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Stochastic models in kinetic theory

Wolfgang Wagner

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Weierstrass Institute for
Applied Analysis and Stochastics
Mohrenstrasse 39
10117 Berlin, Germany
E-Mail: wagner@wias-berlin.de

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Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

The paper is concerned with some aspects of stochastic modelling in kinetic theory. First, an overview of the role of particle models with random interactions is given. These models are important both in the context of foundations of kinetic theory and for the design of numerical algorithms in various engineering applications. Then, the class of jump processes with a finite number of states is considered. Two types of such processes are studied, where particles change their states either independently of each other (mono-molecular processes), or via binary interactions (bi-molecular processes). The relationship of these processes with corresponding kinetic equations is discussed. Equations are derived both for the average relative numbers of particles in a given state and for the fluctuations of these numbers around their averages. The simplicity of the models makes several aspects of the theory more transparent.

Contents

[0]Invited paper submitted to the special issue of *Physics of Fluids* in memory of Carlo Cercignani (1939-2010)

1 Introduction

Kinetic theory describes macroscopic features of gas flows (density, stream velocity, temperature) on the basis of the microscopic behaviour of gas molecules. The starting point for the mathematical treatment of the subject is a nonlinear partial integro-differential equation - the Boltzmann equation [7]. This equation describes the time evolution of a function $f(t,x,v)$ that approximately represents the distribution (relative number) of gas molecules with respect to position x and velocity v at time t. Macroscopic quantities are obtained by integration of appropriate functionals with respect to f. The book "Ludwig Boltzmann. The Man who Trusted Atoms" by Carlo Cercignani [8] provides a profound and enjoyable treatment of the history of kinetic theory.

Though the Boltzmann equation is a deterministic model, the interpretation of its solution as a distribution of gas molecules needs the notion of stochasticity. A precise meaning of this notion is obtained via stochastic models of the form

$$\Big(X_i(t), V_i(t)\Big) \qquad i = 1,\ldots,N(t) \qquad t \geq 0 \tag{1.1}$$

representing systems of a finite number $N(t)$ of particles with position $X_i(t)$ and velocity $V_i(t)$ at time t. When appropriately scaled, such particle systems approximate (in the sense of histograms) the solution of the Boltzmann equation. Models (1.1) can be divided into two classes dependent on how stochasticity is involved. In the first class, the time evolution of the particles is deterministic (Hamiltonian dynamics), taking into account the real size of the molecules and the intermolecular potential. Stochasticity enters the model via the initial condition. Such models are the basis for molecular dynamics simulations. In the second class, there is a random interaction mechanism among particles so that stochasticity enters the model during the time evolution. Physical properties, like the intermolecular potential, are taken into account via intensity functions that govern the random interaction mechanism. Such models are used in the direct simulation Monte Carlo method. Models (1.1) provide a precise description of the stochasticity involved in the Boltzmann equation. However, these models are of importance independently of the deterministic (kinetic) equation, as stochastic models of real gas flows. One advantage of the particle models is that they allow to represent fluctuations in the macroscopic quantities. A particularly useful property of particle models with random interactions is their robustness with respect to generalizations like the inclusion of chemical reaction mechanisms, or coagulation and fragmentation effects.

The original derivation of the Boltzmann equation assumes a deterministic dynamics of the gas molecules (hard spheres moving according to the billiard rules). Systems of particles following the complete Hamiltonian dynamics (with a given intermolecular potential) are often considered to provide the most accurate description of real gas flows, but even they are just idealized models. In my view it is quite natural to model collisions between gas molecules as random events. If you have ever played billiard, or at least watched a snooker match on TV, you understand that there is a lot of stochasticity in collisions of billiard balls. So why should it be different for gas molecules? But this discussion leads to the question whether (and where) there

is stochasticity in the "real system", which is left to philosophers. Relationships between the three types of models (kinetic equations, particle models with deterministic dynamics, particle models with random interactions) can be studied mathematically, without referring to the physical reality. Finally, the results obtained by various models have to be compared with observations of real gas flows, that is, measurements of macroscopic quantities (density, stream velocity, temperature) and their fluctuations. Only this comparison does answer the question which of the models is more appropriate in a particular application area. The main topic of this paper are particle models with random interactions, which provide quite reasonable results in many engineering applications.

The paper is organized as follows. Section 2 gives an overview of the subject. First, the history is briefly reviewed. Then, some numerical algorithms based on particle models with random interactions are discussed. Finally, comments are given concerning other areas (beside rarefied gas dynamics), where similar stochastic models are being applied. Section 3 contains the main part of the paper. The class of jump processes with a finite number of states is considered. Two types of such processes are studied, where particles change their states either independently of each other (mono-molecular processes), or via binary interactions (bi-molecular processes). The relationship of these processes with corresponding kinetic equations is discussed. Equations are derived both for the average relative numbers of particles in a given state and for the fluctuations of these numbers around their averages. The simplicity of the models makes several aspects of the theory more transparent.

