite close to molecular clusters (solid, liquid and gaseous phase)
- hint for phase transitions: nonlinear dynamics (Bando's model)
  - we consider n single cars at position $x_i(t)$ with velocity $v_i(t)$ for $i = 1, \ldots, N$
  - the equation of motion states that the acceleration depends on the difference of the optimal and the real velocity of the cars

$$m\frac{\mathrm{d}v_i}{\mathrm{d}t} = m\frac{1}{\tau}\left(v_{opt}\left(\Delta x_i\right) - v_i\right), \qquad \frac{\mathrm{d}x_i}{\mathrm{d}t} = v_i$$

  - the free headway equals to the distance between two cars: $\Delta x_i = x_{i+1} - x_i$
  - the second equation only represents the definition of the velocity as the change of position

- this model has a stationary point if all cars drive with their optimal velocity $v_i = v_{opt}$
  - since the distance between two cars cannot change any more, all cars have to drive with the same velocity

  $\Rightarrow$ this condition reads as

$$v_i = v = v_{opt}\left(\Delta x_i = \Delta x = \frac{L}{N}\right) = v_{max}\frac{(L/N)^2}{D^2 + (L/N)^2}$$

  $\Rightarrow$ for a small number of cars the behaviour of the system approaches this fixed-point

  $\Rightarrow$ this condition describes the free-flow situation
- for a greater number of cars the solution tends to different stable behaviour
  - cars with small headway again drive with small velocity, for great headway with high velocity
  - for medium headways, the situation differs from the free-flow situation

  $\Rightarrow$ cars coming with high velocity drive faster than accelerating cars although they have the same headway

  $\Rightarrow$ the system contains two different phases: stop-and-go-traffic

- now we compute the mean cluster size of our Master-equation model $\langle n \rangle = \sum_n nP(n,t)$
  - the temporal change can be expressed by the inflow and outflow rate:

$$\frac{\mathrm{d}\langle n \rangle}{\mathrm{d}t} = \langle W_+(n) \rangle - \langle W_-(n) \rangle = W_+\left(\langle n \rangle\right) - W_-\left(\langle n \rangle\right)$$

  - simulations show the characteristics of a phase transition:
    - for small car concentration the mean cluster length equals to zero
    - for a concentration greater than some critical concentration we observe two phases

    $\Rightarrow$ the one phase has a mean cluster length of zero (free flow), the other is characterized by a linear growth of cluster length

    $\Rightarrow$ in this case the probability for the cluster length $P(n)$ has two maximum peaks at $\langle n \rangle = 0$ and some $\langle n \rangle > 0$

2.6 Third example: Radioactive decay

- we now try to describe the radioactive decay with the Master equation
  - a state m describes the number of atoms in the system being able to decay
  - the probability for the decay of one atom is directly proportional to the number of radioactive atoms

$$W_-(n) = \alpha n$$

- the parameter α describes the rate of transitions per time interval

- in closed system the number of radioactive atoms cannot increase:

$$W_+(n) = 0$$

- under these conditions the one-step Master equation reads as

$$\begin{aligned} \frac{\mathrm{d}P(m,t)}{\mathrm{d}t} &= P(m+1,t)W_-(m+1) - P(m,t)W_-(m) \\ &= \alpha(m+1)P(m+1,t) - \alpha m P(m,t) \end{aligned}$$

- we consider an initial amount of N atoms:

$$P(N, t=0) = 1 \quad P(m, t=0) = 0 \quad (0 \le m < N)$$

- the Master equations for $m = 0$ and $m = N$ read as

$$\frac{\mathrm{d}P(0,t)}{\mathrm{d}t} = \alpha P(1,t), \qquad \frac{\mathrm{d}P(N,t)}{\mathrm{d}t} = -N\alpha P(N,t)$$

2.6.1 Solution of the system of linear differential equations

1. since all differential equations are linear in the functions $P(m,t)$, we write this set in terms of vectors and matrices:

$$\begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}t}P(0,t) \\ \frac{\mathrm{d}}{\mathrm{d}t}P(1,t) \\ \frac{\mathrm{d}}{\mathrm{d}t}P(2,t) \\ \vdots \\ \frac{\mathrm{d}}{\mathrm{d}t}P(N-1,t) \\ \frac{\mathrm{d}}{\mathrm{d}t}P(N,t) \end{pmatrix} = \begin{pmatrix} 0 & \alpha & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\alpha & 2\alpha & 0 & \cdots & 0 & 0 \\ 0 & 0 & -2\alpha & 3\alpha & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -(N-1)\alpha & N\alpha \\ 0 & 0 & 0 & 0 & \cdots & 0 & -N\alpha \end{pmatrix} \begin{pmatrix} P(0,t) \\ P(1,t) \\ P(2,t) \\ \vdots \\ P(N-1,t) \\ P(N,t) \end{pmatrix}$$

- since the matrix of coefficient does not depend on the independent variable t, we take the well-known ansatz

$$\vec{P}(t) = \begin{pmatrix} P(0,t) \\ P(1,t) \\ \vdots \\ P(N,t) \end{pmatrix} = \vec{c}\, e^{\lambda t}$$

- inserting this into our equation, we find that the λ have to be eigenvalues of the matrix of coefficients, the vectors $\vec{c}$ are the corresponding eigenvectors:

$$\boldsymbol{M}\vec{c} = \lambda\vec{c} \qquad (\boldsymbol{M} \text{ being the matrix of coefficients})$$

2. for computation of the eigenvalues, we have to calculate the roots of the determinant of $\boldsymbol{M} - \lambda \boldsymbol{I}$:

$$0 \stackrel{!}{=} \begin{vmatrix} -\lambda & \alpha & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\alpha-\lambda & 2\alpha & 0 & \cdots & 0 & 0 \\ 0 & 0 & -2\alpha-\lambda & 3\alpha & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -(N-1)\alpha-\lambda & N\alpha \\ 0 & 0 & 0 & 0 & \cdots & 0 & -N\alpha-\lambda \end{vmatrix}$$

   - this determinant can be computed easily by applying the Laplace expansion. We receive

$$0 = -\lambda(-\alpha-\lambda)(-2\alpha-\lambda)\dots(-N\alpha-\lambda)$$

   - the roots of this equation can be written down directly:

$$\text{eigenvalues:} \quad \lambda_k = -k\alpha \qquad (k = 0, 1, 2, \dots, N)$$

3. in order to determine the eigenvectors, we have to find the solution of the equations

$$(\boldsymbol{M} - \lambda_k \boldsymbol{I})\vec{c}_k = 0 \qquad (k = 0, 1, 2, \dots, N)$$

   - we now fix the index k of the eigenvector and define $\vec{d} = \vec{c}_k$ since we don't want to get confused by too many indices
   - then the set of linear equations explicitly read as

$$\begin{aligned} k\alpha d_0 \quad &+\alpha d_1 &&= 0 \\ (k-1)\alpha d_1 \quad &+2\alpha d_2 &&= 0 \\ (k-2)\alpha d_2 \quad &+3\alpha d_3 &&= 0 \\ &&&\vdots \\ (k-(N-1))\alpha d_{N-1} \quad &+N\alpha d_N &&= 0 \\ &(k-N)\alpha d_N &&= 0 \end{aligned}$$

     or alternatively

$$(k-m)\alpha d_m + (m+1)\alpha d_{m+1} = 0 \quad (0 \le m \le N-1), \quad (k-N)\alpha d_N = 0$$

   - we start with the last equation:
     - if $k \neq N$, we find $d_N = 0$
     - in this case we iteratively find from the equations that d_m equals to zero as long as the index m of the component of $\vec{d}$ is greater than k:

$$d_m = 0 \qquad \forall m > k$$

     - in the equation with $m = k$ we can choose d_m arbitrarily and set $d_{m=k} = 1$

- all equations with lower index k can be written as

$$d_m = -\frac{m+1}{k-m} d_{m+1}$$

- we can insert the same result for d_{m+1} and find by iteration

$$\begin{aligned} d_m &= -\frac{m+1}{k-m} d_{m+1} \\ &= (-1)^2 \frac{(m+1)(m+2)}{(k-m)(k-m-1)} d_{m+2} \\ &= \ldots = (-1)^{k-m} \frac{(m+1)(m+2)\cdots(k-1)k}{(k-m)(k-m-1)\cdots 2 \cdot 1} \, d_k \\ &= (-1)^{k-m} \binom{k}{m} \end{aligned}$$

- in conclusion we found the coefficients of the kth eigenvector as

$$c_m^{(k)} = (-1)^{k-m} \binom{k}{m} \quad (0 \le m \le k), \qquad c_m^{(k)} = 0 \quad (k < m \le N)$$

$\Rightarrow$ the general solution can now be written as a linear combination of our fundamental solutions

$$\vec{P}(t) = \sum_{k=0}^{N} a_k \vec{c}_k e^{-\alpha k t} \quad \text{or}$$

$$P(m,t) = \sum_{k=0}^{N} a_k c_m^{(k)} e^{-\alpha k t} = \sum_{k=m}^{N} a_k (-1)^{k-m} \binom{k}{m} e^{-\alpha k t}$$

4. the coefficients a_m have to be fixed such that the initial condition is fulfilled:

$$P(m, t=0) = \sum_{k=m}^{N} a_k (-1)^{k-m} \binom{k}{m} = \delta_{mN}$$

- the most simple of these equations reads as

$$P(N, t=0) = a_N = 1$$

- continuing iteratively with $a_{N-1},\ a_{N-2}$ we guess that $a_k = \binom{N}{k}$
- we proof this hypothesis by induction over k:
  a) this hypothesis is trivially satisfied for $k = N$
  b) we now assume that it is correct for all $k \ge m+1$

$$a_k = \binom{N}{k} \qquad \forall k \ge m+1$$

c) the step is now to verify the hypothesis for $k = m$:

$$\begin{aligned}
0 &= \sum_{k=m}^{N} a_k (-1)^{k-m} \binom{k}{m} \\
&= a_m + \sum_{k=m+1}^{N} \binom{N}{k} (-1)^{k-m} \binom{k}{m} \\
&= a_m + \binom{N}{m} \frac{m!(N-m)!}{N!} \sum_{k=m+1}^{N} (-1)^{k-m} \frac{N!}{k!(N-k)!} \frac{k!}{m!(k-m)!} \\
&= a_m + \binom{N}{m} \sum_{k=m+1}^{N} (-1)^{k-m} \frac{(N-m)!}{(k-m)!(N-k)!} \\
&= a_m + \binom{N}{m} \sum_{k=m+1}^{N} (-1)^{k-m} \binom{N-m}{N-k} \qquad (k-m \to k,\ l = N-m) \\
&= a_m + \binom{N}{m} \sum_{k=1}^{l} \binom{l}{l-k} (-1)^k 1^{l-k} \\
&= a_m + \binom{N}{m} \left(\sum_{k=0}^{l} \binom{l}{k} (-1)^k 1^{l-k} - 1 \right) \\
&= a_m + \binom{N}{m} \left((1-1)^l - 1 \right) = a_m - \binom{N}{m} \qquad \text{qed.}
\end{aligned}$$

5. we now know that our solution has the following form:

$$P(m,t) = \sum_{k=m}^{N} (-1)^{k-m} \binom{N}{k} \binom{k}{m} e^{-\alpha k t}$$

- with some manipulation we are able to simplify this expression into a very smart form
- we remember that we just used the following identity: $\binom{N}{k}\binom{k}{m} = \binom{N-m}{N-k}\binom{N}{m}$
- using this relation we can carry out the sum

$$\begin{aligned}
P(m,t) &= \sum_{k=m}^{N} (-1)^{k-m} \binom{N-m}{N-k} \binom{N}{m} e^{-\alpha k t} \qquad (k-m \to k,\ l = N-m) \\
&= \binom{N}{m} \sum_{k=0}^{l} (-1)^k \binom{l}{l-k} e^{-\alpha (k+m) t} \\
&= \binom{N}{m} e^{-\alpha N t} \sum_{k=0}^{l} (-1)^k \binom{l}{k} e^{\alpha (l-k) t} \\
&= \binom{N}{m} e^{-\alpha N t} \left(-1 + e^{\alpha t} \right)^{N-m} = \underline{\underline{\binom{N}{m} e^{-\alpha m t} \left(1 - e^{-\alpha} \right)^{N-m}}}
\end{aligned}$$

2.6.2 Discussion of the result

- we found that the radioactive decay can be described by the probabilities of having m atoms at time t as

$$P(m,t) = \binom{N}{m} e^{-\alpha m t} \left(1 - e^{-\alpha t}\right)^{N-m}$$

- this result has a close analogy to the Binomial distribution:

$$P(m,t) = \binom{N}{m} p^m (1-p)^{N-m} \qquad \text{with} \quad p = p(t) = e^{-\alpha t}$$

- thus, we can also determine the first moment as well as the variance easily:
  - first moment: $\langle m \rangle = Np = Ne^{-\alpha t}$
  - variance: $\sigma^2 = Np(1-p) = Ne^{-\alpha t}\left(1 - e^{-\alpha t}\right)$

