Stochastische Prozesse in der Physik

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Montag 15.00 bis 16.30 Uhr, Konferenzraum Wismarsche Str. 44
Montag 16.45 bis 18.15 Uhr, Konferenzraum Wismarsche Str. 44
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This is a joint lecture with the International Study Programme *Master of Science in Physics* at the Institute of Physics.

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

Die Lehrveranstaltung beginnt mit der ersten Vorlesung am Montag, d. 14.10.2013 um 15.15 Uhr im Seminarraum Wismarsche Str. 44

The Importance of Being Noisy – Stochasticity in Science

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

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

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

Textbooks

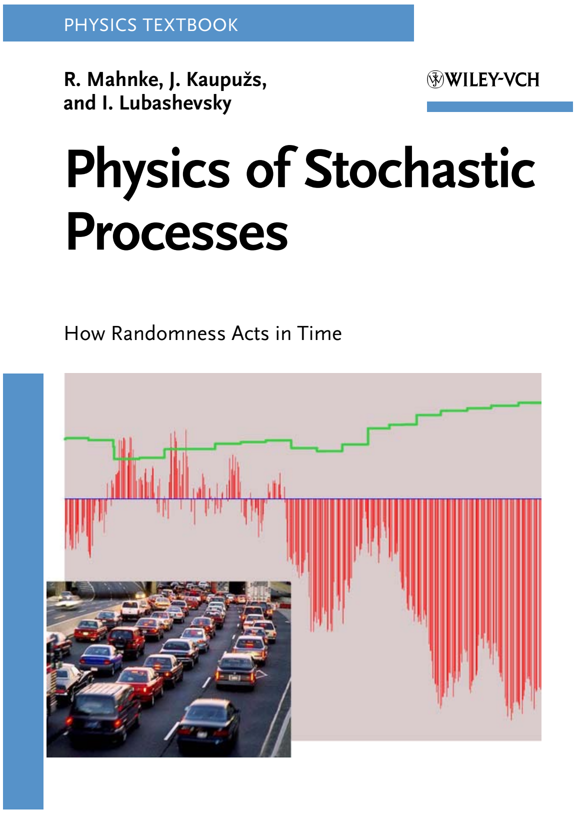

Fig. 1: R. Mahnke, J. Kaupužs and I. Lubashevsky: *Physics of Stochastic Processes*, Wiley-VCH, Weinheim, 2009.

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

Inhaltsverzeichnis

1 Random Walker (Brownian Particle)

1.1 From Random Walk to Diffusion

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

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

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

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

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

$$P(m, n+1) = p\, P(m-1, n) + q\, P(m+1, n) \ . \tag{1}$$

The solution of (1) is the binomial distribution

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

The first moment of this probability distribution is

$$\langle m \rangle (n) = \sum_{m=-n}^{n} m P(m, n) = 2n \left(p - \frac{1}{2} \right) \tag{3}$$

and the second moment is

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

Hence, the root–mean–square is given by

$$\sigma(n) = \sqrt{\left\langle (m - \langle m \rangle)^2 \right\rangle} = \sqrt{\langle m^2 \rangle - \langle m \rangle^2} = \sqrt{4npq} , \tag{5}$$

and the relative width (error)

$$\frac{\sigma}{\langle m \rangle} = \frac{\sqrt{4np(1-p)}}{2n(p-1/2)} = \sqrt{\frac{p(1-p)}{(p-1/2)^2}} \frac{1}{\sqrt{n}} \simeq n^{-1/2} \tag{6}$$

tends to zero when n goes to infinity.

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

$$m = \{-n, -n+1, \ldots, -1, 0, +1, \ldots, n-1, n\} . \tag{7}$$

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

$$m = k - (n-k) = 2k - n . \tag{8}$$

For the k successes we get

$$k = \frac{1}{2}(n+m) . \tag{9}$$

Starting with the well–known binomial distribution for discrete probabilities

$$P(m,n) \equiv B(k,n) = \binom{n}{k} p^k (1-p)^{n-k} \tag{10}$$

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

$$P(m,n) = \frac{n!}{k!(n-k)!} \left(\frac{1}{2}\right)^n = \frac{n!}{[(n+m)/2]!\,[(n-m)/2]!} \left(\frac{1}{2}\right)^n . \tag{11}$$

Further on we introduce (still discrete) coordinate $x_m = d\,m$ and time $t_n = \tau\,n$, where d is the hopping distance (a length unit) and τ is the time step (a time unit) and rewrite the binomial distribution (11) as $P(x_m, t_n)$.

After introducing a new control parameter

$$D = \frac{d^2}{\tau} \ , \tag{12}$$

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

Taking into account the definition (12), we finally obtain the Gaussian distribution

$$p(x,t) = \frac{1}{\sqrt{2\pi Dt}} \exp\left(-\frac{x^2}{2Dt}\right) \ . \tag{13}$$

The dynamics of probability density $p(x,t)$ (13) for a one–dimensional random walk is given by the one–dimensional diffusion equation (partial differential equation)

$$\frac{\partial p(x,t)}{\partial t} = \frac{D}{2} \frac{\partial^2 p(x,t)}{\partial x^2} \ . \tag{14}$$

To obtain certain solution, the diffusion equation (14) has to be completed by initial and boundary conditions. We consider the initial condition $p(x, t = 0) = \delta(x-0)$ given by the delta function (a sharp peak at $x = 0$), which physically means that the random walk starts at $x = 0$, as well as natural boundary conditions $\lim_{x\to\pm\infty} p(x,t) = 0$.

