Interrelations between Stochastic Equations for Systems with Pair Interactions

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Abstract

Several types of stochastic equations are important in thermodynamics, chemistry, evolutionary biology, population dynamics and quantitative social science. For systems with pair interactions four different types of equations are derived, starting from a master equation for the state space: First, general mean value and (co)variance equations. Second, BOLTZMANN-like equations. Third, a master equation for the configuration space allowing transition rates which depend on the occupation numbers of the states. Fourth, a FOKKER-PLANCK equation and a “BOLTZMANN-FOKKER-PLANCK equation”. The interrelations of these equations and the conditions for their validity are worked out clearly. A procedure for a selfconsistent solution of the nonlinear equations is proposed. Generalizations to interactions between an arbitrary number of systems are discussed.

1 Introduction

Stochastic equations have shown to be a useful tool in all fields of science, where fluctuations are involved. Many applications can e.g. be found in chemical kinetics [1], laser theory [2] and biological systems [3], but they also become increasingly important in quantitative social science [4, 5, 6, 7, 8, 9, 10, 11]. Without stochastic models certain phenomena like phase transitions could not be correctly understood [12, 13, 14].

Most often, problems involving fluctuations are handled by master equations, FOKKER-PLANCK equations or BOLTZMANN equations. There are essentially three ways of arriving at these equations:

• A system is influenced by external fluctuations: In this case, a stochastic differential equation (or LANGEVIN equation) would be set up, which can be transformed to a FOKKER-PLANCK equation [15, 16].

• A system consists of a huge number of subsystems: If the entire system behaves conservative, it would be described classically by a LIOUVILLE equation or quantum
mechanically by a von Neumann equation. Both equations can be contracted to a (generalized) master equation \[17, 18, 19, 20, 21, 22, 23, 24, 25\] (which becomes an ordinary master equation in the Markovian limit \[35\]) or to a Boltzmann equation \[26, 27, 28, 29, 30, 31, 32, 33, 34\]. The master equation and the Boltzmann equation contain a few relevant (macroscopic) variables only, and handle the huge remaining number of irrelevant variables as internal fluctuations.

- The state of a system changes to one of several others with a certain probability which depends on the actual state (Markov property): This kind of situation would be modelled by a Chapman-Kolmogorov equation, which can be transformed to a master equation \[36\].

In the following sections the interrelations of master, Fokker-Planck and Boltzmann equations shall be discussed (similar considerations can be made for generalized master equations \[37\], generalized Fokker-Planck equations \[37\] and generalized Boltzmann equations \[33\]): Starting from the master equation for the state space (sect. 2), the Boltzmann equation results in the case of a factorization of the pair distribution function (sect. 2.2), whereas the Fokker-Planck equation follows by a second order Taylor expansion (sect. 3). In addition, a “Boltzmann-Fokker-Planck equation” is derived (sect. 3.1), which can be either obtained from the Fokker-Planck equation by a factorization of the pair distribution function or from the Boltzmann equation by a second order Taylor expansion. The nonlinear dependence of this equation on the probability distribution calls for a selfconsistent method of solution (sect. 3.2).

Having formulated a master equation for the state space, the same can be done for the configuration space (occupation numbers’ space) (sect. 2.4). The mean value equation of the configurational master equation is equivalent to the Boltzmann equation, if simultaneous interactions of more than two systems are neglected (sect. 2.4). The Boltzmann equation is applicable only during a certain time interval in which the (co)variances are small (sect. 2.4). However, the mean value equation can be corrected by methods, which are also suitable for calculating the effects of higher order interactions (sect. 2.5).

## 2 The master equation

Ensembles of statistically behaving systems can often be described by a master equation \[36, 38, 39\]

\[
\frac{d}{dt} P(\vec{X}, t) = \int d\vec{X}' \left[ w(\vec{X}', \vec{X}; t) P(\vec{X}', t) - w(\vec{X}, \vec{X}'; t) P(\vec{X}, t) \right]
\] (1)

with

\[
0 \leq P(\vec{X}, t) \quad \text{and} \quad \int d\vec{X} P(\vec{X}, t) = 1.
\] (2)

\(P(\vec{X}, t)\) is the probability of the ensemble to be at time \(t\) in a state \(\vec{X} = (x_1, \ldots, x_1)\), if a transition from state \(\vec{X}\) to \(\vec{X}'\) occurs with probability \(w(\vec{X}', \vec{X}; t)\) per time unit. The entire state

\[
\vec{X} = (\vec{x}_1; \ldots; \vec{x}_\alpha; \ldots; \vec{x}_N) = (x_{11}, \ldots, x_{1n}; \ldots; x_{\alpha 1}, \ldots, x_{\alpha n}; \ldots; x_{N 1}, \ldots, x_{N n})
\]
is combined of the states \( \vec{x}_\alpha = (x_{\alpha1}, \ldots, x_{\alpha i}, \ldots, x_{\alpha n}) \) of the ensemble’s \( N \) individual systems \((l = n \cdot N)\).

A typical example for the application of (1) is a chemical reaction \( [1, 39, 40, 41, 42, 43, 44, 45] \)

\[
B + C \rightleftharpoons BC,
\]

where \( \vec{x}_\alpha \) could, for example, indicate, if atom \( \alpha \) is bound or free. We would have a discrete state space with \( n = 1 \) then, and the integrals in (1), (2) could be replaced by sums:

\[
\frac{d}{dt} P(\vec{X}, t) = \sum_{\vec{X}'} \left[ w(\vec{X}, \vec{X}'; t) P(\vec{X}', t) - w(\vec{X}', \vec{X}; t) P(\vec{X}, t) \right],
\]

\[
\sum_{\vec{X}} P(\vec{X}, t) = 1.
\]

Methods for solving master equations are discussed in \([46, 47, 48, 23, 49, 50, 51, 52, 53, 39, 54, 55]\).

\[\text{2.1 Mean value equations (Macroscopic equations)}\]

Usually, one is mainly interested in the time evolution of the mean value

\[
\langle f \rangle := \int d^l X f(\vec{X}, t) P(\vec{X}, t)
\]

of \( f(\vec{X}, t) = x_{\alpha i} \). This is given by \([39]\)

\[
\frac{d\langle x_{\alpha i} \rangle}{dt} = \int d^l X x_{\alpha i} \frac{dP(\vec{X}, t)}{dt}
\]

\[
= \int d^l X \int d^l X' \left[ x_{\alpha i} w(\vec{X}, \vec{X}'; t) P(\vec{X}', t) - x_{\alpha i} w(\vec{X}', \vec{X}; t) P(\vec{X}, t) \right]
\]

\[
= \int d^l X \int d^l X' (x'_{\alpha i} - x_{\alpha i}) w(\vec{X}', \vec{X}; t) P(\vec{X}, t)
\]

\[
= \int d^l X m_{\alpha i}(\vec{X}, t) P(\vec{X}, t)
\]

\[
= \langle m_{\alpha i}(\vec{X}, t) \rangle \tag{4}
\]

with the \textit{first jump moments} \([39]\)

\[
m_{\alpha i}(\vec{X}, t) := \int d^l X' \Delta x'_{\alpha i} w(\vec{X}', \vec{X}; t) \quad (\Delta x'_{\alpha i} := x'_{\alpha i} - x_{\alpha i}) \tag{5}
\]

In the derivation of (4) we have exchanged the order of \( \vec{X} \) and \( \vec{X}' \).

If the probability distribution \( P(\vec{X}, t) \) has only small (co)variances, we find in first order \textit{TAYLOR} approximation the relation \([39]\)

\[
\frac{d\langle x_{\alpha i} \rangle}{dt} \approx \left\langle m_{\alpha i}(\langle \vec{X} \rangle, t) + \sum_{\beta j} (x_{\beta j} - \langle x_{\beta j} \rangle) \frac{\partial m_{\alpha i}(\langle \vec{X} \rangle, t)}{\partial (x_{\beta j})} \right\rangle = m_{\alpha i}(\langle \vec{X} \rangle, t). \tag{6}
\]
In many cases, the initial state $X_0$ at a time $t_0$ is known by measurement or preparation, i.e. the initial distribution is
\[ P(X, t_0) = \delta(X - X_0) \]
with the Dirac delta function $\delta(\cdot)$. As a consequence, the (co)variances
\[ \sigma_{\alpha \beta} := \langle (x_\alpha - \langle x_\alpha \rangle)(x_\beta - \langle x_\beta \rangle) \rangle = \langle x_\alpha x_\beta \rangle - \langle x_\alpha \rangle \langle x_\beta \rangle \]
vanish at time $t_0$ and remain small during a certain time interval. Proceeding as above, the equations
\[ \frac{d\sigma_{\alpha \beta}}{dt} = \langle m_{\alpha \beta}(X, t) \rangle + \langle (x_\alpha - \langle x_\alpha \rangle)m_{\beta}(X, t) \rangle + \langle (x_\beta - \langle x_\beta \rangle)m_{\alpha}(X, t) \rangle \] (7)
for the temporal development of the (co)variances are found \[39\], where
\[ m_{\alpha \beta}(X, t) := \int d'X' \Delta x_\alpha \Delta x_\beta w(X', X; t) \] (8)
are the second jump moments. The (co)variance equations (7) have, in first order Taylor approximation
\[ \langle (x_\alpha - \langle x_\alpha \rangle)f(X, t) \rangle \approx \sum_{\gamma, \kappa} \sigma_{\alpha \gamma \kappa} \frac{\partial f(\langle X \rangle, t)}{\partial \langle x_\gamma \rangle}, \]
the form \[39\]
\[ \frac{d\sigma_{\alpha \beta}}{dt} \approx m_{\alpha \beta}(\langle X \rangle, t) + \sum_{\gamma, \kappa} \left( \sigma_{\alpha \gamma \kappa} \frac{\partial m_{\beta}(\langle X \rangle, t)}{\partial \langle x_\gamma \rangle} + \sigma_{\beta \gamma \kappa} \frac{\partial m_{\alpha}(\langle X \rangle, t)}{\partial \langle x_\gamma \rangle} \right). \] (9)
(Since equations (7) and (8) are no closed equations, they can only be approximately solved.)