  $\Rightarrow$ the average number of radioactive atoms can be described by the famous law of decay

2.6.3 The method of generating functions

- we define the generating function as

$$F(z,t) = \sum_n z^n P(n,t)$$

- this function has to satisfy the corresponding differential equation

$$\frac{\partial F(z,t)}{\partial t} = \alpha \frac{\partial F(z,t)}{\partial z} - \alpha z \frac{\partial F(z,t)}{\partial z}$$

- the boundary condition reads as $F(1,t) = 1$ (normalisation), $F(z, t=0) = z^N$

$\Rightarrow$ the solution reads as $F(z,t) = \left(1 - (1-z)e^{-\alpha t}\right)^N$

$\Rightarrow$ the probability $P(n,t)$ can be found as the Taylor coefficient of the generating function:

$$P(n,t) = \frac{1}{n!} \left[\frac{\mathrm{d}^n}{\mathrm{d}z^n} F(z,t)\right]_{z=0}$$

2.7 Phase transition in supersaturated systems

- we now examine systems with constant volume, temperature and number of particles N_{total}

- phase transitions are transitions from a homogeneous into a heterogeneous system (break of symmetry)

- for instance gas phase $\Leftrightarrow$ fluid and gas phase

- microscopic description: N particles at position $\vec{r}_i(t)$ and momentum $\vec{p}_i(t)$

  $\Rightarrow$ $6N$ free variables $\Rightarrow$ problem is unsolvable

- we define an order parameter: distribution of cluster of different sizes

$$N(t) = (N_0, N_1, \ldots, N_n, \ldots, N_{total})$$

  - N_i describes the number of cluster consisting of i atoms

  $\Rightarrow$ N_0 is the number of free particles, N_1 is the number or one-particle-cluster able to build a dimer (consisting of two particles)

  - one free particle (counted in N_0) and one cluster of size i (counted in N_i) form a cluster of size N_{i+1}
  - the number of particles in the system has to be constant: $N_0 + \sum_{n=1} nN_n = N_{total}$

- for reasons of simplicity we now consider the one-cluster situation: there is only one single cluster in the system

  - the order parameter then reads as $N(t) = (N_0, 0, \ldots, N_n = 1, 0, \ldots)$
  - since we have only one independent variable, we introduce $n(t)$ as the cluster size
  - the normalisation condition here reads as $N_{total} = N_0(t) + n(t)$ $\Rightarrow N_0(t) = N_{total} - n(t)$
  - since our system depends on the parameter T, V, N, the thermodynamical potential is the free energy $F(T, V, N)$
  - this quantity can be computed from the partition function $Z(T, V, N)$ by $F = -k_B T \ln Z$

- for computing the partition function $Z(T, V, N)$, we need an appropiate Hamilton function

$$H_n = \sum_j \frac{\left(p_j^{(n)}\right)^2}{2m_j^{(n)}} + \sum_{i<j} U_{ij}^{(n,n)} \left(\vec{r}_i^{(n)}, \vec{r}_j^{(n)}\right)$$

  - the kinetic energy is composed of the momentum $\vec{p}_j^n$ of the cluster and free particles
  - the potential energy U_{ij} is not known in detail
  - the partition function Z can be computed as the product of the partition functions for fixed cluster size n

$$Z = \prod_n \frac{1}{N_n! h^{3N_n}} \int \mathrm{d}^{3N_n} p \int \mathrm{d}^{3N_n} q \; e^{-\frac{H_n}{k_B T}}$$

- if we neglect the interaction term U_{ij}, we can compute the partition function for the ideal gas

$$Z_{id} = \prod_{n=1}^{N} \frac{V^{N_n}}{N_n! h^{3N_n}} \left(\sqrt{2\pi m_n k_B T}\right)^{3N_n}$$

- the interaction term cannot be computed analytically, therefore we take the ansatz

$$Z(T,V,N) = \prod_{n=1}^{N} \frac{V^{N_n}}{N_n!} \left[\left(\frac{\sqrt{2\pi m_n k_B T}}{h} \right)^3 e^{-\frac{f_n}{k_B T}} \right]^{N_n}$$

- the quantity f_n describes the minimum potential energy of the bounded atoms in a n-atom cluster (ground state)
- $\lambda_n = \frac{h}{\sqrt{2\pi m_n k_B T}}$ is the thermal wavelength / de-Broglie wavelength of the particles

- the free energy can now be written as

$$F(T,V,N) = -k_B T \sum_{n=1}^{N} \left(\ln \left\{ \frac{V^{N_n}}{N_n! \lambda_n^{3N_n}} \right\} - \frac{f_n}{k_B T} \right)$$

- using Stirling's formula we receive

$$F(T,V,N) = k_B T \sum_{n=1}^{N} N_n \left(\ln \left\{ \lambda_n^3 \frac{N_n}{V} \right\} - 1 \right) + \sum_{n=1}^{N} N_n f_n$$

- the first term represents the ideal gas, the second is due to the interaction

- for the potential we try the following ansatz

$$f_n(T) = \mu_\infty n + \sigma A(n)$$

- μ_∞ is the chemical potential of the free particles ($\mu_\infty < 0$)
- $A(n)$ is the surface of the cluster depending on n ($A(n) \sim n^{\frac{2}{3}}$)

- on the other hand the dynamics of the change of the cluster size can be described by the Master equation

$$\frac{\partial P(N,t)}{\partial t} = \sum_{N'} \left[w(N,N') P(N',t) - w(N',N) P(N,t) \right]$$

- since we are interested in stationary processes, the probability should not depend on time
- in equilibrium the detailed balance (every summand vanishes) then reads as

$$w(N,N') P^{eq}(N',t) = w(N',N) P^{eq}(N,t)$$

- we further suggest the ansatz that the probability should be Boltzmann-distributed with a maximum at the minima of the free energy

$$P^{eq} \sim e^{-\frac{F}{k_B T}}$$

$\Rightarrow$ the transition rates can now be determined by

$$\frac{w(N', N)}{w(N, N')} = \exp\left\{-\frac{F(N') - F(N)}{k_B T}\right\}$$

- we can now choose one transition rate and then compute the other transition rate by the difference of free energy
- with these transition rates we can examine the dynamics of the complete Master equation

$\Rightarrow$ thus, classical statistics enables us to find a reasonable ansatz for the transition rates in the stochastic description

- at least the long-range development is described correctly

2.7.1 One-cluster-system: Liquid droplets

- we now want to examine a system consisting of free particles and one cluster
- it is useful to start with the free energy

$$F(T, V, N) = k_B T \sum_{n=1}^{N} N_n \left(\ln\left\{\lambda_n^3 \frac{N_n}{V}\right\} - 1\right) + \sum_{n=1}^{N} N_n f_n$$
$$\text{with} \quad f_n(T) = \mu_\infty n + \sigma A(n)$$

- if we only find one cluster, the vector of N has only two non-zero components:

$$N_n = 1, \quad N_0 = N_{total} - n$$

- n is the size of this cluster, we further denote $N = N_{total}$ as the total number of particles

$\Rightarrow$ the corresponding free energy reads as

$$F(T, V, n) = k_B T \left[(N - n)\left(\ln\left\{\lambda_0^3 \frac{N - n}{V}\right\} - 1\right) + \ln\left\{\lambda_n^3 / V\right\} - 1\right] + (N - n) f_0 + f_n$$

$\Rightarrow$ the fraction of $W_-(n)$ and $W_+(n)$ can now be written as

$$\frac{W_-(n)}{W_+(n-1)} = \frac{V\left(1 - \frac{1}{n^{2/3}}\right)}{\lambda_0^3 (N - n)} \exp\left\{\frac{f_n - f_{n-1}}{k_B T}\right\}$$

- for great cluster size n this relation can be approximated by

$$\frac{W_-(n)}{W_+(n)} = \frac{V}{\lambda_0^3(N-n)} \exp\left\{\frac{f_n - f_{n-1}}{k_B T}\right\}$$

- for the growth rate W_+ the ansatz $W_+(n) = \alpha\frac{N-n}{V}A(n)$ is reasonable: the probability for an particle joining the cluster is the greater, the greater the surface and the number of free particle is

$\Rightarrow$ our transition rates then read as

$$W_+(n) = \alpha\frac{N-n}{V}A(n), \qquad W_-(n) = \frac{\alpha A(n)}{\lambda_0^3} \exp\left\{\frac{f_n - f_{n-1}}{k_B T}\right\}$$

- the volume V is proportional to the number of particles, therefore the surface is proportional to $n^{\frac{2}{3}}$

$\Rightarrow$ the difference in the exponent can be approximated by

$$f_n - f_{n-1} = \mu_\infty + \sigma\left(A(n) - A(n-1)\right) = \mu_\infty + \sigma K(n)$$

- we can understand this formula considering that

$$A(n) - A(n-1) \sim n^{\frac{2}{3}} - (n-1)^{\frac{2}{3}} \approx n^{\frac{2}{3}} - n^{\frac{2}{3}}\left(1 - \frac{2}{3n}\right) = \frac{2}{3n^{\frac{1}{3}}} \sim \frac{1}{r_n}$$

$\Rightarrow$ therefore the function $K(n) \sim \frac{1}{r_n}$ describes the curvature of the surface

$\Rightarrow$ we insert this result into our transition rate $W_-(n)$

$$W_-(n) = \frac{\alpha A(n)}{\lambda_0^3} e^{\frac{\mu_\infty}{k_B T}} e^{lK(n)}$$

$\Rightarrow$ the parameter $l = \frac{2\sigma}{c_{clust} k_B T}$ is also referred to as the capillary length

$\Rightarrow$ the quantity $C_{eq} = \frac{1}{\lambda_0^3} e^{\frac{\mu_\infty}{k_B T}}$ describes the equilibrium concentration around the cluster over the surface when the curvature of the cluster surface can be neglected

$\Rightarrow$ the curvature modifies this equilibrium concentration

- the dynamics of the mean cluster size is described by the Master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle n\rangle = W_+\left(\langle n\rangle\right) - W_-\left(\langle n\rangle\right) = \alpha A(n)\left[\underbrace{\frac{N - \langle n\rangle}{V}}_{\text{free particles}} - \underbrace{C_{eq} e^{lK(n)}}_{\text{equilibrium}}\right]$$

- if the concentration of free particles is greater than the equilibrium concentration, the derivative is positive $\Rightarrow$ the cluster grows

- we can find up to two stationary states $\frac{\mathrm{d}\langle n\rangle}{\mathrm{d}t} = 0$
  - the easiest case is $n = 0$ since the surface of a 0-particle cluster equals to zero ($A(n) = 0$)
  - the last factor has two roots depending on the total number of particles N and the volume V
  - if N is too small, no stable cluster is built

  $\Rightarrow$ this system is bistable

2.7.2 Traffic jam

- we can also apply this model for the traffic situation
- we start from

$$\frac{W_+(n-1)}{W_-(n)} = \exp\left\{-\frac{F(n) - F(n-1)}{k_B T}\right\}$$

- the fraction can be expressed by our former ansatz

$$W_- = \frac{1}{\tau} \quad , \quad W_+ = \frac{v_{opt}\left(\Delta x_{free}\right)}{\Delta x_{free}}$$

$$\Rightarrow \quad \frac{W_+(n-1)}{W_-(n)} \approx \frac{W_+(n)}{W_-(n)} = \tau \frac{v_{opt}(\Delta x_{free})}{\Delta x_{free}}$$

- from this ansatz we can compute the free energy:

$$F(n) - F(n-1) = \frac{F(n) - F(n-1)}{n - (n-1)} \approx \frac{\partial F}{\partial n}$$

$$\frac{\partial F}{\partial n} = -k_B T \ln\left\{\frac{W_+}{W_-}\right\} = -k_B T \ln\left\{\tau \frac{v_{opt}(\Delta x_{free})}{\Delta x_{free}}\right\}$$

- from this we get

$$F = F(0) - k_B T \int_0^n \ln\left[\frac{W_+(n')}{W_-(n')}\right] dn'$$

- for performing the integration with respect of n we have to remember the dependence of all quantities on the right side on the cluster length n

$$\Delta x_{free} = \frac{L}{N-n}, \qquad v_{opt}(n) = v_{max} \frac{\left(\frac{L}{N-n}\right)^2}{D^2 + \left(\frac{L}{N-n}\right)^2}$$

- defining car density $\varrho = N/L$ we get

$$\frac{W_+(n)}{W_-(n)} = \tau v_{max} \varrho \frac{1 - n/N}{1 + \varrho^2 D^2 (1 - n/N)^2}$$

$\Rightarrow$ the integration leads us to

$$\begin{aligned} F(n) &= F(0) - k_B T \int_0^n \ln\left\{\tau v_{max} \frac{\left(\frac{L}{N-n'}\right)^2}{D^2 + \left(\frac{L}{N-n'}\right)^2}\right\} \mathrm{d}n' \\ &= F(0) - k_B T \int_0^n \ln\left\{\tau v_{max} \varrho \frac{1 - n'/N}{1 + \varrho^2 D^2 (1 - n'/N)^2}\right\} \mathrm{d}n' \end{aligned}$$

resulting in dimensionless free energy difference $f - f_0 = D(F - F(0))/(k_B T L)$ depending on fraction of congested cars n/N at different densities $\tilde{\varrho} = D\varrho$ (see Figs. 13 and 14)

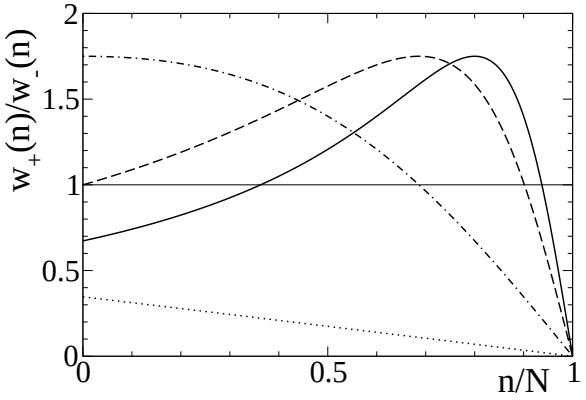

Figure 13: The ratio of transition rates $w_+(n)/w_-(n)$ depending on the fraction of congested cars n/N for four dimensionless densities $\tilde{\rho} = 0.1$ (dotted line), $\tilde{\rho} = 1$ (dot–dashed line), $\tilde{\rho} = 3.186$ (dashed line), and $\widetilde{\rho} = 5$ (solid line).