Home work related to Chapter 1.1 (Abgabe am 28.10.2013)

1. Calculate the zeroth, first and second moment of probability (2).
2. It is known that function (13) solves equation (14). Investigate the general case of drift–diffusion and guess a function which solves the following drift–diffusion equation
$$\frac{\partial p(x,t)}{\partial t} = -v_{drift} \frac{\partial p(x,t)}{\partial x} + \frac{D}{2} \frac{\partial^2 p(x,t)}{\partial x^2} \ .$$
3. Repeat the calculations of zeroth, first and second moment for probability density $p(x,t)$ (drift–diffusion case) and discuss the solutions.
4. Derive from one–dimensional diffusion equation (14) the well–known solution (13) using the following ansatz of product type $p(x,t) = g(t)f(x)$.

1.2 From Random Walker to Vehicular Traffic: Motion on a Circle

1.2.1 Asymmetric Random Walker: Position and time are discrete

Asymmetric random walker. Starting with Markov chain ($p + q = 1$)

$$P(m, n+1) = p\,P(m-1, n) + q\,P(m+1, n) \tag{15}$$

together with a precisely given initial position

$$P(m, n=0) = \delta_{m,m_0} \tag{16}$$

setting $m_0 = 0$ for simplicity. We have discrete position $m = 0, \pm 1, \pm 2, \ldots$ and discrete time $n = 0, 1, 2, \ldots$.
The solution of (15) is well known called Binominal distribution

$$P(m, n) = \frac{n!}{[(n+m)/2]!\,[(n-m)/2]!}\, p^{(n+m)/2}\, q^{(n-m)/2}\ . \tag{17}$$

It is related to the Binominal formula (take $a \equiv p$ and $b \equiv q$)

$$(a+b)^n = \sum_{r=0}^{n} \binom{n}{r} a^r\, b^{n-r} = \sum_{r=0}^{n} \frac{n!}{r!\,(n-r)!}\, a^r\, b^{n-r} \tag{18}$$

with $r = (n+m)/2$ and $n - r = (n-m)/2$.

How to get the solution (17)? We use spatial Fourier transformation given as

$$\widetilde{P}(k, n) = \sum_{m=-n}^{n} P(m, n)\, e^{ikm}\ , \tag{19}$$

$$P(m, n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \widetilde{P}(k, n)\, e^{-ikm}\, dk\ . \tag{20}$$

To prove this we use the orthogonality relation

$$\int_{-\pi}^{\pi} e^{-ik(m-m')}\, dk = 2\pi\, \delta_{m',m}\ . \tag{21}$$

The calculations to get a Markov chain equation in k–space are as follows

$$\sum_m P(m, n+1)\, e^{ikm} = p \sum_m P(m-1, n)\, e^{ikm} + q \sum_m P(m+1, n)\, e^{ikm} \tag{22}$$

$$\begin{aligned} \widetilde{P}(k, n+1) &= p \sum_{m'} P(m', n)\, e^{ik(m'+1)} + q \sum_{m''} P(m'', n)\, e^{ik(m''-1)} \\ &= \left(p\, e^{ik} + q\, e^{-ik}\right) \widetilde{P}(k, n)\ . \end{aligned} \tag{23}$$

This iterative equation has a very simple solution given as

$$\widetilde{P}(k,n) = \left(p\, e^{ik} + q\, e^{-ik}\right)^n \; \widetilde{P}(k,n=0) \tag{24}$$

with initial condition in k–space $\widetilde{P}(k,n=0) = e^{ikm_0} = 1$ if $m_0 = 0$.
Using the inverse transformation (20) we get

$$P(m,n) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \left(p\, e^{ik} + q\, e^{-ik}\right)^n \; e^{-ikm}\, dk\ . \tag{25}$$

Taking the Binominal formula (18) into account we receive

$$\begin{aligned}
P(m,n) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \left[\sum_{r=0}^{n} \binom{n}{r} p^r\, e^{ikr}\, q^{n-r}\, e^{-ik(n-r)}\right] e^{-ikm}\, dk & (26)\\
&= \sum_{r=0}^{n} \binom{n}{r} p^r\, q^{n-r} \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ikr}\, e^{-ikn}\, e^{ikr}\, e^{-ikm}\, dk & (27)\\
&= \sum_{r=0}^{n} \binom{n}{r} p^r\, q^{n-r} \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ik(m-(2r-n))}\, dk & (28)\\
&= \sum_{r=0}^{n} \binom{n}{r} p^r\, q^{n-r}\, \delta_{m,2r-n}\ . & (29)
\end{aligned}$$

Only the term with $m = 2r - n$ remains which gives $r = (n+m)/2$. The solution is therefore

$$P(m,n) = \binom{n}{(n+m)/2} p^{(n+m)/2}\, q^{n-(n+m)/2}\ , \tag{30}$$

which is finally identical with the already known solution (17).