2.2 BOLTZMANN-like equations

The probability distribution $P(X, t)$ rather than the mean value equations should be calculated, if the (co)variances are not negligible. Since the number $N$ of systems is usually tremendous, (4) can be solved neither exactly nor by computer simulations. In order to find a suitable simplification of (4), let us introduce the vectors
\[ X^\alpha := (\vec{0}; \ldots; \vec{0}; \vec{x}_\alpha; \vec{0}; \ldots; \vec{0}), \]
\[ \bar{X}^{\alpha_1 \ldots \alpha_k} := \sum_{i=1}^{k} \bar{X}^{\alpha_i}, \]
and let us decompose the transition rates

$$w(\vec{Y}; \vec{X}; t) = \sum_{k=1}^{N} \sum_{\alpha_1 < \ldots < \alpha_k} w_{\alpha_1 \ldots \alpha_k} \left( \vec{Y}^{\alpha_1 \ldots \alpha_k}; \vec{X}^{\alpha_1 \ldots \alpha_k}; t \right)$$

$$= \sum_{k=1}^{N} \frac{1}{k!} \sum_{\alpha_1 \ldots \alpha_k} w_{\alpha_1 \ldots \alpha_k} \left( \vec{Y}^{\alpha_1 \ldots \alpha_k}; \vec{X}^{\alpha_1 \ldots \alpha_k}; t \right)$$

(10)

into terms

$$w_{\alpha_1 \ldots \alpha_k} \left( \vec{Y}^{\alpha_1 \ldots \alpha_k}; \vec{X}^{\alpha_1 \ldots \alpha_k}; t \right)$$

which describe the interactions between exactly \( k \) systems. Consequently, we have to set

$$w_{\alpha_1 \ldots \alpha_k} \equiv 0, \quad \text{if two indices } \alpha_i, \alpha_j \text{ agree.}$$

For most of the chemical reactions and many other cases the terms with \( k \leq 2 \) are the only important ones, because simultaneous interactions between three or more systems are rare. Therefore, the terms with \( k > 2 \) shall be neglected in the following, but a generalization to an arbitrary number of simultaneously interacting systems is possible (see sect. 2.4) [27, 28, 56, 57, 58]. The master equation (1) has then the form

$$\frac{dP(\vec{X}, t)}{dt} = \sum_{\beta} \int d\vec{Y} \left[ w_{\beta}(\vec{X}; \vec{Y}; t)P(\vec{Y}, t) - w_{\beta}(\vec{Y}; \vec{X}; t)P(\vec{X}, t) \right]$$

$$+ \frac{1}{2} \sum_{\beta, \gamma} \int d\vec{Y} \left[ w_{\beta\gamma}(\vec{X}; \vec{Y}; t)P(\vec{Y}, t) - w_{\beta\gamma}(\vec{Y}; \vec{X}; t)P(\vec{X}, t) \right].$$

(11)

Let us use

$$\int d^n x_{\beta} \, P_{a_{1 \ldots k}}(x_{\alpha_1}; \ldots; x_{\beta}; \ldots; x_{\alpha_k}; t) = P_{a_1 \ldots a_k}(x_{\alpha_1}; \ldots; x_{\alpha_k}; t)$$

(12)

with

$$P_{1 \ldots N}(x_1; \ldots; x_N; t) \equiv P(x_1; \ldots; x_N; t),$$

and assume the factorization

$$P_{a_{1\beta}}(x_{\alpha}; x_{\beta}; t) \approx P_a(x_{\alpha}; t)P_{\beta}(x_{\beta}; t)$$

(13)

of the pair distribution \( P_{a_{\beta}}(x_{\alpha}; x_{\beta}; t) \). Integration of (11) over all variables \( x_{\beta} \) with \( \beta \neq \alpha \) leads to [59, 42]

$$\frac{d}{dt}P_a(\vec{x}_a, t) = \int d^n y_a \left[ w_a(\vec{x}_a; \vec{y}_a; t)P_a(\vec{y}_a, t) - w_a(\vec{y}_a, \vec{x}_a; t)P_a(\vec{x}_a, t) \right]$$

$$+ \int d^n y_a \left[ \sum_{\beta} \left( \int d^n x_{\beta} \, w_{a\beta}(x_{\alpha}; x_{\beta}; \vec{y}_a; \vec{y}_{\beta}; t)P_{\beta}(\vec{y}_{\beta}, t) \right) P_a(\vec{y}_a, t) \right. $$

$$\left. - \left( \sum_{\beta} \int d^n x_{\beta} \, w_{a\beta}(\vec{y}_a, \vec{y}_{\beta}; \vec{x}_a, \vec{x}_{\beta}; t)P_{\beta}(\vec{x}_{\beta}, t) \right) P_a(\vec{x}_a, t) \right]$$

(14)

with

$$\int d^n x_a \, P_a(x_a, t) = 1,$$

(15)
where the conventions
\[ w_\alpha(y_\alpha, x_\alpha; t) \equiv w_\alpha(Y^\alpha; X^\alpha; t), \]
\[ w_{\alpha\beta}(y_\alpha, y_\beta; x_\alpha, x_\beta; t) \equiv w_{\alpha\beta}(Y^{\alpha\beta}; X^{\alpha\beta}; t) \]
have been used. The second and third terms of (14) are similar to those of the BOLTZMANN equation [59, 60, 39].

\[ w_\alpha(y_\alpha, x_\alpha; t) \] describes transitions of system \( \alpha \) from state \( x_\alpha \) to state \( y_\alpha \) occurring spontaneously or being induced by external influences. \( w_{\alpha\beta}(y_\alpha, y_\beta; x_\alpha, x_\beta; t) \) represents interactions between two systems \( \alpha \) and \( \beta \) changing their states from \( x_\alpha \) resp. \( x_\beta \) to \( y_\alpha \) resp. \( y_\beta \). More clearly arranged, (14) can be written in the form
\[
\frac{d}{dt}P_\alpha(\bar{x}; t) = \int d^n x' \left[ w_\alpha(x', \bar{x}; t)P_\alpha(x', t) - w_\alpha(x', \bar{x}; t)P_\alpha(x, t) \right]
\]  
(16)
with the effective transition rates
\[
w^\alpha(x', \bar{x}; t) := w_\alpha(x', \bar{x}; t) + \sum_\beta \int d^n y' \int d^n y w_{\alpha\beta}(x', y'; x, y; t)P_\beta(y, t).
\]  
(17)

The factorization (13) is valid, if each two systems \( \alpha \) and \( \beta \) are statistically independent. This is approximately the case in the limit of weak interactions \( (w_{\alpha\beta} \approx 0) \) or, if correlations between systems \( \alpha \) and \( \beta \) due to pair interactions are soon destroyed, e.g. by external influences (see also (33)). Equation (13) is called the assumption of molecular chaos [61]. Without this assumption, equation (14) would contain the unknown pair distribution \( P_{\alpha\beta}(\bar{x}_\alpha, \bar{x}_\beta, t) \). However, there are methods of calculating corrections, if the factorization (13) is not valid [27, 62] (see sect. 2.5).