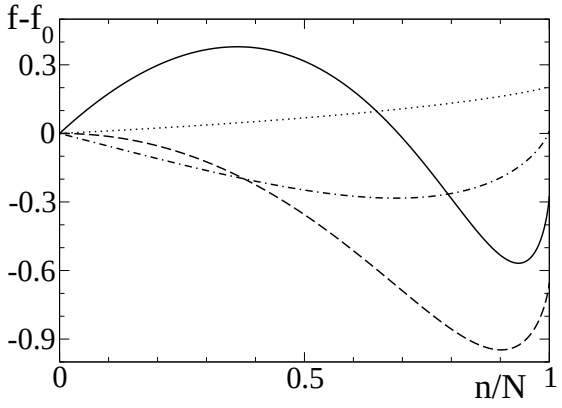

Figure 14: Normalised free energy difference $(F - F_0)/(\widetilde{L}T^*) = f - f_0$ depending on the fraction of congested cars n/N for four dimensionless densities $\tilde{\rho} = 0.1$ (dotted line), $\tilde{\rho} = 1$ (dot–dashed line), $\tilde{\rho} = 3.186$ (dashed line), and $\tilde{\rho} = 5$ (solid line).

2.8 Bifurcation diagramm of first-order phase transitions

- we have to distinguish two different situations: monostable and bistable systems
- monostable systems have only one stable state, bistable systems have two stable and one unstable states (double-well potential)
- the unstable state is also referred to as critical state, the two stable states represent two different phases
- the bifurcation diagram plots the density (extension) of one phase over the concentration of the system
  - for small densities only one phase exists
  - from a critical concentration the second phase appears, its concentration jumps from zero to a finite value
  - increasing the density the concentration of the phase can have two values, one being stable and one being unstable
  - in this case both phases coexist
  - from a second critical density the unstable situation vanishes, therefore only the stable branch exists
  - the stochasticity enables the system to transist from one state to another

2.9 Reaction-diffusion-equation

- we start with a global balance equation for the number of particles in the system

$$\frac{\mathrm{d}N}{\mathrm{d}t} = P\left[N(t)\right] + \phi\left[N(t)\right]$$

  - the first term P describes the production of particles in the system, ϕ refers to the flux of particles out of the system
  - often it is more convenient to formulate this balance equation in the local form
  - therefore we introduce the concentration c, production density q and flux density J

$$N(t) = \int_V n(x,t)\mathrm{d}V, \quad P[N] = \int_V q(x,t)\mathrm{d}V, \quad \phi(N) = -\oint_{\partial V} \vec{J}(x,t)\cdot\mathrm{d}\vec{A}(x)$$

  - using Gauss' theorem we find a generalized continuity equation

$$\frac{\partial n(x,t)}{\partial t} + \mathrm{div}\vec{J}(x,t) = q(x,t)$$

  - the flux can be divided into a convection and a conduction fraction

$$\vec{J}(x,t) = \underbrace{n(x,t)\vec{v}(x,t)}_{\text{convection}} + \underbrace{\vec{j}(x,t)}_{\text{conduction}}$$

- the convection is due to an external velocity field, the conduction term describes the diffusion:

$$\vec{j}(x,t) = -D\text{grad}_x n(x,t)$$

- the production of particles is caused by a chemical reaction rate $q \rightarrow f[n(x,t)]$

$\Rightarrow$ now our local balance can be rewritten in the one-dimensional case as

$$\frac{\partial n(x,t)}{\partial t} + \underbrace{\frac{\partial}{\partial x}\left(v(x,t)n(x,t)\right)}_{\text{drift}} = \underbrace{f\left[n(x,t)\right]}_{\text{reaction}} + \underbrace{D\frac{\partial^2 n(x,t)}{\partial x^2}}_{\text{diffusion}}$$

- we consider this equation in the range of $0 \leq x \leq L$ with boundary conditions according to

$$n(x,t)\Big|_{x\in\partial V} = g(x,t), \qquad \text{grad}_x n(x,t)\Big|_{x\in\partial V} = h(x,t)$$

- our initial condition is generally written as

$$n(x,t=0) = n_0(x)$$

- this problem is similar to the Fokker-Planck-equation

- the forward-Fokker-Planck-equation is known to us as

$$\frac{\partial p(x,t|y,t_0)}{\partial t} = \mathcal{L}_F(x)p(x,t|y,t_0) \qquad \text{with} \qquad \mathcal{L}_F(x) = -\frac{\partial}{\partial x}v(x) + \frac{\partial^2}{\partial x^2}d(x)$$

- the probability density $p(x,t|y,t_0)$ describes the solution $p(x)$ at time t fitted to an initial distribution $p_0(x)$ at time t_0

- on the other hand we can look for a differential equation describing the backward process

- the equation for this problem can be written in a similar form

$$\frac{\partial p(x,t|y,t_0)}{\partial t_0} = \mathcal{L}_B(y)p(x,t|y,t_0) \qquad \text{with} \qquad \mathcal{L}_B(y) = -v(y)\frac{\partial}{\partial y} + d(y)\frac{\partial^2}{\partial x^2}$$

- the initial condition is the same for both problems, for instance $p(x,t = t_0|x_0,t_0) = \delta(x - x_0)$

- the boundary conditions have to be fitted to the direction of the equation

$\Rightarrow$ both equations have the same solution

- we now consider the reaction-diffusion-equation in case of no drift ($v(x,t) \equiv 0$)

$$\frac{\partial n(x,t)}{\partial t} = f\left[n(x,t)\right] + D\frac{\partial^2 n(x,t)}{\partial x^2}$$

Forward Fokker-Planck-equation	Backward Fokker-Planck-equation
$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left[D_1 p\right] + \frac{\partial^2}{\partial p x^2}\left[D_2 p\right]$	$-\frac{\partial p}{\partial t_0} = \frac{\partial p}{\partial t} = -D_1 \frac{\partial p}{\partial x_0} + D_2 \frac{\partial^2 p}{\partial x_0^2}$
reflecting boundary at $x = a$: $j(x = a, t) = 0 \Rightarrow D_1 p - \frac{\partial}{\partial x}\left[D_2 p\right]\Big\|_{x=a} = 0$	reflecting boundary $x_0 = a$: $\frac{\partial p}{\partial x_0}\Big\|_{x=a} = 0$
absorbing boundary at $x = b$: $p(x = b, t \| x_0, t_0) = 0$	absorbing boundary at $x_0 = b$: $p(x, t \| x_0 = b, t_0) = 0$

Table 1: Comparison of the Forward- and Backward-Fokker-Planck-equation

- with boundary conditions

$$\begin{aligned} n(x = 0\,,\, t) &= n_3 \\ n(x = L\,,\, t) &= n_1 \end{aligned}$$

and the initial condition as the step function

$$n(x\,,\, t = 0) = \begin{cases} n_3 & : \quad x \leq x_0 \\ n_1 & : \quad x > x_0 \end{cases}$$

which depends on critical position $x_0 \in [0, L]$

- solutions with homogeneous density have to satisfy the equation

$$\frac{\partial n(x,t)}{\partial t} = f\left[n(x,t)\right] \qquad \left(\frac{\partial n(x,t)}{\partial x} = 0\right)$$

- these solutions describe the fixed points (every solution ends up with a homogeneous density)
- the stationary solutions $\frac{\partial n}{\partial t} = 0$ can be found by the roots of

$$f\left[n(x,t)\right] = -D\frac{\partial^2 n(x,t)}{\partial x^2}$$

- this relation is a nonlinear one-dimensional wave equation, but can also be interpreted as some kind of Newton equation

$$m\frac{\mathrm{d}^2 z}{\mathrm{d}t^2} = F(z)$$

- for this reason we introduce a potential $V(z)$ according to $F(z) = -\frac{dV(z)}{dz}$ and find the conservation of energy

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{m}{2}\left(\frac{\mathrm{d}z}{\mathrm{d}t}\right)^2 + V(z)\right] = 0$$

$\Rightarrow$ transferring this relation by $z \to n,\ t \to z,\ F(z) \to -f(n)$ we receive

$$\frac{D}{2}\left(\frac{\mathrm{d}n}{\mathrm{d}x}\right)^2 + U(n) = E = \text{const} \qquad \text{with } U(n) = \int^n f(n')\mathrm{d}n'$$

$\Rightarrow$ this equation can be formally solved

$$\mathrm{d}x = \frac{\mathrm{d}n}{\sqrt{\frac{2}{D}\left(E - U(n)\right)}} \qquad \Rightarrow \qquad x(n) = \int^{n} \frac{\mathrm{d}n}{\sqrt{\frac{2}{D}\left(E - U(n)\right)}}$$

- the original solution can be found by inversion $n = n(x)$
- unfortunately the boundary conditions can not be handled easily

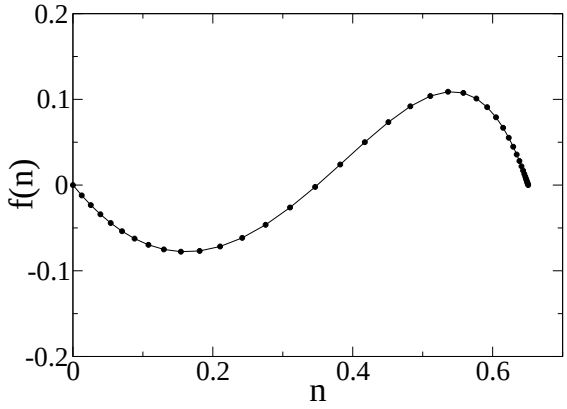

Figure 15: Reaction force $f(n)$ with $\tau = 1$ and $d = 4.4$.

- let us consider as an example the following ansatz of nonlinear reaction force $f(n)$ (see Fig. 15)

$$f(n) = -\frac{1}{\tau}\, n \left[\frac{1}{1-n} - d\, n\right]$$

where constants τ and d are control parameters. The relation $f(n) = 0$ gives the values $0 = n_1 < n_2 < n_3$ for $d > 4$, i. e.

$$n_{2,3} = \frac{1}{2} \pm \frac{1}{2}\sqrt{1 - \frac{4}{d}}$$

- numerical solution is presented in Fig. 16

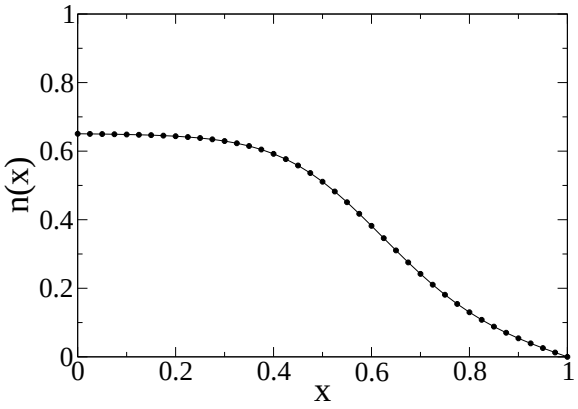

Figure 16: The stationary solution of reaction-diffusion equation called profile obtained by simulation taking into account the reaction force shown in Fig. 15. The diffusion coefficient is $D = 10^{-2}$.