Now we switch to random motion on a closed line of finite length having periodic boundary condition.

1.2.2 Stochastic Motion on a Ring: Position and time are discrete

Once again asymmetric random walker. Starting with Markov chain ($p+q = 1$)

$$P(x_m, t_n + \tau) = p\, P(x_m - a, t_n) + q\, P(x_m + a, t_n) \tag{31}$$

having discrete position and time

$$\begin{aligned}
x_m &= a\, m \quad , \quad m = 0,1,2,\ldots,M-1 & (32)\\
t_n &= \tau\, n \quad , \quad n = 0,1,2,\ldots & (33)
\end{aligned}$$

Using $x_M = a\,M = L$ as length of the ring.
Periodicity means

$$P(x_m, t_n) = P(x_m + L, t_n) \ . \tag{34}$$

Given initial condition

$$P(x_m, t_0 = 0) = \delta_{x_m, x_0} \ . \tag{35}$$

Here x_0 is the initial coordinate of the random walker, which is not necessarily zero. Once again we use spatial Fourier transformation, now given as

$$\widetilde{P}(k, t_n) = \sum_{m=0}^{M-1} P(x_m, t_n)\, e^{ikx_m} \ , \tag{36}$$

$$P(x_m, t_n) = \frac{1}{M} \sum_k \widetilde{P}(k, t_n)\, e^{-ikx_m} \ . \tag{37}$$

with M discrete wave numbers $k = 2\pi l/L$ for $l = 0, 1, \ldots, M-1$.

To prove this we use orthogonality

$$\sum_k e^{-ik(x_m - x_{m'})} = \sum_{l=0}^{M-1} e^{-i(2\pi l/M)(m-m')} = M\,\delta_{m',m} \ . \tag{38}$$

To get a Markov chain equation in discrete k–space similar calculations as before give

$$\widetilde{P}(k, t_n) = \left(p\, e^{ika} + q\, e^{-ika}\right)^{t_n/\tau}\ e^{ikx_0} \tag{39}$$

Inverse transformation generates the following solution

$$P(x_m, t_n) = \frac{1}{M} \sum_k \left(p\, e^{ika} + q\, e^{-ika}\right)^{t_n/\tau}\ e^{-ika(x_m - x_0)/a} \tag{40}$$

with

$$k' \equiv ka = 2\pi l/M \qquad , \qquad l = 0, 1, 2, \ldots, M-1 \ . \tag{41}$$

To consider the limit $M \to \infty$ we replace the sum by the integral as follows

$$\frac{1}{M} \sum_{k'} \ldots \quad \to \quad \frac{1}{2\pi} \int_{-\pi}^{\pi} \ldots\, dk' \ . \tag{42}$$

The periodic solution (40) shows the diffusive relaxation from the initial sharp peak (35) to steady state with or without drift depending on the asymmetry parameter $\Delta = p - q$. Using Δ instead of $p = 1 - q$ we get

$$\left(p\, e^{ika} + q\, e^{-ika}\right) = \cos(ka) + i\Delta \sin(ka) \tag{43}$$

and receive the solution (40) in the following notation

$$P(x_m, t_n) = \frac{1}{M} \sum_k e^{-(\lambda'_k - i\lambda''_k)t_n} \, e^{-ik(x_m - x_0)} \tag{44}$$

with

$$\lambda'_k = -\frac{1}{\tau} \ln\left(\sqrt{\cos^2(ka) + \Delta^2 \sin^2(ka)}\right) \tag{45}$$

$$\lambda''_k = \frac{1}{\tau} \arcsin\left(\frac{\Delta \sin(ka)}{\sqrt{\cos^2(ka) + \Delta^2 \sin^2(ka)}}\right) = \frac{1}{\tau} \arctan\left(\Delta \tan(ka)\right) \tag{46}$$

Finally we rewrite the periodic solution as

$$\begin{aligned} P(x_m, t_n) &= \frac{1}{M} \sum_k e^{-\lambda'_k t_n} \left[\cos(\lambda''_k t_n) \cos(k(x_m - x_0))\right. \\ &\qquad \left. + \sin(\lambda''_k t_n) \sin(k(x_m - x_0))\right] . \end{aligned} \tag{47}$$

This rotating ($\Delta \neq 0$) random walker is, of course, not a model of traffic flow. This stochastic process explains drift–diffusive motion without interaction and active behaviour.

1.2.3 Position is discrete and time is continuous

In this case we have the master equation

$$\frac{\partial}{\partial t} P(x_m, t) = w_+ P(x_{m-1}, t) + w_- P(x_{m+1}, t) - [w_+ + w_-] P(x_m, t) \, . \tag{48}$$

Here $x_m = ma$, $m = 0, 1, 2, \ldots, M-1$ are the discrete coordinates, whereas time t is continuous. The quantities w_+ and w_- are transition rates, which in this case are assumed to be constant. As before, motion is on a ring of lenght L (periodic boundary condition), starting at x_0.