### 2.3 Types of interaction

Normally, the huge number \( N \) of systems \( \alpha \) can be divided into \( A \) types (resp. sets) \( a \) which can be characterized by a special kind of interaction. In example (3), one type would consist of molecules \( B \) and a second type of molecules \( C \). Let \( N_a \) denote the number of systems \( \alpha \in a \) (i.e. of type \( a \)). This implies
\[
\sum_{a=1}^{A} N_a = N.
\]

If we assume systems \( \alpha \in a \) of the same type \( a \) to be indistinguishable, we have
\[
P_a \equiv P_a \quad \text{if} \quad \alpha \in a, \]
\[
w_\alpha \equiv \bar{w}_a \quad \text{if} \quad \alpha \in a, \]
\[
w_{\alpha\beta} \equiv \begin{cases} 
\bar{w}_{ab} & \text{if } \alpha \neq \beta, \ \alpha \in a, \ \beta \in b \\
0 & \text{if } \alpha = \beta,
\end{cases}
\]
where \( \bar{w}_a \) are individual transition rates. We may now introduce the abbreviations
\[
w_a := \bar{w}_a,
\]
\[
w_{ab} := \begin{cases} 
N_b \cdot \bar{w}_{ab} & \text{if } b \neq a \\
(N_a - 1) \cdot \bar{w}_{ab} & \text{if } b = a.
\end{cases}
\]
Then, from (16), (17), (15) we get
\[
\frac{d}{dt} P_a(\vec{x}, t) = \int d^nx' \left[ w^a(\vec{x}, \vec{x}'; t) P_a(\vec{x}', t) - w^a(\vec{x}', \vec{x}; t) P_a(\vec{x}, t) \right]
\]
with the effective transition rates
\[
w^a(\vec{x}', \vec{x}; t) := w_a(\vec{x}', \vec{x}; t) + \sum_b \int d^n y' \int d^n y \ w_{ab}(\vec{x}', \vec{y}'; \vec{x}, \vec{y}; t) P_b(\vec{y}, t)
\]
and
\[
\int d^n x P_a(\vec{x}, t) = 1.
\]
In equations (18), (19) the number of variables has been drastically reduced (if \(A \ll N\) resp. \(N_a \gg 1\)). As a consequence, (18), (19) are tractable with analytical or computer methods. Especially, for \(A = 1, w_1 \equiv 0\),
\[
\int d^n x' \int d^n y' w_{11}(\vec{x}', \vec{y}'; \vec{x}, \vec{y}) = \int d^n x' \int d^n y' w_{11}(\vec{x}, \vec{y}; \vec{x}', \vec{y}')
\]
and
\[
\vec{x} := (\vec{r}, \vec{v})
\]
we obtain the ordinary BOLTZMANN equation for gases [63, 60], where \(\vec{r}\) denotes the place and \(\vec{v}\) the velocity of a particle. A recursive method for solving this special case has been given by CHAPMAN [64, 65] and ENSKOG [66].

2.4 The configuration and its temporal development

In many cases, we are not interested in the states \(\vec{x}_\alpha\) of the single systems \(\alpha\), but in the number \(n^a_{\vec{x}}\) of systems of type \(a\) being in state \(\vec{x}\) (e.g. the number of molecules of type \(B\) being bound). Let us assume that there is only a finite number \(S\) of possible states \(\vec{x} \in \{\vec{x}_1, \ldots, \vec{x}_S\}\) (although analogous considerations can be made for a continuum of states \(\vec{x}\)). Then, the vector
\[
\vec{n} := (n^1_{\vec{x}_1}, \ldots, n^1_{\vec{x}_S}; \ldots; n^A_{\vec{x}_1}, \ldots, n^A_{\vec{x}_S}) = (\vec{n}^1; \ldots; \vec{n}^A)
\]
of occupation numbers \(n^a_{\vec{x}}\) shall be called the configuration of the ensemble of systems. The configuration space consists of all vectors \(\vec{n}\) obeying the relations
\[
\sum_{\vec{x}} n^a_{\vec{x}} \equiv \sum_{s=1}^{S} n^a_{\vec{x}_s} = N_a.
\]
If we neglect pair interactions for a moment (i.e. if we only take terms of order \(k = 1, w_{ab} \equiv 0\)), we can assume the individual systems to be statistically independent from each other. The probability distribution of the configurations \(\vec{n}\) will then be
\[
P(\vec{n}, t) = \prod_{a=1}^{A} P^a(\vec{n}^a, t)
\]
with the multinomial distribution [37]

\[ P^a(\vec{n}, t) \equiv P^a(n_{x_1}^a, \ldots, n_{x_S}^a; t) = \frac{N_a!}{n_{x_1}! \cdots n_{x_S}!} P_a(\vec{x}_1, t)^{n_{x_1}^a} \cdots P_a(\vec{x}_S, t)^{n_{x_S}^a}. \] (21)

By differentiation of (20), (21) and use of (18), we obtain for the temporal change of \( P(\vec{n}, t) \) the master equation

\[ \frac{d}{dt} P(\vec{n}, t) = \sum_{\vec{n}'} \left[ w(\vec{n}, \vec{n}'; t) P(\vec{n}', t) - w(\vec{n}', \vec{n}; t) P(\vec{n}, t) \right] \] (22)

with

\[ 0 \leq P(\vec{n}, t), \quad \sum_{\vec{n}} P(\vec{n}, t) = 1 \]

and

\[ w(\vec{n}', \vec{n}; t) = \begin{cases} n_{x}^a w_a(\vec{y}, \vec{x}; t) & \text{if } \vec{n}' = \vec{n}_{\vec{y}\vec{x}}^a \\ 0 & \text{else} \end{cases}, \] (23)

\[ \vec{n}_{\vec{y}\vec{x}}^a := (n_{x_1}^1, \ldots, n_{x_1}^a; \ldots, n_{x_2}^a; \ldots, n_{x_1}^0 + 1, \ldots, n_{x_2}^0 + 1, \ldots, n_{x_2}^a; \ldots, n_{x_1}^A; \ldots, n_{y_1}^A) \].

According to this, the configurational transition rate \( n_{x}^a \tilde{w}_a(\vec{y}, \vec{x}; t) = n_{x}^a w_a(\vec{y}, \vec{x}; t) \) is proportional to the number \( n_{x}^a \) of systems which can change the state \( \vec{x} \) and proportional to the individual transition rate \( \tilde{w}_a(\vec{y}, \vec{x}; t) \).

The equations for the mean values

\[ \langle f \rangle := \sum_{\vec{n}} f(\vec{n}, t) P(\vec{n}, t) \]

of \( f(\vec{n}, t) = n_{x}^a \) can be obtained from (18) and the first jump moments

\[ m_{x}^a(\vec{n}, t) = \sum_{\vec{n}'} (\Delta \vec{n}')_{x}^a w(\vec{n}', \vec{n}; t) \\
\nonumber = \sum_{\vec{y} \vec{y'}, \vec{b}} (\Delta \vec{n}_{\vec{y}\vec{y'}}^b)_{x}^a w(\vec{n}_{\vec{y}\vec{y'}}^b, \vec{n}; t) \\
\nonumber = \sum_{\vec{y}} \left[ n_{y}^a w_a(\vec{x}, \vec{y}; t) - n_{x}^a w_a(\vec{y}, \vec{x}; t) \right]. \] (24)

(Here, \((\vec{n})_{x}^a\) denotes the component \( n_{x}^a \) of \( \vec{n} \).) After substitution of \( \vec{y} \) by \( \vec{x}' \), the mean value equations of (22), (23) have the explicit form

\[ \frac{d}{dt} \langle n_{x}^a \rangle = \langle m_{x}^a(\vec{n}, t) \rangle = \sum_{\vec{x}'} \left[ w_a(\vec{x}, \vec{x}'; t)\langle n_{x'}^a \rangle - w_a(\vec{x}', \vec{x}; t)\langle n_{x}^a \rangle \right]. \] (25)

Therefore, the equations governing the temporal change of the expected fractions \( \langle n_{x}^a \rangle / N_a \) agree with (18), and we have:

\[ \frac{\langle n_{x}^a \rangle}{N_a} = P_a(\vec{x}, t). \] (26)
Pair interactions