3 Project work

3.1 Project: White noise & Lorentz attractor (Knud Klingbeil)

White noise

- Wiener process $dx(t) = dW(t)$ generates *White noise* (see Fig. 17)
- the initial condition $x(t = t_0) = x_0$
- the properties of the Wiener process
  - the Wiener process $W(t)$ is normally distributed with mean value $\langle W(t) \rangle = 0$ and variance $\langle (W(t))^2 \rangle = t$
  - all increments $\Delta W = W(t + \Delta t) - W(t)$ are independent therefore $\langle \Delta W(t) \rangle = 0$ and $\langle (\Delta W(t))^2 \rangle = \Delta t$
- numerically, the increment $\Delta W(t)$ can be calculated from standard normally distributed random numbers $Z \sim N(0, 1)$ via

$$\Delta W(t) = Z\sqrt{\Delta t}$$

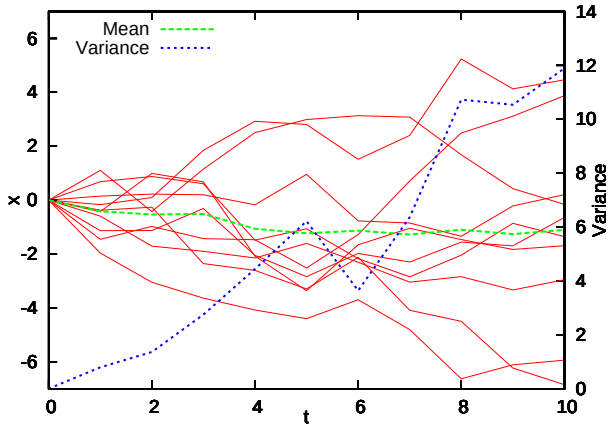

Figure 17: Ensemble of stochastic trajectories with the same initial condition $x_0 = 0$ together with mean value (around 0) and variance (linear increasing).

Lorenz system

- nonlinear system of differential equations:

$$\dot{x} = P(y - x), \qquad \dot{y} = (r - z)x - y, \qquad \dot{z} = xy - bz$$

- there are three given parameter $P,\ r,\ b$
- this system was the first one to be found with chaotic properties

- the parameter define the fixpoints ($\dot{x} = \dot{y} = \dot{z} = 0$)
- if the trajectory starts at a fixpoint, the variables do not leave it
- initial points being close together lead to completely different trajectories (chaos)
- if the initial point is far away from the origin, the trajectory tends to the so-called Lorentz-attractor

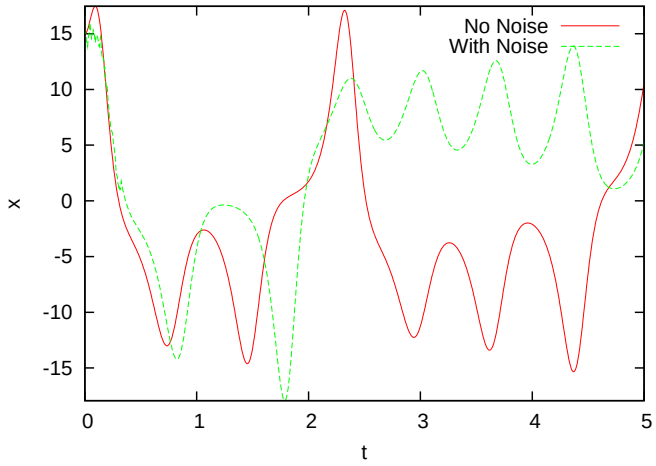

Figure 18: Temperal development $x = x(t)$ with and without noise, parameters: $x_0 = y_0 = z_0 = 15$, $P = 10$, $r = 28$, $b = 8/3$.

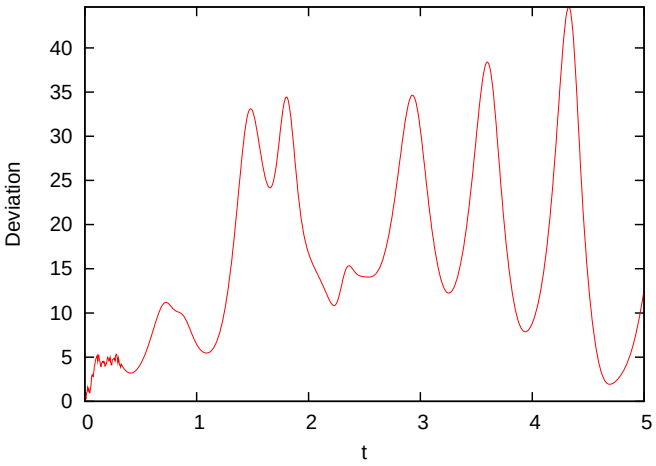

Figure 19: Deviation from initial condition, parameters: $x_0 = y_0 = z_0 = 15$, $P = 10$, $r = 28$, $b = 8/3$.

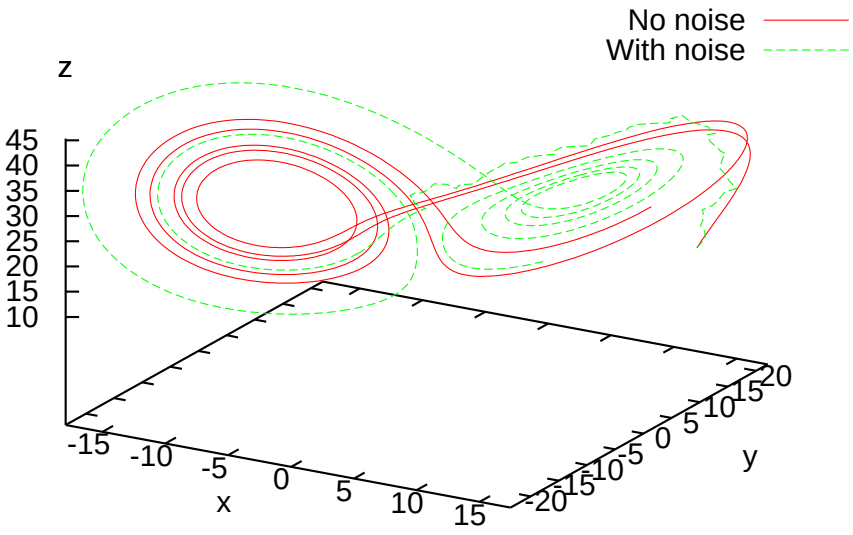

Figure 20: Three-dimensional view of trajectories with and without noise on Lorenz attractor, parameters: $x_0 = y_0 = z_0 = 15$, $P = 10, r = 28, b = 8/3$.

3.2 Project: Sturm-Liouville-Problem (Daniel Münzner)

- we are looking for a solution in the interval $[a, b]$ for the problem

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}y}{\mathrm{d}x}\right) + (q(x) + \lambda g(x))\, y(x) = 0$$

  - the functions $p(x)$ and $q(x)$ have to be positive, $g(x)$ is the weight function
  - the boundary conditions are chosen as

$$y(a) = y(b) = 0$$

  - the considered set of functions shall also contain a scalar product

$$(u, v) = \int_a^b g(x)u(x)v(x)\mathrm{d}x$$

  - we now write the problem as an eigenvalue problem

$$L_y(x)y = \lambda y \qquad \text{with} \quad L_y(x) = -\frac{1}{g(x)}\left((py')' - q(x)y\right)$$

  - there is no explicit solution of the eigenvalue problem, but with the following theory we get information about the structure of the solution

Proposition (Spectrum of a symmetrical, positive definite operator) We assume $O(x)$ a symmetrical, positive definite operator on an infinite-dimensional Hilbert-space. The spectrum of $O(x)$ is compact. [1]

- L_y is symmetrical:

$$\begin{aligned}(L_y u, v) &= \int_a^b g(x)\frac{1}{g(x)}\left(-(pu')' + qu\right)v\mathrm{d}x \\ &= -\int_a^b (pu')'v\mathrm{d}x + \int_a^b quv\mathrm{d}x \\ &= -(pu')v|_a^b + \int_a^b pu'v'\mathrm{d}x + \int_a^b quv\mathrm{d}x\end{aligned}$$

because $v \in L_2(g(x), a, b)$ satisfies $\quad v(a) = 0 = v(b)$

$$\begin{aligned}&= \int_a^b pu'v' + quv\mathrm{d}x \\ &= (u, L_y v)\end{aligned}$$

[1] proof at: Michlin, S.G.: Partielle Differentialgeichungen in der Mathematischen Physik (Mathematische Lehrbücher 30), Berlin, 1978, p. 109f

- L_y is positive definite:

$$\begin{aligned}
(L_y u, u) &= \int_a^b g(x)\left[-\frac{1}{g(x)}\left[(p(x)u'(x))' - q(x)u(x)\right]u(x)\right]\mathrm{d}x \\
&= -\int_a^b \left[(p(x)u'(x))'u(x)\right]\mathrm{d}x \\
&\qquad + \int_a^b q(x)u(x)^2\mathrm{d}x \quad \text{Partielle Integration} \\
&= -p(x)u'(x)u(x)\Big|_a^b + \int_a^b \left[(p(x)u'(x))u'(x)\right]\mathrm{d}x \\
&\qquad + \int_a^b q(x)u(x)^2\mathrm{d}x \\
&= \int_a^b \left[(p(x)u'(x))u'(x) + q(x)u(x)^2\right]\mathrm{d}x \\
&= \int_a^b \left[p(u')^2 + qu^2\right]\mathrm{d}x
\end{aligned}$$

$$\begin{aligned}
(L_y u, u) &= \int_a^b \left[p(u')^2 + qu^2\right]\mathrm{d}x \\
&\geq p_0 \int_a^b (u')^2\mathrm{d}x
\end{aligned}$$

1. g(x) is continuous on [a,b] $\Rightarrow \exists g_1$ with $g(x) \leq g_1\ \forall x \in$ [a,b]

2. $\sqrt{g(x)}u(x) = \sqrt{g(x)}\int_a^x u'(t)\mathrm{d}t$

$$\begin{aligned}
g(x)u^2(x) &\leq g_1\left(\int_a^x u'(t)\mathrm{d}t\right)^2 \\
&\leq g_1\int_a^x u'^2(t)\mathrm{d}t \cdot (x-a) \\
&\leq g_1(b-a)\int_a^b u'^2(t)\mathrm{d}t \\
\Rightarrow \int_a^b\int_a^b u'^2(t)\mathrm{d}t &\geq \frac{1}{g_1(b-a)}\int_a^b r(x)u^2(x)\mathrm{d}x = \|u\|^2 \cdot \frac{1}{g_1(b-a)} \\
(L_y u, u) &\geq p_0\int_a^b u'^2(x)\mathrm{d}x \geq \frac{p_0}{r_1(b-a)}\|u\|^2 \geq 0
\end{aligned}$$

- it is shown, that the operator is symmetrical and positive definite

$\Rightarrow$ L_y defines a series of eigenvalues

$$0 < \lambda_1 < \lambda_2 < \ldots$$

$\Rightarrow$ the eigenfunctions are orthogonal and can be orthonormalized, they represent a complete basis of the set of functions over the interval $[a, b]$

- each eigenvalue leads to an unique eigenfunction

Example (wave equation)

- for instance, we can consider the differential equation for a standing wave

$$y''(x) + \lambda y(x) = 0 \qquad a < x < b$$

- we consider fixed (absorbing) boundaries $y(a) = y(b) = 0$
- the following ansatz satisfies the differential equation:

$$y(x) = c_1 \sin\left(\sqrt{\lambda}(x-a)\right) + c_2 \cos\left(\sqrt{\lambda}(x-a)\right)$$

- the parameter $c_1,\ c_2$ have to fit to the boundary conditions

$$\begin{aligned} y(a) = 0 \quad &\Rightarrow \quad c_2 = 0 \\ y(b) = 0 \quad &\Rightarrow \quad c_1 \sin\left(\sqrt{\lambda}(b-a)\right) \end{aligned}$$

- since c_1 should be different from zero, the sine should vanish:

$$\sqrt{\lambda_n} = \frac{n\pi}{b-a} \quad \Rightarrow \quad \lambda_n = \frac{\pi^2 n^2}{(b-a)^2} \quad (n = 1, 2, \ldots)$$

- if we wish the function to be normalized, the coefficient c_1 has to be determined by

$$\begin{aligned} \|y_n(x)\|^2 &= c_{1,n}^2 \int_a^b \sin^2\left(n\pi \frac{x-a}{b-a}\right) \mathrm{d}x = 1 \\ &= c_{1,n}^2 \int_a^b \sin^2\left(\varphi(x)\right) \mathrm{d}x = 1 \quad \text{with } \varphi(x) = n\pi \frac{x-a}{b-a} \\ \int_a^b \sin^2\left(\varphi(x)\right) \mathrm{d}x &= \underbrace{-\frac{1}{\varphi'(x)} \cos(\varphi(x)) \sin(\varphi(x)) \Big|_a^b}_{=0} + \int_a^b \cos^2(\varphi(x)) \mathrm{d}x \\ &= \int_a^b \mathrm{d}x - \int_a^b \sin^2(\varphi(x)) \mathrm{d}x \\ &\Rightarrow \int_a^b \sin^2(\varphi(x)) = \frac{1}{2} x \Big|_a^b \\ &\Rightarrow \frac{1}{2} c_{1,n} (b-a) = 1 \\ &\Rightarrow c_{1,n} = \sqrt{\frac{2}{b-a}} \end{aligned}$$