To obtain the solution, we use the Fourier transformation

$$\widetilde{P}(k, t) = \sum_{m=0}^{M-1} P(x_m, t) e^{ikx_m} \tag{49}$$

$$P(x_m, t) = \frac{1}{M} \sum_k \widetilde{P}(k, t) e^{-ikx_m} \tag{50}$$

with $k = 2\pi l/L$ for $l = 0, 1, 2, \ldots, M-1$. It gives the equation in the k–space

$$\frac{\partial \widetilde{P}(k,t)}{\partial t} = \left[w_+ e^{ika} + w_- e^{-ika} - (w_+ + w_-)\right] \widetilde{P}(k,t) = -\lambda_k \widetilde{P}(k,t) \ , \tag{51}$$

where

$$\lambda_k = w_+(1 - e^{ika}) + w_-(1 - e^{-ika}) \ . \tag{52}$$

The complex solution reads

$$\widetilde{P}(k,t) = \widetilde{P}(k,0) e^{-\lambda_k t} \ . \tag{53}$$

Using the initial condition $P(x_m, 0) = \delta_{x_m, x_0}$ and (49), we get

$$\widetilde{P}(k,0) = e^{ikx_0} \ . \tag{54}$$

Inserting (53) and (54) into (50), we obtain the solution in the coordinate space,

$$P(x_m, t) = \frac{1}{M} \sum_k e^{-\lambda_k t - ik(x_m - x_0)} \ . \tag{55}$$

Further on we represent the complex rate parameter λ_k as

$$\lambda_k = \lambda'_k - i\lambda''_k \ , \tag{56}$$

where

$$\lambda'_k = (w_+ + w_-)(1 - \cos(ka)) \tag{57}$$
$$\lambda''_k = (w_+ - w_-)\sin(ka) \ . \tag{58}$$

It allows us to write the solution in real form as

$$P(x_m, t) = \frac{1}{M} \sum_k e^{-\lambda'_k t} \Big(\cos(\lambda''_k t) \cos(k[x_m - x_0]) + \sin(\lambda''_k t) \sin(k[x_m - x_0]) \Big) \ . \tag{59}$$

1.2.4 From discrete to continuous time

The solution $P(x_m, t_n)$ of the model with discrete time and coordinate is different for odd and even n, i. e., it always makes jumps in time in such a way that it is zero for odd m and nonzero for even m at one time step and vice versa at the next time step. Therefore, we consider the probability function

$$\bar{P}(x_m, t_n) = \frac{1}{2}\Big(P(x_m, t_n) + P(x_m, t_n + \tau)\Big) \ , \tag{60}$$

which is obtained by an averaging over two succesive time steps. This function is expected to be smoother in time. Considering two succesive steps of the Markov chain (31),

$$P(x_m, t_n + \tau) = p\,P(x_m - a, t_n) + q\,P(x_m + a, t_n) \tag{61}$$

$$P(x_m, t_n + 2\tau) = p\,P(x_m - a, t_n + \tau) + q\,P(x_m + a, t_n + \tau) \ , \tag{62}$$

we obtain the Markov chain

$$\bar{P}(x_m, t_n + \tau) = p\bar{P}(x_m - a, t_n) + q\bar{P}(x_m + a, t_n) \tag{63}$$

for $\bar{P}(x_m, t_n)$. If the initial condition for $P(x_m, t_n)$ is $P(x_m, 0) = \delta_{x_m, x_0}$, then for $\bar{P}(x_m, t_n)$ we have

$$\bar{P}(x_m, 0) = \frac{1}{2}\Big(q\,\delta_{x_m, x_0 - a} + \delta_{x_m, x_0} + p\,\delta_{x_m, x_0 + a}\Big) \ . \tag{64}$$

Taking into account that $p + q = 1$, we can write

$$\begin{aligned} \frac{\bar{P}(x_m, t_n + \tau) - \bar{P}(x_m, t_n)}{\tau} &= \frac{p}{\tau}\,\bar{P}(x_m - a, t_n) + \frac{q}{\tau}\,\bar{P}(x_m + a, t_n) \\ &- \frac{p + q}{\tau}\,\bar{P}(x_m, t_n) \ . \end{aligned} \tag{65}$$

The expression on the left hand side of (65) is approximately equal to the time derivative $\partial\bar{P}(x_m, t)/\partial t$ at $t = t_n$ for $\tau \ll t_n$, i. e., for a large number of time steps or large time scale, when the probability distribution $\bar{P}(x_m, t)$ (but not $P(x_m, t)$) changes very slightly in one time step. It leads to the master equation

$$\frac{\partial\bar{P}(x_m, t)}{\partial t} = w_+\bar{P}(x_m - a, t) + w_-\bar{P}(x_m + a, t) - (w_+ + w_-)\bar{P}(x_m, t) \ , \tag{66}$$

where $w_+ = p/\tau$ and $w_- = q/\tau$ are the transition rates. Here we consider the limit $t/\tau \to \infty$ for a finite τ, since the transition rates have to be finite. For large t/τ, the solution of (66) with the initial condition (64) is practically the same as the solution with the initial condition $\bar{P}(x_m, 0) = \delta_{x_m, x_0}$, since the shift of the initial coordinate by one lattice constant a is not important.

Thus, at large time scales $t/\tau \gg 1$, the solution for $\bar{P}(x_m, t)$ is given by the expression on the right hand side of (59), which is expected to be approximately consistent with (60), where $P(x_m, t_n)$ and $P(x_m, t_n + \tau)$ are calculated from (47).