In order to take pair interactions into account, we apply the method of section 2.2. The master equation (22) then reads

$$\frac{d}{dt} P(\vec{n}, t) = \sum_{a,\vec{x},a',\vec{x}'} [w(\vec{n}; \vec{n}_a^{a', a}, t) P(\vec{n}_a^{a', a}, t) - w(\vec{n}_a^{a', a}, \vec{n}; t) P(\vec{n}_a^{a', a}, t)]$$

$$+ \frac{1}{2} \sum_{a,\vec{x},a',\vec{y},b,\vec{y}',\vec{y}'} \sum_{\vec{n},t} \left[ w(\vec{n}; \vec{n}_a^{a', ab}, t) P(\vec{n}_a^{a', ab}, t) - w(\vec{n}_a^{a', ab}, \vec{n}; t) P(\vec{n}_a^{a', ab}, t) \right]$$

with

$$\vec{n}_a^{a', a} := (\ldots, (n_{a'} - 1), \ldots),$$

$$\vec{n}_a^{a', ab} := (\ldots, (n_{a'} - 1), \ldots, (n_{ab} - 1), \ldots)$$

Usually, the transition rates will depend on the changing occupation numbers only, which results in

$$\frac{d}{dt} P(\vec{n}, t) = \sum_{a,\vec{x},a',\vec{x}'} \left[ w_{a,\vec{x}}^{a', a}(n_a^{a', a}, t) P(n_a^{a', a}, t) - w_{a,\vec{x}}^{a', a}(n_a^{a', a}, t) P(n_a^{a', a}, t) \right]$$

$$+ \frac{1}{2} \sum_{a,\vec{x},a',\vec{y},b,\vec{y}',\vec{y}'} \sum_{\vec{n},t} \left[ w_{a,\vec{x}}^{a', ab}(n_a^{a', ab}, t) P(n_a^{a', ab}, t) - w_{a,\vec{x}}^{a', ab}(n_a^{a', ab}, t) P(n_a^{a', ab}, t) \right]$$

analogous to (11). Let us in the following consider the special case

$$w_{a,\vec{x}}^{a', a}(n_a^{a', a}, t) := n_a^{a'} \bar{w}_a(\vec{x}', \vec{x}; t) \delta_{a,a'}$$

$$+ n_a^{a'} \bar{w}_a(\vec{x}', \vec{x}; t) \delta_{a,a'},$$

$$w_{a,\vec{x}}^{a', ab}(n_a^{a', ab}, t) := n_a^{a'} \bar{w}_{ab}(\vec{x}', \vec{y}; \vec{x}, \vec{y}; t) \delta_{a,a'} \delta_{bb'}$$

$$+ n_a^{a'} \bar{w}_{ab}(\vec{x}', \vec{y}; \vec{x}, \vec{y}; t) \delta_{a,a'} \delta_{bb'}$$

that means

$$w(\vec{n}', \vec{n}; t) = \begin{cases} n_a^{a'} \bar{w}_a(\vec{x}', \vec{x}; t) & \text{if } \vec{n}' = \vec{n}_a^{a', a} \\ n_a^{a'} n_b^{b} \bar{w}_{ab}(\vec{x}', \vec{y}; \vec{x}, \vec{y}; t) & \text{if } \vec{n}' = \vec{n}_a^{a', ab} \\ 0 & \text{else} \end{cases}$$

(28)

(where $\delta_{a,a'}$ denotes the KRONECKER function). The configurational transition rates are proportional to the individual transition rates $\bar{w}_a$ resp. $\bar{w}_{ab}$ and proportional to the numbers $n_a^{a'}$ of systems which can change the state $\vec{x}$ resp. to the numbers $n_a^{a'} n_b^{b}$ of possible pair interactions between states $\vec{x}$ and $\vec{y}$. Therefore, if $\vec{n}' = \vec{n}_a^{a', a}, n_a^{a'} n_b^{b} \bar{w}_{ab}(\vec{x}', \vec{y}; \vec{x}, \vec{y}; t)$ has to be replaced by $n_a^{a'} (n_a^{a'} - 1) \bar{w}_{aa}(\vec{x}', \vec{y}; \vec{x}, \vec{x}; t)$ in order to exclude self-interactions again. However, (28) is approximately valid, if $n_a^{a'} \gg 1$ for all configurations $\vec{n}$, where $P(\vec{n}, t)$ cannot be neglected. For simplicity, the validity of this assumption will be also presupposed in the following sections.
Mean value equations (Macroscopic equations)

Noticing
\[ w_{\beta\alpha}(\vec{y}', x''; \vec{y}, x'; t) = w_{\alpha\beta}(\vec{x}', \vec{x}; \vec{y}, t) \]
(since the transition rates are independent from the arbitrary numeration of the systems),
the first jump moments can be calculated analogously to equation (24). They are found to be
\[ m_{i,x}^a(\vec{n}, t) = \sum_{x'} [n_{x'}^a \overline{w}^a(\vec{x}', x''; t) - n_{x''}^a \overline{w}^a(\vec{x}', x; t)] \tag{29} \]
with
\[ \overline{w}^a(\vec{x}', \vec{x}; t) := w_a(\vec{x}', \vec{x}; t) + \sum_b \sum_{\vec{y}} \sum_{\vec{y}'} w_{ab}(\vec{x}', \vec{y}; \vec{x}, \vec{y}; t) \frac{n_{b}^b}{N_b} \tag{30} \]
(if \( N_a \gg 1 \)). Therefore, the approximate mean value equations (see [3]) are
\[ \frac{d}{dt} \langle n_{x'}^a \rangle \approx m_{i,x}^a(\langle \vec{n} \rangle, t) = \sum x' \left[ \overline{\hat{w}}^a(\vec{x}', \vec{x}; t)\langle n_{x'}^a \rangle - \overline{\hat{w}}^a(\vec{x}', x'; t)\langle n_{x'}^a \rangle \right] \tag{31} \]
with the mean transition rates
\[ \overline{\hat{w}}^a(\vec{x}', \vec{x}; t) := w_a(\vec{x}', \vec{x}; t) + \sum_b \sum_{\vec{y}} \sum_{\vec{y}'} w_{ab}(\vec{x}', \vec{y}; \vec{x}, \vec{y}; t) \frac{n_{b}^b}{N_b}. \tag{32} \]

Again, equations (31), (32) for the expected fractions \( \langle n_{x'}^a \rangle/N_a \) agree with equations (18), (19) for the probabilities \( P_a(x', t) \) if making the identification (26). However, the approximate equations (31), (32) are only valid under the condition
\[ \langle n_{x'}^a n_{x'}^b \rangle \approx \langle n_{x'}^a \rangle \langle n_{x'}^b \rangle, \]
which obviously corresponds to the factorization assumption (13). This condition is fulfilled if the absolute values of the (co)variances
\[ \sigma_{x,x'}^{ab} = \langle n_{x'}^a n_{x'}^b \rangle - \langle n_{x'}^a \rangle \langle n_{x'}^b \rangle \]
are small, i.e., if
\[ |\sigma_{x,x'}^{ab}| \ll \langle n_{x'}^a \rangle \langle n_{x'}^b \rangle. \tag{33} \]
(This is often the case in the thermodynamic limits \( N \rightarrow \infty \)). According to (3), approximate equations for the temporal development of the (co)variances are
\[ \frac{d\sigma_{x,x'}^{ab}}{dt} \approx m_{x,x'}^{ab}(\langle \vec{n} \rangle, t) + \sum_{c,y} \left( \frac{\sigma_{x,y}^{ac}}{\partial \langle n_{y'}^c \rangle} \frac{\partial m_{x,y}^{bc}(\langle \vec{n} \rangle, t)}{\partial \langle n_{y'}^c \rangle} + \frac{\sigma_{y,y'}^{bc}}{\partial \langle n_{y'}^c \rangle} \frac{\partial m_{x,y}^{bc}(\langle \vec{n} \rangle, t)}{\partial \langle n_{y'}^c \rangle} \right) \tag{34} \]
with the second jump moments
\[ m_{x,x'}^{ab}(\vec{n}, t) = \sum_{\vec{n}'} (\Delta \vec{n'})^a_{\vec{x}} (\Delta \vec{n'})^b_{\vec{x}} w(\vec{n}', \vec{n}; t) \]
\[ = \sum_{\vec{y}, \vec{y}', c} (\Delta \vec{n'}_{\vec{y}'}^c)^a_{\vec{x}} (\Delta \vec{n'}_{\vec{y}'}^c)^b_{\vec{x}} w(\vec{n'}_{\vec{y}'}^c, \vec{n}; t) \]
In section 2.4 the exact mean value equations (31), (29), (30) and the approximate (co)variance equations (34), (35) can also be used for mean field approaches in physics, e.g. the ISING model [70, 71]. Equations (27) resp. (31), (29), (30) and (34), (35) can also be applied in quantitative social science, where the decisions or the behavior of individuals may depend on the configuration $\vec{n}$ [6, 8, 54, 55, 68, 69]. Equations (27) resp. (31), (29), (30) and (34), (35) can also be used for mean field approaches in physics, e.g. the ISING model [70, 71].

### 2.5 Corrections and higher order interactions

In section 2.4 the exact mean value equations

$$\frac{d\langle n_x^a \rangle}{dt} = \langle m_x^a(\vec{n}, t) \rangle \quad (37)$$

are, according to equations (29), (30) for $m_x^a$, dependent on $\langle n_x^a n_x^b \rangle$. However, the exact equation

$$\frac{d\langle n_x^a n_x^b \rangle}{dt} = \langle m_x^a(\vec{n}, t) \rangle + \langle n_x^a m_x^b(\vec{n}, t) \rangle + \langle n_x^b m_x^a(\vec{n}, t) \rangle$$

governing the temporal development of $\langle n_x^a n_x^b \rangle$ depends on $\langle n_x^a n_x^b n_x^c \rangle$, because of equation (33). So, we are confronted with the problem of having no closed set of equations.