$\Rightarrow$ the orthonormalized eigenfunctions then read as

$$y_n(x) = \sqrt{\frac{2}{b-a}} \sin\left(\frac{n\pi(x-a)}{b-a}\right)$$

with the corresponding eigenvalue

$$\lambda_n = \left(\frac{n\pi}{b-a}\right)^2$$

3.3 Project: Space-dependent diffusion (Thomas Kiesel)

- talking about diffusion we always assumed that the diffusion constant D does not depend on space or time

- we are now going to consider a linearly space dependent diffusion parameter

$$D = D(x) = D_0(1+gx)$$

- first we have to find the corresponding diffusion equation

  - we start with Fick's laws:

$$\text{the continuity equation:} \qquad \frac{\partial c(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0$$

$$\text{flux ansatz:} \qquad j(x,t) = -D\frac{\partial c(x,t)}{\partial x}$$

  - $c(x,t)$ is the concentration of particles at time t and position x and can be considered as directly proportional to the probability density
  - it is normalised to the number of particles in the system
  - we can find the corresponding diffusion equation by inserting the flux ansatz into the first relation

$$\frac{\partial c(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial c(x,t)}{\partial x}\right) = Dg\frac{\partial c(x,t)}{\partial x} + D(1+gx)\frac{\partial^2 c(x,t)}{\partial x^2}$$

  - we choose a reflecting boundary at $x = -\frac{1}{g}$ and a standard initial condition

$$j\left(x = -\frac{1}{g}, t\right) = 0 \quad , \quad c(x, t=0) = \delta(x - x_0)$$

Solution of this problem

1. as a first step we rewrite the diffusion equation in such a form which contains only a linear combination of first and second derivatives of some functions:

$$\begin{aligned}\frac{\partial c(x,t)}{\partial t} &= D_0 g \frac{\partial c(x,t)}{\partial x} + D_0(1+gx)\frac{\partial^2 c(x,t)}{\partial x^2} \\ &= D_0 g \frac{\partial c(x,t)}{\partial x} + \frac{\partial^2}{\partial x^2}\left(D_0(1+gx)c(x,t)\right) - 2D_0 g \frac{\partial c(x,t)}{\partial x} \\ &= -D_0 g \frac{\partial c(x,t)}{\partial x} + \frac{\partial^2}{\partial x^2}\left(D_0(1+gx)c(x,t)\right)\end{aligned}$$

   - this equation can be checked easily by applying Leibniz' product formula for derivatives twice
   - comparing the result with the definition of the flux we find

$$j(x,t) = D_0 g c(x,t) - \frac{\partial}{\partial x}\left(D_0(1+gx)c(x,t)\right)$$

2. we now search for a new space coordinate $\bar{x} = \bar{x}(x)$ which removes the space dependence of the diffusion constant

   - therefore we have to transform the derivatives with respect to x as well:

$$\frac{\partial}{\partial x} = \frac{\partial \bar{x}}{\partial x}\frac{\partial}{\partial \bar{x}}, \qquad \frac{\partial^2}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial \bar{x}}{\partial x}\frac{\partial}{\partial \bar{x}}\right) = \frac{\partial^2 \bar{x}}{\partial x^2}\frac{\partial}{\partial \bar{x}} + \left(\frac{\partial \bar{x}}{\partial x}\right)^2 \frac{\partial^2}{\partial \bar{x}^2}$$

   - the concentration should be transformed into a new function $w(\bar{x},t)$ such that the normalisation condition is conserved:

$$c(x,t)\mathrm{d}x = w(\bar{x},t)\mathrm{d}\bar{x} \qquad \Rightarrow \quad c(x,t) = w(\bar{x},t)\frac{\partial \bar{x}}{\partial x}$$

   - since we are interested to simplify the second-derivative term, we concentrate on

$$\begin{aligned}\frac{\partial^2}{\partial x^2}\left(D_0(1+gx)c(x,t)\right) &\rightarrow D_0(1+gx)\frac{\partial^2 c(x,t)}{\partial x^2} \\ &\rightarrow D_0(1+gx)\left(\frac{\partial \bar{x}}{\partial x}\right)^2 \frac{\partial^2}{\partial \bar{x}^2}\left(w(\bar{x},t)\frac{\partial \bar{x}}{\partial x}\right)\end{aligned}$$

     - we neglected all terms which did not contain any second derivative with respect to $\bar{x}$
   - now we choose the transform $\bar{x}(x)$ such that the factor does not depend on $\bar{x}$:

$$D_0(1+gx)\left(\frac{\partial \bar{x}}{\partial x}\right)^2 = D_0 = \text{constant}$$

$\Rightarrow$ we receive

$$\frac{\partial \bar{x}(x)}{\partial x} = \sqrt{\frac{1}{1+gx}} \quad \Rightarrow \quad \bar{x}(x) = \frac{2}{g}\sqrt{1+gx}, \quad \frac{\partial \bar{x}(x)}{\partial x} = \frac{2}{g\bar{x}}$$

- in this case the derivatives and the concentration field transform as

$$\frac{\partial}{\partial x} = \frac{2}{g\bar{x}}\frac{\partial}{\partial \bar{x}}, \qquad \frac{\partial^2}{\partial x^2} = \frac{\partial \bar{x}}{\partial x}\frac{\partial}{\partial \bar{x}}\left(\frac{2}{g\bar{x}}\frac{\partial}{\partial \bar{x}}\right) = -\frac{4}{g^2\bar{x}^3}\frac{\partial}{\partial \bar{x}} + \frac{4}{g^2\bar{x}^2}\frac{\partial^2}{\partial \bar{x}^2}$$

$$c(x,t) = \frac{2w(\bar{x},t)}{g\bar{x}}$$

- furthermore we transform the diffusion equation

$$\begin{aligned}
\frac{\partial}{\partial t}\left(\frac{2w(\bar{x},t)}{g\bar{x}}\right) &= D_0 g \frac{2}{g\bar{x}}\frac{\partial}{\partial \bar{x}}\left(\frac{2w(\bar{x},t)}{g\bar{x}}\right) \\
&+ D_0\frac{g^2\bar{x}^2}{4}\left[-\frac{4}{g^2\bar{x}^3}\frac{\partial}{\partial \bar{x}}\left(\frac{2w(\bar{x},t)}{g\bar{x}}\right) + \frac{4}{g^2\bar{x}^2}\frac{\partial^2}{\partial \bar{x}^2}\left(\frac{2w(\bar{x},t)}{g\bar{x}}\right)\right] \\
\Rightarrow \frac{\partial w(\bar{x},t)}{\partial t} &= D_0\frac{\partial}{\partial \bar{x}}\left(\frac{w(\bar{x},t)}{\bar{x}}\right) + D_0\bar{x}\frac{\partial^2}{\partial \bar{x}^2}\left(\frac{w(\bar{x},t)}{\bar{x}}\right) \\
&= D_0\frac{1}{\bar{x}^2}w(\bar{x},t) - D_0\frac{1}{\bar{x}}\frac{\partial w(\bar{x},t)}{\partial \bar{x}} + D_0\frac{\partial^2 w(\bar{x},t)}{\partial \bar{x}^2}
\end{aligned}$$

- last but not least we should not forget the boundary and initial conditions

1. $$\begin{aligned}
j(x=-g^{-1},t) &= D_0 g c(x,t) - \frac{\partial}{\partial x}\left(D_0(1+gx)c(x,t)\right)\Big|_{x=-\frac{1}{g}} = 0 \\
\Rightarrow^{\frac{2w(\bar{x},t)}{\bar{x}}} &= \frac{2}{g\bar{x}}\frac{\partial}{\partial \bar{x}}\left(\frac{g^2\bar{x}^2}{4}\frac{2w(\bar{x},t)}{g\bar{x}}\right) = \frac{1}{\bar{x}}\frac{\partial}{\partial \bar{x}}\left(\bar{x}w(\bar{x},t)\right)\Big|_{\bar{x}=0} \\
\Rightarrow^{\frac{w(\bar{x},t)}{\bar{x}}} &= \frac{\partial w(\bar{x},t)}{\partial \bar{x}}\Big|_{\bar{x}=0}
\end{aligned}$$

2. $$\begin{aligned}
c(x,t=0) &= \delta(x-x_0) \qquad \Rightarrow \qquad \frac{2w(\bar{x},t=0)}{g\bar{x}} = \delta\left(\frac{g}{4}\left(\bar{x}^2-\bar{x}_0^2\right)\right) \\
\Rightarrow w(\bar{x},t=0) &= \frac{\bar{x}}{\bar{x}_0}\delta\left(\bar{x}-\bar{x}_0\right) = \frac{\bar{x}_0}{\bar{x}_0}\delta\left(\bar{x}-\bar{x}_0\right) = \delta\left(\bar{x}-\bar{x}_0\right)
\end{aligned}$$

- here we used the relation $\delta(f(x)) = \frac{1}{|f'(x_0)|}\delta(x-x_0)$ with x_0 as a root of $f(x)$

3. if one wants to eliminate the diffusion constant D_0, he should introduce a new time coordinate $T = D_0 t$

   - simple calculations show that D_0 vanishes in each equation, the time t is replaced by the new variable T

4. for solving this new problem, we now try the separation ansatz $w(\bar{x},T) = \chi(T)\psi(\bar{x})$

- inserting it and dividing by $\chi(T)\psi(\bar{x})$ we find

$$\frac{1}{\chi(T)}\frac{\partial\chi(T)}{\partial T} = \frac{1}{\bar{x}^2} - \frac{1}{\bar{x}\psi(\bar{x})}\frac{\partial\psi(\bar{x})}{\partial\bar{x}} + \frac{1}{\psi(\bar{x})}\frac{\partial^2\psi(\bar{x})}{\partial\bar{x}^2}$$

- since both sides dependent only on different variables, they have to be constant
- choosing $-\lambda^2$ as the separation constant we get a simple relation for the temporal evolution:

$$\frac{\partial\chi(T)}{\partial T} = -\lambda^2\chi(T) \qquad \Rightarrow \qquad \chi(T) = e^{-\lambda^2 T}$$

5. the spatial solution has to satisfy a more complicated differential equation

$$\bar{x}^2\frac{\partial^2\psi(\bar{x})}{\partial\bar{x}^2} - \bar{x}\frac{\partial\psi(\bar{x})}{\partial\bar{x}} + \left(1+\lambda^2\bar{x}^2\right)\psi(\bar{x}) = 0$$

- this equation is quite similar to the Bessel equation

$$x^2y''(x) + xy'(x) + (n^2+x^2)y(x) = 0$$

- we can transfer our equation into this form by

$$y = \lambda\bar{x}, \quad \psi(\bar{x}) = y\phi(y)$$

- now we compute

$$\begin{aligned}
(1+\lambda^2\bar{x}^2)\,\psi(\bar{x}) &= y\phi(y) + y^3\phi(y) \\
\bar{x}\tfrac{\partial\psi(\bar{x})}{\partial\bar{x}} &= y\frac{\partial}{\partial y}\left(y\phi(y)\right) = y\phi(y) + y^2\frac{\partial\phi(y)}{\partial y}, \\
\bar{x}^2\tfrac{\partial^2\psi(\bar{x})}{\partial\bar{x}^2} &= y^2\frac{\partial^2}{\partial y^2}\left(y\phi(y)\right) = 2y^2\frac{\partial\phi(y)}{\partial y} + y^3\frac{\partial^2\phi(y)}{\partial y^2} \\
\Rightarrow \qquad 0 &= y^2\frac{\partial^2\phi(y)}{\partial y^2} + y\frac{\partial\phi(y)}{\partial y} + y^2\phi(y)
\end{aligned}$$

$\Rightarrow$ the solution of this equation is given by a linear combination of Bessel functions of zeroth order

$$\phi(y) = \frac{1}{\lambda}\left(c_1J_0(y) + c_2Y(0)\right)$$

- written in terms of $\bar{x}$ and $\psi(\bar{x})$ it reads as

$$\psi(\bar{x}) = c_1\bar{x}J_0(\lambda\bar{x}) + c_2\bar{x}Y_0(\lambda\bar{x})$$

6. this solution has to fit to our boundary condition

$$\frac{w(\bar{x},t)}{\bar{x}} = \frac{\partial w(\bar{x},t)}{\partial\bar{x}}\Big|_{\bar{x}=0} \qquad \Rightarrow \qquad \frac{\psi(\bar{x})}{\bar{x}} = \frac{\partial\psi(\bar{x})}{\partial\bar{x}}\Big|_{\bar{x}=0}$$

- inserting our solution into this equation we receive

$$0 = \bar{x}\left(c_1 J_0'(\lambda\bar{x}) + c_2 Y_0'(\lambda\bar{x})\right)_{\bar{x}\to 0}$$

- it can be shown that the Bessel functions can be approximated in the limit $x \to 0$ by

$$\lim_{\lambda x\to 0} J_0'(\lambda x) = 0, \qquad \lim_{\lambda x\to 0} Y_0'(\lambda x) = \frac{2}{\pi x}$$