1.2.5 Position and time are continuous

We consider now the limit $a \to 0$ in the master equation (48) or (66). These two equations are similar, with the only difference that (66) is for the averaged over two succesive time steps probability distribution. We can rewrite (48) as

$$\begin{aligned}\frac{\partial P(x_n,t)}{\partial t} &= a^2 \frac{w_+ + w_-}{2} \frac{P(x_n+a,t) - 2P(x_n,t) + P(x_n-a,t)}{a^2} \\ &- a\,(w_+ - w_-) \frac{P(x_n+a,t) - P(x_n-a,t)}{2a} \, . \end{aligned} \tag{67}$$

Considering the probability density $p(x,t) = P(x,t)/a$ as a continous function of coordinate x and taking the limit $a \to 0$, we obtain from (67) the drift–diffusion equation

$$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2} - v_{\mathrm{drift}} \frac{\partial p(x,t)}{\partial x} \tag{68}$$

with the diffusion coefficient D and drift coefficient v_{drift} given by

$$D = \frac{a^2}{2}\Big(w_+ + w_-\Big) \tag{69}$$

$$v_{\mathrm{drift}} = a\,(w_+ - w_-) \, . \tag{70}$$

To get this result, the following relations have been used

$$\lim_{a\to 0} \frac{p(x+a,t) - p(x-a,t)}{2a} = \frac{\partial p(x,t)}{\partial x} \tag{71}$$

$$\lim_{a\to 0} \frac{p(x+a,t) - 2p(x,t) + p(x-a,t)}{a^2} = \frac{\partial^2 p(x,t)}{\partial x^2} \, . \tag{72}$$

To solve (68) with the initial condition $p(x,0) = \delta(x - x_0)$, we use the Fourier transformation

$$\widetilde{p}(k,t) = \int_0^L p(x,t) e^{ikx} dx \tag{73}$$

$$p(x,t) = \frac{1}{L} \sum_k \widetilde{p}(k,t) e^{-ikx} dk \, , \tag{74}$$

where $k = 2\pi l/L$ with $l = 0, \pm 1, \pm 2, \ldots$ The Fourier–transformed drift–diffusion equation reads

$$\frac{\partial \widetilde{p}(k,t)}{\partial t} = (-Dk^2 + ik\, v_{\mathrm{drift}})\, \widetilde{p}(k,t) \, . \tag{75}$$

The solution is

$$\widetilde{p}(k,t) = \widetilde{p}(k,0)\, e^{-\lambda_k t} \;, \tag{76}$$

where the complex rate parameter λ_k is

$$\lambda_k = \lambda_k' - i\lambda_k'' \tag{77}$$

with

$$\begin{aligned} \lambda_k' &= Dk^2 && (78) \\ \lambda_k'' &= k\, v_{\rm drift} \;. && (79) \end{aligned}$$

Using the initial condition $p(x,0) = \delta(x - x_0)$, we obtain $\widetilde{p}(k,0) = e^{ikx_0}$ and thus

$$\widetilde{p}(k,t) = e^{-\lambda_k t + ikx_0} \;. \tag{80}$$

The solution in the coordinate space

$$p(x,t) = \frac{1}{L} \sum_k e^{-(\lambda_k' - i\lambda_k'')t} e^{-ik(x-x_0)} \tag{81}$$

is obtained via the transformation (74). In can be written in a real form as

$$\begin{aligned} p(x,t) &= \frac{1}{L} \sum_k e^{-\lambda_k' t} \Big(\cos(\lambda_k'' t) \cos(k[x - x_0]) \\ &\qquad + \sin(\lambda_k'' t) \sin(k[x - x_0]) \Big) \;. && (82) \end{aligned}$$

1.2.6 Transformation from discrete to continuos coordinate in the solution

The solution (82) can be obtained from that one (59) with discrete coordinate x_n in a certain limit, where this solution is quasi–continuous (it holds for large $w_+ t$ and $w_- t$) and therefore only small–k contribution is relevant, if the summation interval in (59) is made more symmetric around $k = 0$ (otherwise the vicinity of $k = 2\pi$ is also important). For this purpose, first we shift the range of l for $k = 2\pi l/L$ in (59) by $-[M/2]$. In the continuum limit $a \to 0$, where we have $M = L/a \to \infty$, this yields $k = 2\pi l/L$ with $l = 0, \pm 1, \pm 2, \ldots$ Further on, we expand λ_k' in (57) and λ_k'' in (58) in a Taylor series around $k = 0$, which yields λ_k' and λ_k'' consistent with (78) and (79), i. e.,

$$\begin{aligned} \lambda_k' &= (w_+ + w_-)(1 - \cos(ka)) \approx (w_+ + w_-)\, \frac{(ka)^2}{2} = Dk^2 && (83) \\ \lambda_k'' &= (w_+ - w_-) \sin(ka) \approx (w_+ - w_-)\, ka = k\, v_{\rm drift} \;. && (84) \end{aligned}$$

Dividing both sides of (59) by a (it yields $P(x,t) \to p(x,t)$ and $1/M \to 1/L$), and applying the considered here shift of k values and the approximations for λ'_k and λ''_k, we obtain the continuum solution (82).