Let us consider the general case of up to $k$ interactions. In the master equation (22) we have then to take the transition rates

$$w(\vec{n}', \vec{n}; t) = \begin{cases} n_x^a \tilde{w}_a(x', x_1; t) & \text{if } \vec{n}' = \vec{n}_x^a \vec{n} \\ n_x^a n_x^b \tilde{w}_{ab}(x', x_1, x_2; \vec{n}) & \text{if } \vec{n}' = \vec{n}_x^a \vec{n}_x^b \vec{n} \\ 0 & \text{else} \end{cases} \quad (38)$$

This generalization is necessary, if the individual transition rates $\tilde{w}_a$, $\tilde{w}_{ab}$ are themselves functions of the occupation numbers. Such cases appear e.g. in quantitative social science, where the decisions or the behavior of individuals may depend on the socioconfiguration $\vec{n}$ [6, 8, 54, 55, 68, 69]. Equations (27) resp. (31), (29), (30) and (34), (35) can also be used for mean field approaches in physics, e.g. the ISING model [70, 71].
with
\[
\hat{n}_{\bar{x}_1 \ldots \bar{x}_k}^{a_1 \ldots a_k} := (\ldots, (n_{\bar{x}_1}^{a_1} + 1), \ldots, (n_{\bar{x}_1}^{a_1} - 1), \ldots, (n_{\bar{x}_k}^{a_k} + 1), \ldots, (n_{\bar{x}_k}^{a_k} - 1), \ldots).
\]

The temporal development of the \(l\)th moments \(\langle n_{\bar{x}_1}^{a_1} \ldots n_{\bar{x}_1}^{a_l} \rangle\) is governed by the equations
\[
\frac{d}{dt} \langle n_{\bar{x}_1}^{a_1} \ldots n_{\bar{x}_1}^{a_l} \rangle = \sum_{\bar{n}} \sum_{\bar{n}'} \Big[ (\Delta \hat{n})_{\bar{x}_1}^{a_1} \ldots (\Delta \hat{n})_{\bar{x}_1}^{a_l} \Big] w(\bar{n}', \bar{n}; t) P(\bar{n}, t)
\]
\[
- \sum_{\bar{n}} \Big[ (\Delta \hat{n})_{\bar{x}_1}^{a_1} + n_{\bar{x}_1}^{a_1} \Big] \ldots \Big[ (\Delta \hat{n})_{\bar{x}_1}^{a_l} + n_{\bar{x}_1}^{a_l} \Big] w(\bar{n}', \bar{n}; t) P(\bar{n}, t)
\]
\[
= \sum_{m=1}^{l} \sum_{\mathcal{M}_m} \langle m_{\bar{x}_1 \ldots \bar{x}_m}^{a_1 \ldots a_m} \cdot n_{\bar{x}_{m+1}}^{a_{m+1}} \ldots n_{\bar{x}_1}^{a_1} \rangle
\]
\[
= \sum_{m=1}^{l} \frac{1}{m!(l-m)!} \sum_{(i_1, \ldots, i_l)\in\sigma(l)} \langle m_{\bar{x}_1 \ldots \bar{x}_m}^{a_1 \ldots a_m} \cdot n_{\bar{x}_{m+1}}^{a_{m+1}} \ldots n_{\bar{x}_1}^{a_1} \rangle. \tag{39}
\]

Here,
\[
m_{\bar{x}_1 \ldots \bar{x}_m}^{a_1 \ldots a_m}(\bar{n}, t) := \sum_{\bar{n}'} (\Delta \hat{n})_{\bar{x}_1}^{a_1} \ldots (\Delta \hat{n})_{\bar{x}_m}^{a_m} w(\bar{n}', \bar{n}; t)
\]
are the \(m\)th jump moments, and \(\sigma(l)\) is the set of all \(l!\) permutations of the indices \(1, \ldots, l\). \(\sum_{\mathcal{M}_m}\) means the summation over all subsets \(\{i_1, \ldots, i_m\}\) of \(\{1, \ldots, l\}\) consisting of \(m\) elements. Notice, that the solutions for the moments should, in the case of time independent transition rates \(w(\bar{n}', \bar{n})\), converge to certain values in the limit \(t \to \infty\), since \(P(\bar{n}, t)\) approaches an unique equilibrium distribution \([17]\).

Because of (38), the \(m\)th jump moments are polynomials of order \(k\) of the occupation numbers \(n_{\bar{x}_1}^{a_1}\). Therefore, the equations (39) for the \(l\)th moments depend on the 1st up to the \((l-1+k)\)th moments. As a consequence, the exact moment equations (39) represent a closed system of equations only for \(k = 1\) (exclusion of multiple interactions). For interactions of up to \(k > 1\) systems we have to take a suitable approximation of (39) or, in other words, of
\[
\langle n_{\bar{x}_1}^{a_1} \ldots n_{\bar{x}_n}^{a_n} \rangle = \left[ \left( n_{\bar{x}_1}^{a_1} - \langle n_{\bar{x}_1}^{a_1} \rangle \right) + \langle n_{\bar{x}_1}^{a_1} \rangle \right] \ldots \left[ \left( n_{\bar{x}_n}^{a_n} - \langle n_{\bar{x}_n}^{a_n} \rangle \right) + \langle n_{\bar{x}_n}^{a_n} \rangle \right]
\]
\[
= \sum_{m=0}^{n} \sum_{\mathcal{M}_m} \left( n_{\bar{x}_1}^{a_1} - \langle n_{\bar{x}_1}^{a_1} \rangle \right) \ldots \left( n_{\bar{x}_m}^{a_m} - \langle n_{\bar{x}_m}^{a_m} \rangle \right) \langle n_{\bar{x}_{m+1}}^{a_{m+1}} \rangle \ldots \langle n_{\bar{x}_1}^{a_1} \rangle. \tag{40}
\]
\((41)\) is the exact TAYLOR expansion of (11). If we are interested in the 1st up to the \(j\)th moments \((1 \leq l \leq j, j \geq 1)\), we have essentially two possibilities of getting approximate moment equations:

(a) Replacing all jump moments \(m_{\bar{x}_1 \ldots \bar{x}_m}^{a_1 \ldots a_m}\) by first order TAYLOR approximations:
\[
m_{\bar{x}_1 \ldots \bar{x}_m}^{a_1 \ldots a_m}(\bar{n}, t) \approx m_{\bar{x}_1 \ldots \bar{x}_m}^{a_1 \ldots a_m}(\langle \bar{n} \rangle, t) + \sum_{a, \bar{x}} (n_{\bar{x}}^a - \langle n_{\bar{x}}^a \rangle) \frac{\partial}{\partial (n_{\bar{x}}^a)} m_{\bar{x}_1 \ldots \bar{x}_m}^{a_1 \ldots a_m}(\langle \bar{n} \rangle, t).
\]
Then, the equations for the \( l \)th moments depend on the 1st up to the \( l \)th moments only, but each equation is an approximation. This method has been used in sections 2.1 and 2.4. According to (11), it corresponds to the assumption

\[
\left| \langle (n_{\tilde{x}_{1}}^{a_{1}} - \langle n_{\tilde{x}_{1}}^{a_{1}} \rangle) \ldots (n_{\tilde{x}_{m}}^{a_{m}} - \langle n_{\tilde{x}_{m}}^{a_{m}} \rangle) \rangle \right| \ll \langle n_{\tilde{x}_{1}}^{a_{1}} \rangle \ldots \langle n_{\tilde{x}_{m}}^{a_{m}} \rangle \quad \text{for} \quad 1 < m \leq k,
\]

which can be checked by considering the 1st up to the \( k \)th moments (i.e. \( j \geq k \)).