- therefore we find that the constant c_2 has to vanish to zero
- in conclusion the solution for each λ reads as

$$w_\lambda(\bar{x}, T) = \chi_\lambda(T)\psi_\lambda(\bar{x}) = c_\lambda e^{-\lambda^2 T}\bar{x} J_0(\lambda\bar{x})$$

7. the general solution can be written as a linear combination of the solutions for each single λ

- since we have a continuous set of eigenvalues λ, we have to formulate the linear combinations with an integral

$$w(\bar{x}, T) = \int_0^\infty \mathrm{d}\lambda C(\lambda) e^{-\lambda^2 T}\bar{x} J_0(\lambda\bar{x})$$

- the weight function $C(\lambda)$ is determined by the initial condition

$$w(\bar{x}, T = 0) = \frac{\bar{x}}{\bar{x}_0}\delta\left(\bar{x} - \bar{x}_0\right)$$

$\Rightarrow$ in our example we have to solve the equation

$$\delta\left(\bar{x} - \bar{x}_0\right) = \int_0^\infty \mathrm{d}\lambda C(\lambda)\bar{x} J_0(\lambda\bar{x})$$

- for this purpose we intend to use the orthogonality of the Bessel functions
  - it can be shown that the Bessel functions are orthogonal when we consider the scalar product

$$(f, g) = \int_0^\infty f(x) g(x) x \mathrm{d}x$$

  $\Rightarrow$ thus, the corresponding relation reads as

$$(J_0(\lambda\bar{x}), J_0(\kappa\bar{x})) = \lambda\int_0^\infty J_0(\lambda\bar{x}) J_0(\kappa\bar{x})\,\bar{x}\,\mathrm{d}\bar{x} = M^2\delta(\lambda - \kappa)$$

  - M is the normalisation constant

- therefore, we multiply both sides of our equation with $\kappa J_0(\kappa\bar{x})$ and integrate over $\bar{x}$

$$\begin{aligned}
\kappa\int_0^\infty J_0(\kappa\bar{x})\delta\left(\bar{x}-\bar{x}_0\right)\mathrm{d}\bar{x} &= \kappa\int_0^\infty \mathrm{d}\bar{x}J_0(\kappa\bar{x})\int_0^\infty \mathrm{d}\lambda C(\lambda)\bar{x}J_0(\lambda\bar{x}) \\
&= \int_0^\infty \mathrm{d}\lambda C(\lambda)\int_0^\infty \kappa J_0(\kappa\bar{x})J_0(\lambda\bar{x})\,\bar{x}\,\mathrm{d}\bar{x} \\
\Rightarrow \kappa J_0(\kappa\bar{x}_0) &= \int_0^\infty \mathrm{d}\lambda C(\lambda)M^2\delta(\lambda-\kappa) \\
\Rightarrow C(\kappa) &= \frac{\kappa}{M^2}J_0(\kappa\bar{x}_0)
\end{aligned}$$

$\Rightarrow$ our final solution reads as

$$\begin{aligned}
w(\bar{x},T) &= \int_0^\infty \mathrm{d}\lambda\,\left(\frac{1}{M^2}\lambda J_0(\lambda\bar{x}_0)\right)\,\left(\bar{x}J_0\left(\lambda\bar{x}\right)e^{-\lambda^2 T}\right) \\
&= \frac{\bar{x}}{M^2}\int_0^\infty \mathrm{d}\lambda\;\lambda J_0(\lambda\bar{x}_0)J_0(\lambda\bar{x})e^{-\lambda^2 T} \\
&= \frac{\bar{x}}{M^2}\left(\frac{1}{2T}\exp\left\{-\frac{\bar{x}^2+\bar{x}_0^2}{4T}\right\}I_0\left(\frac{\bar{x}_0\bar{x}}{2T}\right)\right)
\end{aligned}$$

  - here we used an integral taken from [1]

$\Rightarrow$ replacing $\bar{x}=\frac{2}{g}\sqrt{1+gx}$, $T=D_0t$ and $c(x,t)=\frac{2w(\bar{x},T)}{g\bar{x}}$ we find the concentration in variables of x,t:

$$\underline{\underline{c(x,t)=\frac{1}{M^2gD_0t}\exp\left\{-\frac{2+g(x+x_0)}{g^2D_0t}\right\}I_0\left(\frac{2\sqrt{1+gx}\sqrt{1+gx_0}}{g^2D_0t}\right)}}$$

Properties of the moments

- for a founded discussion it is convenient to compute the first moments of the concentration

$$\langle x^n\rangle=\int_{-\frac{1}{g}}^\infty x^n c(x,t)\mathrm{d}x$$

- for reasons of simplicity we perform a linear transformation $y=1+gx$ such that the lower boundary equals to zero

  - inserting our solution for the concentration we find the following integral

$$\langle x^n\rangle=\frac{1}{M^2gD_0t}\exp\left\{-\frac{1+gx_0}{g^2D_0t}\right\}\int_0^\infty\frac{(y-1)^n}{g^n}\exp\left\{-\frac{y}{g^2D_0t}\right\}I_0\left(2\frac{\sqrt{1+gx_0}}{g^2D_0t}\sqrt{y}\right)\frac{\mathrm{d}y}{g}$$

  - these integrals can be solved analytically with the help of appropiate integral tables

- in [1] we can find the following formula:

$$\int_0^\infty x^{\mu-\frac{1}{2}} e^{-\alpha x} I_{2\nu}(2\beta\sqrt{x}) = \frac{\Gamma\left(\mu+\nu+\frac{1}{2}\right)}{\beta\alpha^\mu\Gamma(2\nu+1)} e^{\frac{\beta^2}{2\alpha}} M_{-\mu,\nu}\left(\frac{\beta^2}{\alpha}\right)$$
$$\Re\left\{\mu+\nu+\frac{1}{2}\right\} > 0$$

- since we want to compute the zeroth, first and second moment, we are interested in the parameters $\mu = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$ and $\nu = 0$
- the functions $M_{-\mu,\nu}$ read in these cases

$$\begin{aligned} M_{-\frac{1}{2},0}(x) &= \sqrt{x}e^{\frac{1}{2}z}, & \Gamma(1) = 1 \\ M_{-\frac{3}{2},0}(x) &= \sqrt{x}(1+x)e^{\frac{1}{2}z}, & \Gamma(2) = 1 \\ M_{-\frac{5}{2},0}(x) &= \tfrac{1}{2}\sqrt{x}(2+4x+x^2)e^{\frac{1}{2}z}, & \Gamma(3) = 2 \end{aligned}$$

- therefore we can use the following formulae

$$\begin{aligned} \int_0^\infty e^{-\alpha x} I_0(2\beta\sqrt{x})\mathrm{d}x &= \frac{1}{\alpha} e^{\frac{\beta^2}{\alpha}} \\ \int_0^\infty x e^{-\alpha x} I_0(2\beta\sqrt{x})\mathrm{d}x &= \frac{1}{\alpha^2}\left(1+\frac{\beta^2}{\alpha}\right) e^{\frac{\beta^2}{\alpha}} \\ \int_0^\infty x^2 e^{-\alpha x} I_0(2\beta\sqrt{x})\mathrm{d}x &= \frac{1}{\alpha^3}\left(2+4\frac{\beta^2}{\alpha}+\frac{\beta^4}{\alpha^2}\right) e^{\frac{\beta^2}{\alpha}} \end{aligned}$$

- in our calculations the parameters α and β are given by

$$\alpha = \frac{1}{g^2 D_0 t}, \quad \beta = \frac{\sqrt{1+gx_0}}{g^2 D_0 t}$$

- the zeroth moment is due to the normalization of the distribution: the integral of the concentration over the total space gives us the total number of particles in the system

- thus, we are able the determine the parameter M

$$\begin{aligned} \langle x^0 \rangle = \int_{-\frac{1}{g}}^\infty c(x,t)\mathrm{d}x &= \frac{1}{M^2 g D_0 t} e^{-\frac{1+gx_0}{g^2 D_0 t}} \int_0^\infty e^{-\alpha y} I_0(2\beta\sqrt{y})\frac{\mathrm{d}y}{g} \\ &= \frac{1}{M^2 g^2 D_0 t} e^{-\frac{1+gx_0}{g^2 D_0 t}} \frac{1}{\alpha} e^{\frac{\beta^2}{\alpha}} \\ &= \frac{1}{M^2 g^2 D_0 t} e^{-\frac{1+gx_0}{g^2 D_0 t}} g^2 D_0 t e^{\frac{1+gx_0}{g^2 D_0 t}} \\ &= \frac{1}{M^2} \stackrel{!}{=} N \end{aligned}$$

- if we consider a probability density, we have to choose $N = 1$

- the first moment describes the center of mass of the concentration

$$\begin{aligned}
\langle x \rangle &= \int_{-\frac{1}{g}}^{\infty} x c(x,t) \mathrm{d}x \\
&= \frac{1}{gD_0 t} e^{-\frac{1+gx_0}{g^2 D_0 t}} \int_0^{\infty} \frac{y-1}{g} e^{-\alpha y} I_0(2\beta\sqrt{y}) \frac{\mathrm{d}y}{g} \\
&= \frac{1}{g^3 D_0 t} e^{-\frac{1+gx_0}{g^2 D_0 t}} \int_0^{\infty} y e^{-\alpha y} I_0(2\beta\sqrt{y}) \mathrm{d}y - \frac{1}{g}\langle x^0 \rangle \\
&= \frac{1}{g^3 D_0 t} e^{-\frac{1+gx_0}{g^2 D_0 t}} \frac{1}{\alpha^2} \left(1 + \frac{\beta^2}{\alpha}\right) e^{\frac{\beta^2}{\alpha}} - \frac{1}{g} \\
&= \frac{1}{g^3 D_0 t} e^{-\frac{1+gx_0}{g^2 D_0 t}} (g^2 D_0 t)^2 \left(1 + \frac{1+gx_0}{g^2 D_0 t}\right) e^{\frac{1+gx_0}{g^2 D_0 t}} - \frac{1}{g} \\
&= \frac{1}{g}\left(g^2 D_0 t + 1 + g x_0\right) - \frac{1}{g} = \underline{\underline{g D_0 t + x_0}}
\end{aligned}$$

$\Rightarrow$ the center of mass drifts with a constant velocity $v_{drift} = gD_0$ to the area with a higher diffusion parameter

$\Rightarrow$ it is important to mention that the center of mass can not be estimated by the position of the maximum

$\Rightarrow$ Fig.21 shows that the maximum of the concentration profile moves to the left boundary although the center of mass shifts to the other side

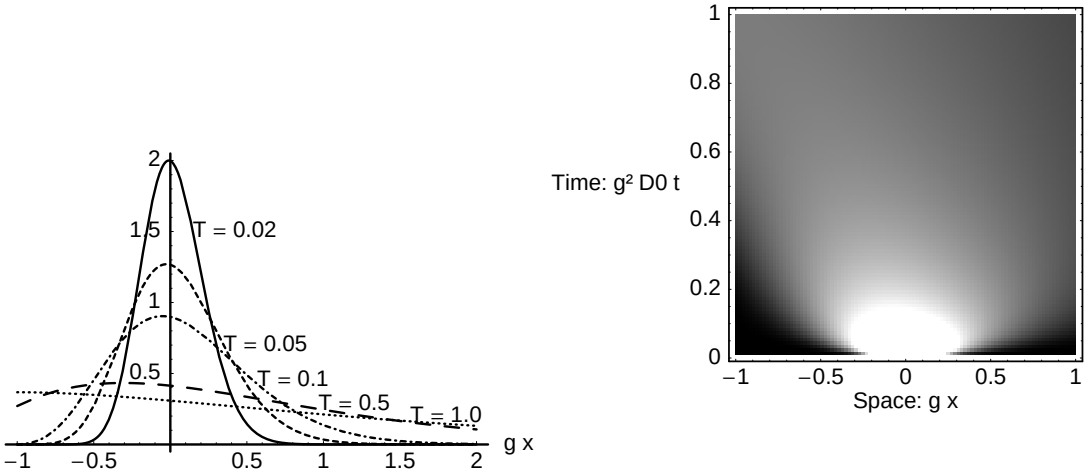

Figure 21: Plot of the concentration profile in dimensionless quantities $X = gx$ and $T = g^2 D_0 t$ for an initial distribution at $x_0 = 0$. The left graph shows the shape of the profile at different times, the right graph demonstrates the spread of the particles with time.