1.2.7 What do we need for traffic flow?

Discrete stochastic model of Ornstein-Uhlenbeck type with 'staying together parameter' γ, drift or speed v, diffusion or stochasticity D

$$\frac{\partial}{\partial t}p(x,t) = -v\frac{\partial}{\partial x}p(x,t) + \gamma\frac{\partial}{\partial x}\left(xp(x,t)\right) + D\frac{\partial^2}{\partial x^2}p(x,t) \tag{85}$$

1.2.8 Fourier transforms in the case of discrete coordinates with finite period L

At any given time moment t_n we have

$$\widetilde{P}(k,t_n) = \sum_{m=0}^{M-1} P(x_m,t_n)e^{ikx_m} \tag{86}$$

$$P(x_m,t_n) = \frac{1}{M}\sum_k \widetilde{P}(k,t_n)e^{-ikx_m}\,, \tag{87}$$

where $k = 2\pi\ell/L$ with $\ell = 0,1,2,\ldots,M-1$ are the set of discrete wave vectors and $x_m = m\ell/M$ with $m = 0,1,2,\ldots,M-1$ are the discrete coordinates. To prove (check) these relations, first we insert (87) into (86). It yields

$$\begin{aligned}\widetilde{P}(k,t_n) &= \sum_{m=0}^{M-1}\left(\frac{1}{M}\sum_q \widetilde{P}(q,t_n)e^{-iqx_m}\right)e^{ikx_m}\\ &= \frac{1}{M}\sum_q \widetilde{P}(q,t_n)\sum_{m=0}^{M-1} e^{ix_m(k-q)} = \sum_q \widetilde{P}(q,t_n)\,\delta_{k,q}\\ &= \widetilde{P}(k,t_n)\,.\end{aligned} \tag{88}$$

Here the orthoganality relation

$$\sum_{m=0}^{M-1} e^{ix_m(k-q)} = \sum_{m=0}^{M-1} e^{2\pi i\,m(\ell-\ell')/M} = M\,\delta_{\ell-\ell',0} \tag{89}$$

for $k = 2\pi\ell/L$ and $q = 2\pi\ell'/L$ has been used.

Now we insert (86) into (87). It yields

$$\begin{aligned} P(x_m, t_n) &= \frac{1}{M} \sum_k \left(\sum_{n=0}^{M-1} P(x_n, t_n) e^{ikx_n} \right) e^{-ikx_m} \\ &= \frac{1}{M} \sum_{n=0}^{M-1} P(x_n, t_n) \sum_k e^{ik(x_n - x_m)} \\ &= \frac{1}{M} \sum_{n=0}^{M-1} P(x_n, t_n)\, M \delta_{x_n, x_m} = P(x_m, t_n) \;, \end{aligned} \tag{90}$$

using again the orthogonality of the wave functions e^{ikx_m}.

1.2.9 The limit $L \to \infty$ for discrete coordinates

To take this limit, it is convenient to write (86) as

$$\widetilde{P}(k, t_n) = \sum_{m=-[M/2]}^{M-1-[M/2]} P(x_m, t_n) e^{ikx_m} \;, \tag{91}$$

shifting the coordinate system by $-[M/2]$, where $[M/2]$ is the integer part of $M/2$. In this case, we obtain all possible coordinates x_m ranging from $-\infty$ to ∞ at $M \to \infty$. Further on, we rewrite (87) as

$$P(x_m, t_n) = \frac{1}{M\Delta k} \sum_k \widetilde{P}(k, t_n) e^{-ikx_m} \Delta k \;, \tag{92}$$

where $\Delta k = 2\pi/L$ is the distance between points in the k–space, and then change the variables $q = k\,L/M$, $\hat{P}(q, t_n) = \widetilde{P}(k, t_n)$. We consider the limit $L \to \infty$ at a given lattice constant $a = L/M$, i. e., the limit $M \to \infty$ or $\Delta q = 2\pi/M \to 0$. In this case we obtain

$$\begin{aligned} P(x_m, t_n) &= \lim_{\Delta q \to 0} \frac{1}{M\Delta q} \sum_q \hat{P}(q, t_n) e^{-iq\,(M/L)x_m} \Delta q \\ &= \frac{1}{2\pi} \int_0^{2\pi} \hat{P}(q, t_n) e^{-iqm} dq = \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{P}(q, t_n) e^{-iqm} dq \;. \end{aligned} \tag{93}$$

In the latter transformation, the periodicity relation $\widetilde{P}(k + 2\pi M/L, t_n) = \widetilde{P}(k, t_n)$, i. e., $\hat{P}(q + 2\pi, t_n) = \hat{P}(q, t_n)$ has been used. Changing now the notations in such a way that $\widetilde{P}(k, t_n)$ again is the Fourier transform of $P(x_m, t_n)$, we have

$$\begin{aligned} \widetilde{P}(k,t_n) &= \sum_{m=-\infty}^{\infty} P(x_m,t_n)e^{ikm} && (94) \\ P(x_m,t_n) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \widetilde{P}(k,t_n)e^{-ikm}dk\ . && (95) \end{aligned}$$