(b) Replacing \((m_{\tilde{x}_{1}}^{a_{1}} \ldots n_{\tilde{x}_{m+1}}^{a_{m+1}} \ldots n_{\tilde{x}_{l}}^{a_{l}})\) by \( j \)th order TAYLOR approximations. Then, the equations for the 1st up to the \((j - k + 1)\)th moments are exact (see (11)), but the equation for an \( l \)th moment depends on the 1st up to the \((l - 1 + k)\)th moments, some of which may be determined by approximate equations. Method (b) corresponds to the assumption

\[
\left| \langle (n_{\tilde{x}_{1}}^{a_{1}} - \langle n_{\tilde{x}_{1}}^{a_{1}} \rangle) \ldots (n_{\tilde{x}_{m}}^{a_{m}} - \langle n_{\tilde{x}_{m}}^{a_{m}} \rangle) \rangle \right| \ll \langle n_{\tilde{x}_{1}}^{a_{1}} \rangle \ldots \langle n_{\tilde{x}_{m}}^{a_{m}} \rangle \quad \text{for} \quad j < m \leq l - 1 + k
\]

with \( 1 \leq l \leq j \). For large \( m \) (12) is normally fulfilled: If the (co)variances are small in the sense of

\[
|\sigma_{T}^{a_{b}}| < \langle n_{T}^{a} \rangle \langle n_{T}^{b} \rangle
\]

(which is often true in the thermodynamic limes \( N \to \infty \)), the absolute value of

\[
\left( \frac{n_{\tilde{x}_{1}}^{a_{1}}}{\langle n_{\tilde{x}_{1}}^{a_{1}} \rangle} - 1 \right) \ldots \left( \frac{n_{\tilde{x}_{m}}^{a_{m}}}{\langle n_{\tilde{x}_{m}}^{a_{m}} \rangle} - 1 \right)
\]

is usually small where \( P(\tilde{n}, t) \) is large [13]. Note, that (13) has to be checked only for the variances \( \sigma_{T}^{a_{a}} \), since the CAUCHY-SCHWARZ inequality implies

\[
|\sigma_{T}^{a_{b}}| \leq \sqrt{\sigma_{T}^{a_{a}} \sigma_{T}^{b_{b}}}
\]

As higher order approximation, method (b) will usually yield better results than (a) if \( j \geq 2 \). For \( k = 2 \) (i.e. pair interactions) and \( j = 2 \) it would e.g. result in corrected mean value equations (37), (29), (30) containing terms of the form \((\langle n_{\tilde{y}}^{a_{1}} \rangle, \langle n_{\tilde{y}}^{b_{1}} \rangle, \langle n_{\tilde{y}}^{b_{2}} \rangle, \langle \tilde{n} \rangle, t)\) and \((\sigma_{T}^{c_{y}} \partial n_{\tilde{y}}^{b_{2}}(\langle \tilde{n} \rangle, t) + \sigma_{T}^{b_{y}} \partial m_{\tilde{x}}^{a_{2}}(\langle \tilde{n} \rangle, t))\), using

\[
\langle n_{\tilde{x}_{1}}^{a_{1}} n_{\tilde{x}_{2}}^{a_{2}} n_{\tilde{x}_{3}}^{a_{3}} \rangle \approx \langle n_{\tilde{x}_{1}}^{a_{1}} \rangle \langle n_{\tilde{x}_{2}}^{a_{2}} \rangle \langle n_{\tilde{x}_{3}}^{a_{3}} \rangle + \sigma_{\tilde{x}_{1} \tilde{x}_{2}}^{a_{1} a_{2}} \langle n_{\tilde{x}_{3}}^{a_{3}} \rangle + \sigma_{\tilde{x}_{1} \tilde{x}_{3}}^{a_{1} a_{3}} \langle n_{\tilde{x}_{2}}^{a_{2}} \rangle + \sigma_{\tilde{x}_{2} \tilde{x}_{3}}^{a_{2} a_{3}} \langle n_{\tilde{x}_{1}}^{a_{1}} \rangle
\]

and (35).

Methods (a) and (b) are also applicable in the case of configuration dependent individual transition rates (see (56)).
The master equation (1) can (by substitution of $\vec{Z} := -\Delta \vec{X}' \equiv \vec{X} - \vec{X}'$ in the first term and of $\vec{Z} := +\Delta \vec{X}'$ in the second term) be written in the form

$$
\frac{d}{dt} P(\vec{X}, t) = \int d'Z \left[ w(\vec{X}, \vec{X} - \vec{Z}; t) P(\vec{X} - \vec{Z}, t) - w(\vec{X} + \vec{Z}, \vec{X}; t) P(\vec{X}, t) \right]
$$

with

$$
w[\vec{X}; \vec{Z}; t] := w(\vec{X} + \vec{Z}, \vec{X}; t) \quad (\vec{Z} \equiv \Delta \vec{X}').
$$

According to Kramers [72] and Moyal [73], equation (44) may be transformed into the Fokker-Planck equation [15]

$$
\frac{d}{dt} P(\vec{X}, t) = -\sum_{\alpha,i} \frac{\partial}{\partial x_{\alpha i}} \left[ m_{\alpha i}(\vec{X}, t) P(\vec{X}, t) \right] + \frac{1}{2} \sum_{\alpha,i} \sum_{\beta,j} \frac{\partial}{\partial x_{\alpha i}} \frac{\partial}{\partial x_{\beta j}} \left[ m_{\alpha i \beta j}(\vec{X}, t) P(\vec{X}, t) \right]
$$

(45)

by a second order Taylor approximation. This approximation will be the better the smaller the (co)variances $\sigma_{\alpha i \beta j}$ are (see the van Kampen system size expansion [74, 39, 15] for a more systematic derivation). However, the Fokker-Planck equation implies the same mean value and (co)variance equations as the master equation [54], and is compatible with

$$
0 \leq P(\vec{X}, t), \quad \int d^dX P(\vec{X}, t) = 1
$$

(see the Pawula theorem [37]). Interpreting equation (45), $m_{\alpha i}$ (see (3)) have the meaning of drift coefficients and $m_{\alpha i \beta j}$ (see (8)) the meaning of diffusion coefficients [37, 39].

The Fokker-Planck equation corresponding to the master equation (22), (28) is

$$
\frac{d}{dt} P(\vec{n}, t) = -\sum_{a,x} \frac{\partial}{\partial n_{a x}} \left[ m_{a x}^b(\vec{n}, t) P(\vec{n}, t) \right] + \frac{1}{2} \sum_{a,x} \sum_{b,x'} \frac{\partial}{\partial n_{a x}} \frac{\partial}{\partial n_{b x'}} \left[ m_{a x b}^b(\vec{n}, t) P(\vec{n}, t) \right].
$$

(46)

Equation (46) should be transformed to variables $n_{a x}^a := n_{a x}^a / N_a$. These variables can be approximately handled as continuous ones; see [54].

A reason for using the Fokker-Planck equation instead of the master equation is the variety of methods existing for its solution [37, 75, 13, 76, 77, 78, 79, 80], since it is a partial differential equation. Especially, the Fokker-Planck equation has some analogies to the Schrödinger equation [37, 77].

3.1 The “Boltzmann-Fokker-Planck equation”

We shall now proceed with equation (45) as in section 2.2. Let us decompose the transition rates as in equation (10) and neglect interactions of $k > 2$ systems, again. We find

$$
m_{\alpha i}(\vec{X}, t) = m_{\alpha i}^a(\vec{X}^a, t) + \sum_{\beta} m_{\alpha i}^{a \beta}(\vec{X}^{a \beta}, t),
$$

$$
m_{\alpha i \beta j}(\vec{X}, t) = \delta_{\alpha \beta} \left[ m_{\alpha a \beta}^a(\vec{X}^{a \alpha}, t) + \sum_{\gamma} m_{\alpha a \beta}^{a \gamma}(\vec{X}^{a \gamma}, t) \right] + m_{\alpha i \beta j}^{a \beta}(\vec{X}^{a \beta}, t)
$$
with

\[ m_\alpha^\gamma(\vec{x}^\gamma, t) := \int d^dZ \, z_\alpha w_\gamma [\vec{X}^\gamma; \vec{Z}^\gamma; t], \]
\[ m_\alpha^\delta(\vec{x}^\gamma, t) := \int d^dZ \, z_\alpha w_\delta [\vec{X}^\gamma; \vec{Z}^\delta; t], \]
\[ m_{\alpha i j}^\gamma(\vec{x}^\gamma, t) := \int d^dZ \, z_\alpha z_\beta w_\gamma [\vec{X}^\gamma; \vec{Z}^\gamma; t], \]
\[ m_{\alpha i j}^\delta(\vec{x}^\gamma, t) := \int d^dZ \, z_\alpha z_\beta w_\delta [\vec{X}^\delta; \vec{Z}^\gamma; t]. \]

By integration over all variables \( \vec{x}_\beta \) with \( \beta \neq \alpha \) (see (12)) and assumption of the factorization (13), one obtains

\[ \frac{d}{dt} P_\alpha(\vec{x}_\alpha, t) = -\sum_i \frac{\partial}{\partial x_i} \left[ M_\alpha(\vec{x}_\alpha, t) P_\alpha(\vec{x}_\alpha, t) \right] + \frac{1}{2} \sum_{i,j} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \left[ M_{\alpha i j}(\vec{x}_\alpha, t) P_\alpha(\vec{x}_\alpha, t) \right] \]

with

\[ M_\alpha(\vec{x}_\alpha, t) := m_\alpha^\alpha(\vec{x}_\alpha, t) + \sum_\beta \int d^n x_\beta \, m_{\alpha i}^\beta(\vec{x}_\alpha, \vec{x}_\beta, t) P_\beta(\vec{x}_\beta, t), \]
\[ M_{\alpha i j}(\vec{x}_\alpha, t) := m_{\alpha i a j}(\vec{x}_\alpha, t) + \sum_\beta \int d^n x_\beta \left[ m_{\alpha i a j}^\beta(\vec{x}_\alpha, \vec{x}_\beta, t) + m_{\alpha i j b}^\beta(\vec{x}_\alpha, \vec{x}_\beta, t) \right] P_\beta(\vec{x}_\beta, t) \]

and

\[ \int d^n x_\alpha \, P_\alpha(\vec{x}_\alpha, t) = 1. \]

Here, the conventions

\[ m_\alpha^\gamma(\vec{x}_\alpha, t) \equiv m_{\gamma}^\alpha(\vec{x}^\alpha, t), \]
\[ m_{\alpha i j}^\gamma(\vec{x}_\alpha, \vec{x}_\beta, t) \equiv m_{\alpha i j}^{\alpha \beta}(\vec{x}^\alpha, \vec{x}^\beta, t) \]

have been used.