- the second moment can be computed analogically

$$\begin{aligned}
\langle x^2\rangle &= \int_{-\frac{1}{g}}^{\infty} x^2 c(x,t)\mathrm{d}x \\
&= \frac{1}{gD_0t}e^{-\frac{1+gx_0}{g^2D_0t}}\int_0^{\infty}\frac{(y-1)^2}{g^2}e^{-\alpha y}I_0(2\beta\sqrt{y})\frac{\mathrm{d}y}{g} \\
&= \frac{1}{g^4D_0t}e^{-\frac{1+gx_0}{g^2D_0t}}\int_0^{\infty} y^2e^{-\alpha y}I_0(2\beta\sqrt{y})\mathrm{d}y - \frac{2}{g}\left(\langle x\rangle + \frac{1}{g}\right) + \frac{1}{g^2}\langle x^0\rangle \\
&= \frac{1}{g^4D_0t}e^{-\frac{1+gx_0}{g^2D_0t}}\frac{1}{\alpha^3}\left(2+4\frac{\beta^2}{\alpha}+\frac{\beta^4}{\alpha^2}\right)e^{\frac{\beta^2}{\alpha}} - 2\frac{1}{g^2}\left(g^2D_0t+gx_0+1\right)+\frac{1}{g^2} \\
&= \frac{1}{g^4D_0t}e^{-\frac{1+gx_0}{g^2D_0t}}(g^2D_0t)^3\left(2+4\frac{1+gx_0}{g^2D_0t}+\frac{(1+gx_0)^2}{(g^2D_0t)^2}\right)e^{\frac{1+gx_0}{g^2D_0t}} \\
&\quad -\frac{1}{g^2}\left(2g^2D_0t+2gx_0+1\right) \\
&= \frac{1}{g^2}\left(2(g^2D_0t)^2+4(g^2D_0t)(1+gx_0)+(1+gx_0)^2-2gx_0-1-2g^2D_0t\right) \\
&= \frac{1}{g^2}\left(2(g^2D_0t)^2+4(g^2D_0t)(1+gx_0)+g^2x_0^2-2g^2D_0t\right) \\
&= 2g^2D_0^2t^2+2D_0t(1+2gx_0)+x_0^2
\end{aligned}$$

$\Rightarrow$ thus, the variance is given by

$$\begin{aligned}
\langle x^2\rangle - \langle x\rangle^2 &= 2g^2D_0^2t^2+2D_0t(1+2gx_0)+x_0^2-(D_0gt+x_0)^2 \\
&= \underline{\underline{g^2D_0^2t^2+2D_0t(1+gx_0)}}
\end{aligned}$$

$\Rightarrow$ we find that the standard deviation $\sigma = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$ grows linearly in time

Remark: This work is a generalization with arbitrary initial condition compared to the solution given by Martin [2].

References

[1] I. S. Gradshteyn, I. M. Ryzhik: Tables of Integrals, Series and Products, Fifth Edition, Academic Press, 1994

[2] M. Martin: The source solution for diffusion with a linearly position dependent diffusion coefficient, Zeitschrift für Physikalische Chemie, NF, **162**(1989)245

3.4 Project: Schlögl reaction (Peter Grünwald)

- Schlögl considered a chemical reaction

$$\mathrm{A} + 2\ \mathrm{X} \underset{k_1'}{\overset{k_1}{\rightleftharpoons}} 3\ \mathrm{X} \quad , \quad \mathrm{X} \underset{k_2'}{\overset{k_2}{\rightleftharpoons}} \mathrm{F}$$

- the concentrations for all components are given by $c_A = A,\ c_F = F,\ c_X = C$
- the transition rates shall be given by some constants k_1, k_2, k_1', k_2'

$\Rightarrow$ we can describe the temporal evolution by the Schlögl equation

$$\frac{\mathrm{d}C}{\mathrm{d}T} = \underbrace{k_1 A C^2 - k_1' C^3}_{\text{left reaction}} + \underbrace{k_2' F - k_2 C}_{\text{right reaction}}$$

- this equation is bistable:
  - in case of equilibrium $\frac{\mathrm{d}C}{\mathrm{d}T} = 0$ we find a polynomial of third order in C

  $\Rightarrow$ substitutions for dimensionless equations: $V_0,\ \tau_0,\ \tau,\ X$

$$V_0,\ \tau_0 = \frac{V_0^2}{k_1'},\ \tau = \frac{T}{\tau_0},\ X = V_0 C$$

  $\Rightarrow$

$$\frac{\mathrm{d}X}{\mathrm{d}\tau} = -X^3 + aX^2 - bX + c$$

  with $a = \frac{k_1}{k_1'} A V_0 \geq 0,\ b = \frac{k_2}{k_1'} V_0^2 \geq 0,\ c = \frac{k_2'}{k_1'} F V_0^3 \geq 0$
  - the roots of this polynomial define the stationary states

  $\Rightarrow$ if this polynomial has one single root, the equation is monostable
  - the polynomial can also have three roots

  $\Rightarrow$ this equation creates two stable solutions at the outer roots
  - we can understand it when we introduce a potential:

$$\frac{\mathrm{d}C}{\mathrm{d}T} = -\frac{\mathrm{d}V}{\mathrm{d}C} \qquad \Rightarrow \qquad V = -\frac{1}{3} A C^3 + \frac{1}{4} k_1' C^4 - k_2' F C + \frac{1}{2} k_2 C^2$$

  $\Rightarrow$ the potential can have two minima (=stable points)

$\Rightarrow$ we now try to find a stochastic description with the one-step Master equation

- the concentration is proportional to the number of particles N which is now our stochastic variable
- the one-step Master equation has the well-known form

$$\frac{\partial P(N,T)}{\partial T} = W_{N-1}^{+} P(N-1,T) + W_{N+1}^{-} P(N+1,T) - (W_N^{+} + W_N^{-}) P(N,T)$$

- we need to define reasonable transition rates:

$$W_N^+ = k_1 A \frac{N(N-1)}{V^2} V + k_2' F V, \qquad W_N^- = k_1' V \frac{N(N-1)(N-2)}{V^3} + k_2 V \frac{N}{V}$$

  $\Rightarrow$ they directly correspond to the positive and negative terms in the Schlögl equation

  $\Rightarrow$ the concentration C is replaced here by $\frac{N}{V}$

  - we replaced $N \to N-1$ or $N-2$ because of the needed impact of two or more particles for the reaction
  - from this transformation we receive an additional factor V

- an analytical solution can be expected to be very complicated if it exists at all
  - the solution has two stable states like the Schlögl equation above
  - however, the system can change stochastically between both states
  - the probability density has two maxima at these points, but is also greater than zero between both states

- we can try to find analytical solutions for some special cases
  - for instance in case of detailed balance $\frac{\mathrm{d}P(N,T)}{\mathrm{d}T} = 0$
  - from the Master equation we achieve then a recursive form

$$P^{eq}(N) = \frac{W_{N-1}^+}{W_N^-} P^{eq}(N-1)$$

  - because of the Schlögl reaction it must be $N \geq 2$
  - with normalization relation

$$\sum_{N=2}^{\infty} P^{eq}(N) = P^{eq}(2) \sum_{N=2}^{\infty} \frac{W_{N-1}^+}{W_N^-} \equiv 1$$

  $\Rightarrow$ a solution can be written down, but would still be quite complicated in explicit form

  - simplify process by assuming $b \equiv 0,\ c \equiv 0$, i.e. there is no reaction $X \leftrightharpoons F$

  $\Rightarrow$

$$\frac{P^{eq}(N)}{P^{eq}(2)} = \frac{W_{N-1}^+ W_{N-2}^+ \ldots W_2^+}{W_N^- W_{N-1}^- \ldots W_3^-} = \ldots = \left(a \frac{V}{V_0}\right)^{N-2} \frac{2}{N!} \quad \text{for } N \geq 3$$

  - we substitute the prefactor to k

$$k = a \frac{V}{V_0} = \frac{k_1}{k_1'} A V \propto V$$

$\Rightarrow$ now $P^{eq}(2)$ can be calculated with the exponential series

$$1 = P^{eq}(2)\frac{2}{k^2}\sum_{N=2}^{\infty}\frac{k^N}{N!} = P^{eq}(2)\frac{2}{k^2}(e^k - k - 1)$$

$\Rightarrow$ therefore we achieve as a result for detailed balance without a second reaction

$$P^{eq}(N) = \frac{k^N}{N!}e^{-k}\frac{1}{1 - e^{-k}(1+k)}$$

- remarkable is the asymptotic behaviour in the thermodynamic limit $V \to \infty, k \to \infty$

$$P^{eq}(N, k \to \infty) \approx \frac{k^N}{N!}e^{-k} = P^{eq}_{Poisson}(N)$$

$\Rightarrow$ Poisson statistics as the classical result in big volumina!

Remark: See for further Information:

- *R. Mahnke "Nichtlineare Physik in Aufgaben", Teubner Studienbücher Physik, Stuttgart, 1994*

3.5 Projekt: Analyse der stochastischen Dynamik des diskreten Galton–Bretts mit Kontinuumsgrenzübergang (Elisabeth Schöne)

Aufgabenstellung:

- **Studium der historischen Grundlagen**
  Informieren Sie sich über den britischen Forscher *Sir Francis Galton*, der in der Physik durch das nach ihm benanntes Galton–Brett weltbekannt ist. Können Sie aufgrund der Lebensdaten, Ausbildung, Beruf, Mitarbeiter, etc Angaben zu seiner Motivation machen, sich mit der Zeitentwicklung eines statistischen Ensembles zu beschäftigen, das durch eine Binominalverteilung beschrieben wird.

Biographie:

Francis Galton, *16.02.1822 in Sparkbrook, Birmingham †17.01.1911 in Haslemere, Surrey

Francis Galton war das neunte und letzte Kind von Samuel Tertius Galton und Frances Anne Violetta, der Tochter von Erasmus Darwin. Somit stammt Francis Galton väterlicherseits aus einer Familie der Waffenhersteller und Banker und mütterlicherseits aus einer medizinisch–naturwissenschaftlichen Familie.

Bereits als Kind zeigte sich Francis Galton als sehr intelligent. Mit schon 18 Monaten konnte er alle Buchstaben lesen und beherrschte Latein- und Französischvokabeln mit nur vier Jahren. Ab seinem 5.Lebensjahr besuchte er verschiedene Schulen im In- und Ausland.

Nach einer Studienreise durch Europa im Jahr 1838 und der ersten Stufe seiner medizinischen Ausbildung im Birmingham General Hospital widmete er sich bereits ein Jahr später am Trinity College in London der Mathematik. Er verließ die Universität mit dem Bachelor of Arts, als er nach dem Tod seines Vaters 1844 ein großes Vermögen geerbt hatte.

Ab 1845 folgten viele Reisen. Galton zog es bis zum Nil bzw. Jordan und schließlich bis nach Afrika. Aus diesen Reisen entstanden eine Vielzahl von publizieren Berichten und weitere Arbeiten, wie z.B. Kartierungen, wofür er wiederholt Auszeichnungen und Medaillen erhielt.

Seit 1853 war Galton mit Louisa Butler verheiratet, wobei die Ehe kinderlos blieb. Für seine Arbeiten wurde Galton 1909 von der Krone geadelt.

Ab den 1860er Jahren engagierte sich Galton stark in der British Association for the Advancement of Science. Auch in dieser Zeit folgten zahlreiche Veröffentlichungen.

Galton interessierte sich für vielerlei Bereiche. So entwickelte er Wetterkarten in der Meteologie, beschäftigte sich, angeregt durch seinen Cousin Charles Darwin, mit der Vererbungslehre und gilt sogar als (Mit-)Begründer der Differentialpsychologie. Weiterhin untersuchte er den mathematischen Aspekt bei Personenerkennungssytemen in der Daktyloskopie. In der Statistik arbeitete er mit Karl Pearson zusammen (Korrelationskoeffizient) und beschäftigte sich hierbei mit der Normalverteilung und der Methode der Regression. Zudem entwickelte er ein Modell zur Demonstration von Wahrscheinlichkeiten, das Galtonbrett.

Mögliche Gründe für seine Motivation:

Angeregt durch seine fernen Auslandsreisen konnte Galton genug Beobachtungen über fremde Rassen machen. Diese Grundlagen wurde durch seinen Cousin Charles Darwin, der sich intensiv mit Vererbungslehre beschäftigte, erweitert. Weiterhin beschäftigte sich Galton mit der Differentialpsychologie, wobei er hier auch Testverfahren zur Erfassung psychologischer Eigenschaften entwickelte. So entsteht bei Galton ein Interesse für den Menschen, jedoch auf wissenschaftlicher Basis. Später versucht er sogar die "Dummheit der Masse" mit Hilfe eines Experimentes statistisch zu beweisen.

- **Das (asymmetrische) Galtonbrett als Modell für die Brownsche Bewegung**
  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).

Wirkungsweise des Galtonbretts:

Das Galtonbrett ist ein Modell zur Veranschaulichung der Binomialverteilung. Es besteht aus einer regelmäßigen Anordnung von Hindernissen, an denen eingeworfene Kugeln vorbei müssen. Aufgrund der zwei Wege, die die einzelne Kugel laufen kann, liegt hier Binomialverteilung vor. Durch das Durchlaufen der Einzelkugel durch das gesamte Galtonbrett, welches aus vielen Hindernisstufen besteht, erfolgt eine mehrstufige Bernoulli-Kette, wobei die Kettenlänge gleich der Anzahl der waagerechten Reihen von Hindernissen ist, n genannt. Am Ende fallen die nacheinander eingeworfenen Kugeln in so genannte Fächer, mit k bezeichnet, und zwar mit entsprechender Gauß-Verteilung.