1.2.10 Continuum limit for an infinite L and discrete time

Consider now the continuum limit in (94) and (95), where the lattice constant a goes to zero. One has to take into account that in the model with discrete time the random walker always jumps from an odd to an even lattice site or vice versa at each time step. According to this, we first rewrite (94) as

$$\widetilde{P}(k,t_n) = \frac{1}{\Delta x}\sum_{m=-\infty}^{\infty} P(x_m,t_n)e^{ikm}\Delta x\ , \qquad (96)$$

where $\Delta x = 2a$ is the distance between lattice sites of an odd or an even sublattice, on which $P(x_m, t_n)$ has nonzero values. Furter on, we introduce the probability density $p(x, t_n) = P(x, t_n)/\Delta x = P(x, t_n)/(2a)$ and rescaled wave vector $q = k/a$. Taking into account that $x_m = m/a$ and denoting $\widetilde{p}(q, t_n) = \widetilde{P}(k, t_n)$, we obtain in the continuum limit

$$\widetilde{p}(q,t_n) = \lim_{\Delta x\to 0}\left(\sum_{m=-\infty}^{\infty}(P(x_m,t_n)/\Delta x)e^{iqx_m}\right) = \int_{-\infty}^{\infty} p(x,t_n)e^{iqx}dx \qquad (97)$$

$$\begin{aligned} p(x,t_n) &= \lim_{a\to 0}\left(\frac{1}{2a}\,\frac{1}{2\pi}\int_{-\pi/a}^{\pi/a}\widetilde{p}(q,t_n)e^{-iqx}dq\cdot a\right) \\ &= \frac{1}{4\pi}\int_{-\infty}^{\infty}\widetilde{p}(q,t_n)e^{-iqx}dq\ . && (98) \end{aligned}$$

Changing the notations in such a way that $\widetilde{p}(k, t_n)$ is the Fourier transform of $p(x, t_n)$, we have

$$\widetilde{p}(k, t_n) = \int_{-\infty}^{\infty} p(x, t_n) e^{ikx} dx \tag{99}$$

$$p(x, t_n) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \widetilde{p}(k, t_n) e^{-ikx} dk \; . \tag{100}$$

1.2.11 Continuum limit for a finite L and discrete time

We consider the continuum limit $a \to 0$ at a given time moment, taking again into account that the random walker always jumps from an odd to an even lattice site or vice versa at each time step. In this case, Eq. (86) gives us

$$\widetilde{P}(k, t_n) = \lim_{\Delta x \to \infty} \left(\frac{1}{\Delta x} \sum_{m=0}^{M-1} P(x_m, t_n) e^{ikx_m} \Delta x \right) = \int_0^L p(x, t_n) e^{ikx} dx \; . \tag{101}$$

Here $\Delta x = 2a = 2L/M$ is the distance between lattice sites of an odd or an even sublattice, on which $P(x_m, t_n)$ has nonzero values, and $p(x, t_n) = P(x, t_n)/\Delta x = P(x, t_n)\, M/(2L)$. For the sum over $k = 2\pi\ell/L$ in (87), we shift ℓ by $-[M/2]$. It is correct for any given M owing to the periodicity property $\widetilde{P}(k, t_n) = \widetilde{P}(2\pi M/L + k, t_n)$. Such a choice of ℓ interval is appropriate for the limit case $M \to \infty$ or $a \to 0$, since one can expect that the main contribution comes from the terms with finite ℓ values (for the initial asymmetric choice, terms with finite index ℓ and infinite at $M \to \infty$ index $M - \ell$ are equally important). In such a way, in this limit case we obtain

$$p(x, t_n) = \frac{1}{2L} \sum_k \widetilde{P}(k, t_n) e^{-ikx} \; , \tag{102}$$

where $k = 2\pi\ell/L$ with $\ell = 0, \pm 1, \pm 2, \ldots$ Changing the notations in such a way that $\widetilde{p}(k, t_n)$ is the Fourier transform of $p(x, t_n)$, we have

$$\widetilde{p}(k, t_n) = \int_0^L p(x, t_n) e^{ikx} dx \tag{103}$$

$$p(x, t_n) = \frac{1}{2L} \sum_k \widetilde{p}(k, t_n) e^{-ikx} \; . \tag{104}$$

1.2.12 The limit $L \to \infty$ in the case of continuous coordinate and discrete time

To take the limit $L \to \infty$ in (103) and (104) first we shift the coordinate system by $-L/2$ to ensure that all possible values of the coordinates ranging from $-\infty$ to ∞ are obtained at $L \to \infty$. Then we rewrite (104) as

$$p(x, t_n) = \frac{1}{\Delta k} \frac{1}{2L} \sum_k \widetilde{p}(k, t_n) e^{-ikx} \Delta k \; , \tag{105}$$

where $\Delta k = 2\pi/L$ is the distance between points in the k–space. In the limit $L \to \infty$ we have $\Delta k \to 0$, and the sum over k is replaced by the integral. It finally yields

$$\widetilde{p}(k, t_n) = \int_{-\infty}^{\infty} p(x, t_n) e^{ikx} dx \tag{106}$$

$$p(x, t_n) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \widetilde{p}(k, t_n) e^{-ikx} dk \; . \tag{107}$$

These equations are consistent with (99) and (100).