Distinguishing \( A \) types \( a \) of interaction only (see section 2.3), we have

\[ P_a \equiv P_a \quad \text{if} \quad \alpha \in a, \]
\[ m_\alpha^\alpha \equiv \tilde{m}_\alpha^\alpha \quad \text{if} \quad \alpha \in a, \]
\[ m_{\alpha i j}^{\alpha \beta} \equiv \begin{cases} \tilde{m}_{\alpha i j}^{\alpha \beta} & \text{if} \; \alpha \neq \beta, \; \alpha \in a, \; \beta \in b \\ 0 & \text{if} \; \alpha = \beta. \end{cases} \]

Therefore, we arrive at

\[ \frac{d}{dt} P_a(\vec{x}, t) = -\sum_i \frac{\partial}{\partial x_i} \left[ M_\alpha(\vec{x}, t) P_a(\vec{x}, t) \right] + \frac{1}{2} \sum_{i,j} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \left[ M_{\alpha i j}(\vec{x}, t) P_a(\vec{x}, t) \right] \quad (47) \]

with the effective drift coefficients

\[ M_\alpha(\vec{x}, t) := m_\alpha^\alpha(\vec{x}, t) + \sum_b \int d^n y \, m_{\alpha i}^{\alpha b}(\vec{x}, \vec{y}, t) P_b(\vec{y}, t) \]
\[ = \int d^n x' \Delta x'_i w^\alpha(\vec{x}', \vec{x}, t), \quad (48) \]
The effective diffusion coefficients
\[ M_{aij}(\vec{x}, t) := m^a_{aij}(\vec{x}, t) + \sum_b \int d^n y \left[ m^{ab}_{aij}(\vec{x}, \vec{y}, t) + m^{ab}_{ahj}(\vec{x}, \vec{y}, t) \right] P_b(\vec{y}, t) \] (49)
\[ = \int d^n x' \Delta x'_i \Delta x'_j w^a(\vec{x}', \vec{x}; t) + \sum_b \int d^n x' \int d^n y' \int d^n y \Delta x'_i \Delta y'_j w_{ab}(\vec{x}', \vec{y}', \vec{x}, \vec{y}; t) P_b(\vec{y}, t) \]

and
\[ m^a_a := \widetilde{m}_a, \]
\[ m^{ab} := \begin{cases} N_b \cdot \widetilde{m}^{ab} & \text{if } b \neq a \\ (N_a - 1) \cdot \widetilde{m}^{ab} & \text{if } b = a. \end{cases} \]

The result (47), (48), (49) could have also been obtained by a second order Taylor expansion of the BOLTZMANN-like equations (18), (19) (compare to [81, 82, 83]). Therefore, the author suggests to term equations (47), (48), (49) the “BOLTZMANN-FOKKER-PLANCK equation”.

### 3.2 Selfconsistent solution

Equation (47) is difficult to solve, since it is nonlinear in \( P^a(\vec{x}, t) \) due to (48), (49). However, the stationary solution \( P^{st}_a(\vec{x}) \) of (47) to (49) can, with time independent jump moments \( m^a_a(\vec{x}), m^{ab}(\vec{x}) \), be obtained by recursive solution of the linear differential equations
\[ 0 = -\sum_i \frac{\partial}{\partial x_i} \left[ M^k_{ai}(\vec{x}) P^{k+1}_a(\vec{x}) \right] + \frac{1}{2} \sum_{i,j} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \left[ M^k_{aij}(\vec{x}) P^{k+1}_a(\vec{x}) \right]. \] (50)

Here, we have used the definitions
\[ M^k_{ai}(\vec{x}) := m^a_{ai}(\vec{x}) + \sum_b \int d^n y \, m^{ab}_{ai}(\vec{x}, \vec{y}) P^k_b(\vec{y}), \]
\[ M^k_{aij}(\vec{x}) := m^a_{aij}(\vec{x}) + \sum_b \int d^n y \left[ m^{ab}_{aij}(\vec{x}, \vec{y}) + m^{ab}_{aihj}(\vec{x}, \vec{y}) \right] P^k_b(\vec{y}). \] (51)

Starting with suitable distributions \( P^0_a(\vec{x}) \), e.g. the solutions of (47) with neglected interaction terms \( m^{ab}(\vec{x}, \vec{y}) \equiv 0 \), we have
\[ P^{st}_a(\vec{x}) = \lim_{k \to \infty} P^k_a(\vec{x}), \]
if the sequence of functions \( P^k_a(\vec{x}) \) converges. The procedure given by equations (50), (51) is completely analogous to HARTREE’s method for calculating selfconsistent fields in quantum mechanics [84, 85]. In a slightly generalized form, it can also be used to get dynamic solutions \( P_a(\vec{x}, t) \). A recursive solution of BOLTZMANN-like equations (18), (19) or mean value equations (31), (32) is obtained in a similar way.
4 Summary and fields of application

Starting from a master equation for the state space, several equations for statistically behaving systems with pair interactions have been derived. For the case of small (co)variances, approximate mean value and (co)variance equations have been found. However, if the (co)variances are not negligible, BOLTZMANN-like equations are more appropriate. A drastic reduction of the tremendous number of variables is obtained, if the systems can be divided into a few types of interaction. Generalizations to interactions between an arbitrary number of systems have also been discussed.

Important applications of these equations are not only known from thermodynamics [33, 39, 59, 61] and chemistry [39, 1, 40, 41, 42, 43, 44, 45], but also from mathematical population dynamics [54, 86, 87, 88] and from the biology of evolution [89, 90]. For example, the equation

$$\frac{d}{dt} P(x, t) = \sum_{x'} \left[ w(x, x') P(x', t) - w(x', x) P(x, t) \right]$$

(52a)

$$+ \left[ f(x) - \sum_y f(y) P(y, t) \right] P(x, t)$$

(52b)

describes mutations by the left-hand side of (52a), and a selection due to pair interactions by term (52b) [33, 61]. It results from equations (18), (19) with $n = 1, A = 1, w_1(x', x) \equiv w(x', x)$ and

$$w_{11}(x', y'; x, y; t) := \max \left( f(x) - f(y), 0 \right) \delta_{xx'} \delta_{yy'} + \max \left( f(y) - f(x), 0 \right) \delta_{yx'} \delta_{yy'} .$$

$f(x)$ can be interpreted as the fitness of a species or strategy $x$ and $\sum_y f(y) P(y, t) = \langle f \rangle$ as the average fitness.

In addition, a master equation has been introduced allowing transition rates which depend on the occupation numbers of the states. This equation has important applications in quantitative social science [3, 24, 52, 58, 92], e.g. opinion formation [54, 8].

Finally, a FOKKER-PLANCK equation and a “BOLTZMANN-FOKKER-PLANCK equation” for pair interactions have been derived, since they will often be easier solvable or interpretable [9] than the corresponding master equation resp. BOLTZMANN-like equation.

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References

[1] I. Oppenheim, K. E. Schuler and G. H. Weiss, eds., Stochastic Processes in Chemical Physics: The Master Equation (MIT Press, Cambridge, Mass. 1977).

[2] H. Haken, Laser Theory (Springer, Berlin, 1984).

[3] L. Arnold and R. Lefever, eds., Stochastic Nonlinear Systems in Physics, Chemistry and Biology, Springer Series in Synergetics, Vol. 8 (Springer, Berlin, 1981).
[4] J. S. Coleman, *Introduction to Mathematical Sociology* (The Free Press of Glencoe, New York, 1964).

[5] D. J. Bartholomew, *Stochastic Models for Social Processes* (Wiley, London, 1967).

[6] W. Weidlich, *Physics Reports* **204** (1991) 1.

[7] D. Helbing, “A Fluid Dynamic Model for the Movement of Pedestrians”, submitted to *Transportation Research*.

[8] D. Helbing, “A mathematical model for attitude formation by pair interactions”, submitted to *Behavioral Science*.

[9] D. Helbing, “A mathematical model for the behavior of individuals in a social field”, in preparation.

[10] D. Helbing, “Chaos in mathematical models of attitude formation”, in preparation.

[11] D. Helbing, “Spatial aspects of attitude formation”, in preparation.

[12] S.-K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, Reading, Mass., 1976).

[13] W. Horsthemke and R. Lefever, *Noise-Induced Transitions*, Springer Series in Synergetics, Vol. 15 (Springer, Berlin, 1984).