Wahrscheinlichkeiten:

Symmetrie:

Ohne äußere Einflüsse, d.h. bei ordentlichen Standortbedingungen des Galtonbrettes, liegt Symmetrie und somit reine Diffusion vor. Für die allgemeine Formel für das k-te Fach bei n-Reihen

$$B(k,n) = \binom{n}{k} p^k q^{n-k}$$

gilt bei Symmetrie aufgrund $p = 1/2$ und $q = 1/2$

$$B(k,n) = \binom{n}{k} \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{n-k} = \binom{n}{k} \left(\frac{1}{2}\right)^n$$

Asymmetrie:

Treten allerdings Störungen auf, d.h. dass das Galtonbrett beispielsweise nicht ordentlich steht, so gibt es bei den Wahrscheinlichkeiten Änderungen. In diesem Fall tritt neben dem Zufall auch die Notwendigkeit ein.

Es gilt

$$B(k,n) = \binom{n}{k} p^k q^{n-k}$$

Totale Asymmetrie:

Als drittes gibt es die Möglichkeit, dass nur Notwendigkeit eintritt, man spricht vom reinen Drift. Die Wahrscheinlichkeiten betragen dann $p = 0$ und $q = 1$ bzw. $p = 1$ und $q = 0$

Formal lässt sich die totale Asymmetrie durch das Kronecker-Symbol beschreiben.

$$\delta_{nk} = B(n,k) = \begin{cases} 0 & n \neq k \\ 1 & n = k \end{cases}$$

- **Kontinuumsgrenzübergang**

  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).

Kontinuumsgrenzübergang:

Nach der Einführung neuer Parameter x (distance) und t (time) erhält man statt der bisherigen Wahrscheinlichkeit bei n Versuchen, von welchen k erfolgreich sind, $P(k,n) = \binom{n}{k}(1/2)^n$ folgende Gleichung:

$$\widetilde{P}(x,t) \equiv P(k,n) = \binom{t/\tau}{(t/2*\tau)+(x/2*a)}(1/2)^{1/\tau}$$

Da sich jene Formel jedoch als wenig günstig erweist, müssen im Anschluss noch einige elementare Schritte durchgeführt werden. Die Ausgangsformel $P(k,n) = \binom{n}{k}(1/2)^n$ wird für große k und n abgeschätzt. Bei dieser Abschätzung muss für die Fakultät die Stirlingsche Formel verwendet werden. Nach dem Einsetzen der Stirlingschen Formel in die Ausgangsgleichung erhält man:

$$\widetilde{P}(x,t) \equiv P(k,n) = A \cdot B \cdot C \cdot F,$$

, wobei A,B,C und F Terme sind, die weitgehend vereinfacht werden müssen. Anschließend wird die Diffusionskonstante $D = a^2/\tau$ eingeführt. Es wird weiter gefordert, dass die Hüpfzeit τ als auch die Sprungweite a gegen Null gehen. Die Zwischenergebnisse von A,B,C und F werden nun in $\widetilde{P}(x,t) \equiv P(k,n) = A \cdot B \cdot C \cdot D$ eingesetzt und man erhält

$$\widetilde{P}(x,t) = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{2\tau}{t}}\exp\left\{-\frac{x^2}{2Dt}\right\}$$

Da τ gegen Null läuft, ist es an dieser Stelle wenig störend.

Nach der Abschätzung

$$\sum_{k_1}^{k_2} P(k,n) \approx \int_{k_1}^{k_2} P(k,n)dk$$

erfolgt das Einsetzen der Gleichung $\widetilde{P}(x,t) \equiv P(k,n) = A \cdot B \cdot C \cdot D$ in die Abschätzung, so dass man nach Kürzen

$$\sum_{k_1}^{k_2} P(k,n) = \int_{x_1}^{x_2} f(x,t)dx$$

erhält. Bei der Einfügung der Wahrscheinlichkeitsverteilung
$\widetilde{P}(x,t) \equiv P(k,n) = A \cdot B \cdot C \cdot D$ erhält man schließlich die endgültige Form

$$\int_{x_1}^{x_2} exp\left\{-\frac{x^2}{2Dt}\right\} \frac{1}{\sqrt{2\pi Dt}} dx.$$

Diese ergibt die Wahrscheinlichkeitsdichte $f(x,t) = \frac{1}{\sqrt{2\pi Dt}} \exp\left\{-\frac{x^2}{2Dt}\right\}$.

Literaturhinweis:
H. Haken: Synergetik, Springer–Verlag, Berlin, div. Auflagen ab 1977

Stochastik II
für LA an Gymnasien und Physiker

PD Dr. Reinhard Mahnke

Lehrveranstaltung (2 SWS V + 2 SWS Ü) im Rahmen des Graduiertenkollegs *Stark korrelierte Vielteilchensysteme* und im Rahmen des Studiengangs *Master in Physics*

Dienstag 13.00 bis 15.00 Uhr, Seminarraum
Freitag 13.00 bis 15.00 Uhr, Seminarraum Didaktik
Institut für Physik, Universitätsplatz 3
Sommersemester 2006

About the contents:

1. **Random Walks and Diffusion** (04.04.2006, R. Mahnke)
   Introduction of simple stochastic processes like Brownian motion, diffusion, Galton board, random walker, concept of probability, Markov chain, Binominal distribution, Master equation, drift–diffusion equation (Fokker–Planck equation)

2. **Exercise: Binominal distribution** (07.04.2006, R. Mahnke)
   Calculation of moments by generating functions, computing 0th, 1st and 2nd moment of Binominal distribution, Stirling formula

3. **From discrete walk on a line to 1dim diffusion** (11.04.06, Mahnke)
   Continuous approximation of symmetric Binominal distribution resulting in Gaussian probability density, definition of diffusion coefficient, diffusion equation, phenomenological understanding by Fick's laws, Einstein's derivation (*Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen* in `Annalen der Physik, 1905`)

4. **Diffusion in a finite interval** (18.04.06, R. Mahnke)
   Example of initial and boundary value diffusion problem in a finite interval with one reflecting (left) and one absorbing boundary (right); transformation to dimensionless variables, separation ansatz, wave equation, discrete set of wave numbers, superposition, outflow at right boundary

5. **Exercise: Diffusion equation and its solution** (21.04.06, R. Mahnke)
   Discussion of outflow function at right boundary (probability per time) and its properties, limit case for left boundary tends to minus infinity, solution of diffusion equation with natural boundaries and initial delta peak by method of Fourier transformation

6. (25.04.06, Verlegung in Projektwoche)

7. **The master equation** (28.04.06, J. Kaupužs)
   Introduction into 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

8. **Solution of one–step master equation** (02.05.06, J. Kaupužs)
   One–step master equation and its stationary solution for a closed finite system, discussion of a particular case: dissolution of traffic congestion, finding the solution recursively and calculation of moments, an alternative way of solution by means of generating function

9. **Exercise: Properties of Gaussian distribution** (05.05.06, R. Mahnke)
   Method of getting solution of diffusion equation by Fourier transformation, calculation of moments of Gaussian distribution, checking normalisation (zeroth moment), computing mean value and variance

10. **Drift–diffusion dynamics in finite interval** (09.05.06, J. Hinkel)
    Introduction of drift–diffusion equation in a finite interval taking into account specific boundary conditions, i. e. reflecting boundary on the left hand side and absorbing border on the right hand side, formulation of corresponding mathematical description (Fokker–Planck equation), explanation of algorithm to get the analytical solution in term of probability density, influence of drift value on final result

11. **Stochastic description by different concepts** (12.05.06, R.Mahnke)
    Based on drift–diffusion equation the notation of Fokker–Planck equation in the general one–dimensional form has been introduced, relationship to Master equation via Kramers–Moyal expansion, introduction of stochastic differential equation in Ito notation and its relationship to Fokker–Planck equation, definition of Wiener process (white noise) and numerical realizations

12. **Ornstein–Uhlenbeck process** (16.05.06, Ch. Liebe)
    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) as well as special cases (analytically), especially the well–known stationary Maxwell–Boltzmann velocity distribution of an ideal gas

13. **Summeries and home works** (19.05.06, R. Mahnke)
    Ornstein–Uhlenbeck process revisited and underlining basis equations once again, showing probability density distribution for different time moments as computer graphics (via gnu plot).
    Discussing of home works (orthogonality, completness) concerning eigenfunctions for drift–diffusion in finite interval

14. **Car cluster formation I** (23.05.06, R. Mahnke)
    Example of one–step master equation with jam formation and dissolution, introducing the concept of optimal velocity function and discussing the phase transition between dilute and dense traffic, from free flow to stop–and–go motion (congestion)

15. (26.05.06, R. Mahnke) Keine Lehrveranstaltung (Brückentag)

16. **Car cluster formation II** (30.05.06, R. Mahnke)
    Hint for phase transition by phase space analysis of nonlinear vehicular dynamics called Bando's model, transition from fixed point to limit cycle behaviour in space of headways and velocities, calculation of mean cluster size: zero at small densities, nonzero value at larger densities

17. **Stochastics of a decay process** (02.06.06, R. Mahnke)
    Having in mind the well–known radioactive decay process, the one–step master equation has been solved by two different methods:
    (1) Solution of a system of linear differential equations (algebraic method, presented by Th. Kiesel)
    (2) Method of generating functions to solve a partial differential equation

18. **Projects** (06.06.06, R. Mahnke)
    Consultations concerning project tasks: 09.06.06 + 13.06.06 (Projektwoche)

    a) Coordinate dependent diffusion (Thomas Kiesel)
    b) Bistable Schlögl reaction (Peter Grünwald)
    c) Galton board (Elisabeth Schöne)
    d) Sturm–Liouville theory (Daniel Münzner)
    e) Stochastic trajectories + Lorenz attractor
       (Knut Klingbeil & Sebastian Helm)

19. **Project work** (16.06.06, R. Mahnke)
    Presentation of two projects by
    Knut Klingbeil: Stochastic trajectories and Lorenz attractor
    (Generation of random numbers, white noise trajectories, Lorenz system as set of nonlinear deterministic differential equations, chaotic properties)
    and
    Daniel Münzner: Sturm–Liouville theory
    (Sturm-Liouville equation as initial–boundary value problem searching for eigenvalues and eigenfunctions, special case: wave equation looking for standing waves)

20. **Project work** (20.06.06, R. Mahnke)
    Presentation of the project 'Coordinate dependent diffusion' by Thomas Kiesel (Introducing linearly space dependent diffusion coefficent into Fick's law, solving the corresponding (more complicated) one–dimensional diffusion equation by transformations, separation ansatz, solution is represented by Bessel functions)

21. **Nucleation in supersaturated systems I** (23.06.06, R. Mahnke)
    Phase transition in a finite isothermal–isochoric systems by symmetry breaking. Formation of small clusters of a new dense phase in a dilute surrounding, e. g. liquid–gas transition. Cluster distribution function as order parameter. Calculation of state function 'free energy' from the canonical partition function

22. **Project work** (27.06.06, R. Mahnke)
    Presentation of two projects by
    Elisabeth Schöne: Galton board
    (Sir Francis Galton and its life, discrete finite board, general Binominal distribution with two special cases: pure diffusion and pure drift, transition to Gaussian distribution by vanishing hopping rate and lattice parameter as well)
    and
    Peter Grünwald: Bistable Schlögl reaction
    (Kinetics of Schlögl reaction, deterministic description by cubic equation for temporal development of concentration, comparison with stochastic description by one–step master equation, discussion of transition rates and detailed balance solution)

23. **Nucleation in supersaturated systems II** (30.06.06, R. Mahnke)
    Free energy (ideal part and binding energy) of a finite one–cluster–system with monomers (in a heat bath), ansatz for attachment rate due to condensation, using detailed balance relation to obtain detachment rate (evaporation), solving master equation numerically, dynamics of mean cluster size and determination of its stationary solutions depending on overall concentration, discussion of bistability

24. **Summeries and case studies** (04.07.06, R. Mahnke)
    Master equation, stationary solution, detailed balance as equilibrium case, probability distribution as Boltzmann function with free energy, relationship between transition rates and free energy difference, calculation of free energy of vehicular traffic based on given ratio of transition rates for a specified traffic flow model (optimal velocity model), discussion of free energy difference as function of car cluster size for different overall densities, bifurcation diagram of first–order phase transition (subcritical and supercritical)

25. **Reaction–diffusion equation** (07.07.06, R. Mahnke)
    Formulation of reaction–diffusion equation by empirical arguments based on general balance equation, relationship to Fokker–Planck equation, without diffusion only homogeneous solutions possible, fixed point analysis, Schlögl reaction with diffusion showing moving profils

26. **Fokker–Planck equation** (11.07.06, R. Mahnke)
    Discussion of general Fokker–Planck equation, forward and backword notation, comparison of different boundary conditions, identical conditional probability density as solution in both cases

27. **Concluding remarks** (14.07.06, R. Mahnke)
    Final presentation of project 'Coordinate dependent diffusion' by Thomas Kiesel, round table disussion (with ice cream)

Acknowledgements

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