1.3 Tasks for students: Projects

1.3.1 Random walk with discrete position and time for natural boundary conditions

Ludwig Scheibe

Perform Monte Carlo (MC) simulations for a random walk on an infinite line with discrete positions $x_m = am$, $m = 0, \pm 1, \pm 2, \ldots$ and discrete time $t_n = \tau n$, $n = 0, 1, 2, \ldots$, starting at $x_0 = 0$. Make the transformation to dimensionless coordinates $x_m/a = m$ and dimensionless time $t_n/\tau = n$. At each time step the random walker jumps forwards ($m \to m + 1$) with probability p or backwards ($m \to m - 1$) with probability q, where $p + q = 1$. Perform MC simulations for several p values, including the symmetric case $p = 1/2$ and the asymmetric case $p \neq 1/2$, and estimate the probability distribution $P(m, n)$ to be at a position m after n time steps for different n values and compare the results with the theoretical Binomial distribution (17).

1.3.2 Random walk with discrete position and continuous time for natural boundary conditions

Julius Zimmermann

Consider the master equation (48), describing a random walk on an infinite line with discrete positions $x_m = ma$, $m = 0, \pm 1, \pm 2, \ldots$ and continuous time t. Find the probability distribution $P(x_m, t)$ at different time moments t for several sets of constant transition rates w_+ and w_- by solving the master equation via simulation of stochastic trajectories, starting at $x_0 = 0$. Compare the results with the analytical solution (59) for large $M \to \infty$ (or taking aM larger than the difference between the largest and the smallest coordinate reached in the simulations).

1.3.3 Random walk with continuous position and time for natural boundary conditions

Kai Wardelmann
Heinrich Behle

Consider the Fokker–Planck equation (68), describing a random walk on an infinite line with continuous coordinate x and time t. Find the probability density $p(x,t)$ by solving numerically (68) with the initial condition $p(x, t = 0) = \delta(x - x_0)$ for different sets of diffusion and drift coefficients, D and v_{drift}, and compare the results with the known analytical solution in the form of the Gaussian distribution

$$p(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{(x - x_0 - v_{\mathrm{drift}} t)^2}{4Dt} \right) . \tag{108}$$

1.3.4 Random walk on a ring with discrete position and time

Nicolas Künzel
Sören Lobback

Perform Monte Carlo (MC) simulations for a random walk on a ring of length L (periodic boundary conditions) with discrete positions $x_m = am$, $m = 0, 1, 2, \ldots, M-1$, and discrete time $t_n = \tau n$, $n = 0, 1, 2, \ldots$, starting at $x_0 = 0$. At each time step the random walker jumps forwards ($x_m \to x_m + a$) with probability p or backwards ($x_m \to x_m - a$) with probability q, where $p+$

$q = 1$. Perform MC simulations for several p values, including the symmetric case $p = 1/2$ and the asymmetric case $p \neq 1/2$, and estimate the probability distribution $P(x_m, t_n)$ to be at a position x_m at a time t_n for different n values and compare the results with the theoretical distribution (47).

1.3.5 Random walk on a ring with discrete position and continuous time

Helge Dobbertin

Consider the master equation (48), describing a random walk on a ring of length L (periodic boundary conditions) with discrete positions $x_m = ma$, $m = 0, 1, 2, \ldots, M-1$ and continuous time t. Find the probability distribution $P(x_m, t)$ at different time moments t for several sets of constant transition rates w_+ and w_- by solving the master equation via simulation of stochastic trajectories, starting at $x_0 = 0$. Compare the results with the analytical solution (59).

1.3.6 Random walk on a ring with continuous position and time

Björn Thorben Kruse
Philipp Henning

Consider the Fokker–Planck equation (68), describing a random walk on a ring of length L (periodic boundary conditions) with continuous coordinate x and time t. Find the probability density $p(x, t)$ by solving numerically (68) with the initial condition $p(x, t = 0) = \delta(x - x_0)$ for different sets of diffusion and drift coefficients, D and v_{drift}, and compare the results with the theoretical distribution (82).

1.3.7 Comparison between the random walk on a ring for discrete and continuos coordinates, time being continuous

Tobias Deffge

Consider a random walk on a ring with continuous time. Compare the theoretical probability density (82) for the continuous–coordinate model with $P(x_m, t)/a$, where $P(x_m, t)$ is the solution (59) of the model with discrete coordinate $x_m = am$. Choose the transition rates w_+ and w_- consistent with (69) and (70) and consider the limit case, where a is very small for given finite values D and $v_{\rm drift}$.

1.3.8 Comparison between the random walk on a ring for discrete and continuous time, position being discrete

Hannes Wernicke

Consider a random walk on a ring with discrete positions $x_m = ma$, $m = 0, 1, 2, \ldots, M-1$ and discrete time $t_n = \tau n$, $n = 0, 1, 2, \ldots$ and calculate the averaged over two succesive time steps probability $\bar{P}(x_m, t_n)$ given by (60) and (47) for different p and q (τ and a can be fixed, e. g., set to unity). Compare the result for large n with the solution of the continuous–time model (master equation) given by (59) at $t = \tau n$, $w_+ = p/\tau$ and $w_- = q/\tau$.