[14] G. Nicolis and I. Prigogine *Self-Organization in Nonequilibrium Systems. From Dissipative Structures to Order through Fluctuations* (Wiley, New York, 1977).

[15] C. W. Gardiner, *Handbook of Stochastic Methods*, 2nd ed. (Springer, Berlin, 1985).

[16] R. L. Stratonovich, *Introduction to the Theory of Random Noise* (Gordon and Breach, New York, London, 1963).

[17] I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Wiley, New York, 1962).

[18] L. van Hove, *Physica* **21** (1955) 517.

[19] L. van Hove, *Physica* **23** (1957) 441.

[20] P. Réssibois, *Physica* **27** (1961) 541.

[21] I. Prigogine and P. Réssibois, *Physica* **27** (1961) 629.

[22] P. Réssibois, *Physica* **29** (1963) 721.

[23] E. W. Montroll: In *Fundamental Problems in Statistical Mechanics* ed. by E. G. D. Cohen (North-Holland, Amsterdam, 1962).

[24] R. W. Zwanzig, *Boulder Lectures in Theoretical Physics* **3** (1962) 106.

[25] R. Zwanzig, *Physica* **30** (1964) 1109.

[26] R. L. Liboff, *Kinetic Theory. Classical, Quantum, and Relativistic Descriptions* (Prentice Hall, Englewood Cliffs, N.J., 1990).
[27] N. Bogolyubov: In *Studies in Statistical Mechanics, Vol. 1* ed. by G. E. Uhlenbeck and J. deBoer (North-Holland, Amsterdam, 1962).

[28] E. G. D. Cohen: In *Fundamental Problems in Statistical Mechanics* ed. by E. G. D. Cohen (North-Holland, Amsterdam, 1962).

[29] G. E. Uhlenbeck, *Probability and Related Topics in Physical Sciences*, compiled by M. Kac (Wiley, New York, 1959).

[30] J. G. Kirkwood, *J. Chem. Phys.* **15** (1947) 72.

[31] H. Grad, *Principles of the Kinetic Theory of Gases*, Hand. d. Physik, Vol. 12 (Springer, Berlin, 1958).

[32] A. Rieckers and H. Stumpf, *Thermodynamik, Vol. 2* (Vieweg, Braunschweig, 1977).

[33] H.-J. Czerwon, R. Der and R. Haberlandt, *Molecular Physics* **33** (1977) 1743.

[34] H. Grabert and W. Weidlich, *Z. Phys.* **268** (1974) 139.

[35] V. M. Kenkre: In *Statistical Mechanics and Statistical Methods in Theory and Application* ed. by U. Landman (Plenum, New York, 1977).

[36] H. Haken, *Synergetics. An Introduction*, 3rd ed. (Springer, Berlin, 1983).

[37] H. Risken, *The Fokker-Planck Equation*, 2nd ed. (Springer, Berlin, 1989).

[38] N. G. van Kampen, *Adv. Chem. Phys.* **34** (1976) 245.

[39] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).

[40] N. Saitô, *J. Chem. Phys.* **61** (1974) 3644.

[41] D. A. McQuarrie, *J. Appl. Prob.* **4** (1967) 413.

[42] C. W. Gardiner, K. J. McNeil, D. F. Walls and I. S. Matheson, *J. Stat. Phys.* **14/4** (1976) 307.

[43] H. K. Janssen, *Z. Phys.* **270** (1974) 67.

[44] G. Czajkowski, *Z. Phys.* **270** (1974) 25.

[45] G. Nicolis, M. Malek-Mansour, A. van Nypelseer and K. Kitahara, *J. Stat. Phys.* **14** (1976) 5.

[46] J. W. Haus and K. W. Kehr, *Physics Reports* **150** (1987) 263.

[47] E. W. Montroll and B. J. West: In *Fluctuation Phenomena* ed. by E. W. Montroll and J. L. Lebowitz (North-Holland, Amsterdam, 1979).

[48] E. W. Montroll and M. F. Shlesinger: In *Nonequilibrium Phenomena II: From Stochastics to Hydrodynamics* ed. by J. L. Lebowitz and E. W. Montroll (North-Holland, Amsterdam, 1984).
[49] G. Haag, W. Weidlich and P. Alber, Z. Phys. B 26 (1977) 207.

[50] J. Schnakenberg, Rev. Mod. Phys. 48/4 (1976) 571.

[51] W. Weidlich, Z. Phys. B 30 (1978) 345.

[52] G. Haag, Z. Phys. B 29 (1978) 153.

[53] G. Haag and P. Hänggi, Z. Phys. B 34 (1979) 411.

[54] W. Weidlich and G. Haag, Concepts and Models of a Quantitative Sociology (Springer, Berlin, 1983).

[55] W. Weidlich and G. Haag (eds.) Interregional Migration (Springer, Berlin, 1988).

[56] G. E. Uhlenbeck and G. W. Ford, Lectures in Statistical Mechanics (American Mathematical Society, Providence, R. I., 1963).

[57] E. G. D. Cohen: In Lectures in Theoretical Physics ed. by W. E. Brittin, Vol. IXC (Gordon and Breach, New York, 1967).

[58] E. G. D. Cohen: In Transport Phenomena in Fluids ed. by H. J. M. Hanley (Dekker, New York, 1969).

[59] R. Kubo, M. Toda and N. Hashitsume, Statistical Physics II (Springer, Berlin, 1985).

[60] L. Boltzmann, Lectures on Gas Theory (University of California, Berkeley, 1964).

[61] J. Keizer, Statistical Thermodynamics of Nonequilibrium Processes (Springer, New York, 1987).

[62] J. R. Dorfman: In Perspectives in Statistical Physics ed. by H. J. Raveché (North-Holland, Amsterdam, 1981).

[63] L. D. Landau and E. M. Lifshitz, Course of Theoretical Physics, Vol. 10: Physical Kinetics (Pergamon, Oxford, 1981).

[64] S. Chapman, Phil. Trans. A 211 (1912) 433; 216 (1915) 279. Also Mem. Manchester Lit. Philos. Soc. 66 (1922) 66.

[65] S. Chapman and T. G. Cowling, The Mathematical Theory of Non-Uniform Gases, 3rd ed. (Cambridge University, London, 1970).

[66] D. Enskog, Kinetische Theorie der Vorgänge in mässig verdünnten Gasen. Inaug. Diss., Uppsala, 1917.

[67] J. R. Blum and J. I. Rosenblatt, Probability and Statistics (Saunders, Philadelphia, 1972).

[68] W. Weidlich, Physica Scripta 35 (1987) 380.

[69] W. Weidlich and G. Haag, Journal of Regional Science 27 (1987) 529.

[70] N. W. Ashcroft and N. D. Mermin, Solid State Physics (Holt-Saunders, Tokyo, 1976).
[71] J. M. Ziman, *Principles of the Theory of Solids*, 2nd ed. (Cambridge University, London, 1972).

[72] H. A. Kramers, *Physica* 7 (1940) 284.

[73] J. E. Moyal, *J. R. Stat. Soc.* 11 (1949) 151.

[74] N. G. van Kampen, *Can. J. Phys.* 39 (1961) 551.

[75] H. Risken and H. D. Vollmer: In *Noise in Nonlinear Dynamical Systems, Vol. 1* ed. by F. Moss and P. V. E. McClintock (Cambridge University, Cambridge, 1989).

[76] M.-O. Hongler, *Physics Letters* 75A (1979) 3.

[77] R. Graham, *Z. Phys. B* 40 (1980) 149.

[78] H. Brand and A. Schenzle, *Physics Letters* 81A (1981) 321.

[79] L. Garrido and J. Masoliver, *J. Math. Phys.* 23/6 (1982) 1155.

[80] H. Gang, *Physical Review A* 39 (1989) 1286.

[81] R. L. Liboff, *The Theory of Kinetic Equations* (Wiley, New York, 1969).

[82] D. Montgomery, *The Physics of Fluids* 14 (1971) 2088.

[83] R. F. Pawula, *Physical Review* 162 (1967) 186.

[84] D. R. Hartree, *Proc. Cambridge Philos. Soc.* 24 (1928) 111.

[85] V. Fock, *Z. Physik* 61 (1930) 126.

[86] N. S. Goel, S. C. Maitra and E. W. Montroll, *Reviews of Modern Physics* 43/2 (1971) 231.

[87] Th. G. Hallam and S. A. Levin (eds.), *Mathematical Ecology* (Springer, Berlin, 1986).

[88] R. M. May, *Stability and Complexity in Model Ecosystems*, 2nd ed. (Princeton University, Princeton, N. J., 1974).

[89] M. Eigen, *Naturwissenschaften* 58 (1971) 465.

[90] R. Feistel and W. Ebeling, *Evolution of Complex Systems* (Kluwer Academic, Dordrecht, 1989).