2 Overview

In this section we address some general aspects of particle models (1.1) with random interactions and their relationship with kinetic equations. This provides the background for the more detailed (and technical) studies in Section 3.

2.1 History

Here we sketch some stochastic particle models of the form (1.1) that have been used in the context of foundations of kinetic theory. More details can be found, e.g., in [16, Section 2.3.3].

Ehrenfest model

In [9] a particle system $x_1(t), \ldots, x_N(t)$ is considered, where each particle has the state 1 or 2. The state is interpreted as the number of the box, where the particle is located. The random evolution is defined by choosing (with equal probability) one of the particles and moving it to the other box. This model is used to illustrate statements

from kinetic theory about averaged quantities and fluctuations. More details will be given in Section 3.4.2.

Leontovich model

In [13] a particle model (1.1) (with $N(t) = N(0) = N$) is introduced, which leads to the Boltzmann equation in the limit $N \to \infty$. The connection is given by the formula

$$f(t,x,v) = \lim_{N\to\infty} p_1^{(N)}(t,x,v)\,, \tag{2.1}$$

where $p_k^{(N)}$ ($k = 1,2,\ldots$) denotes the k-particle marginal density of the N-particle distribution function. Particles move along straight lines according to their velocities (in the absence of an external field). The random interactions (collisions) consist in the change of velocities of a pair of particles. The corresponding transition probabilities depend on the positions of the particles and are different from zero only if their distance does not exceed a certain quantity.

Leontovich provided the description of a model with random spatial interaction, which is a conceptual breakthrough. Particles can be considered either as points interacting at random distances, or as spheres that interact randomly while interpenetrating each other. Leontovich did not prove property (2.1), but he made the asymptotic connection with the Boltzmann equation very clear. In particular, the factorization property

$$\lim_{N\to\infty} p_2^{(N)}(t,x_1,v_1,x_2,v_2) = \lim_{N\to\infty} p_1^{(N)}(t,x_1,v_1) \times \lim_{N\to\infty} p_1^{(N)}(t,x_2,v_2) \tag{2.2}$$

was pointed out as a key element in the proof of (2.1). Moreover, a motivation for the introduction of the stochastic particle system was modelling the fluctuations that are actually observed in real gas flows.

Kac model

In [12] a particle system $V_1(t),\ldots,V_N(t)$ is studied. Spatial dependence is skipped and random interactions consist in choosing pairs of particles and changing their velocities. A theorem is formulated claiming the "propagation" of the factorization property

$$\lim_{N\to\infty} p_k^{(N)}(t,v_1,\ldots,v_k) = \prod_{i=1}^{k} \lim_{N\to\infty} p_1^{(N)}(t,v_i)\,. \tag{2.3}$$

Namely, if (2.3) holds for $t = 0$, then it holds for any $t > 0$. As a consequence, the function $f(t,v) = \lim_{N\to\infty} p_1^{(N)}(t,v)$ (cf. (2.1)) is shown to solve the spatially homogeneous Boltzmann equation. Property (2.3) means asymptotic independence of particles, which is sometimes called "chaos". Kac proved "propagation of chaos" for a simplified model in the case of two-dimensional velocities. A very instructive account of results related to the Kac model is given in [4].

The clear formulation of the “propagation” property is a major achievement. This property has to be proved for the stochastic particle system in order to make the connection with the Boltzmann equation rigorous. It should be noted that the “assumption of molecular chaos” concerns real gas flows, being related to the observation that velocities of colliding particles are uncorrelated. Its approximate validity, which has to be established by experiments, indicates that the Boltzmann equation correctly describes the real gas flow. As far as the stochastic particle model is concerned, the property “propagation of chaos” has to be *proved*. *Assuming* “molecular chaos” in the sense of (2.3) makes the transition to the Boltzmann equation almost trivial.

Cercignani model

In [6] a particle model (1.1) similar to the Leontovich model is studied, namely a system of “soft spheres”. These spheres can inter-penetrate each other and have a certain probability density of scattering each other for each value of the distance between their centers. In the limiting case when the probability is concentrated on a single distance (the particle diameter) the traditional hard sphere gas is re-obtained.

Carlo Cercignani proved a limit theorem for this system, obtaining the factorization (2.2) and the characterization (2.1) for the solution of a spatially smoothed (mollified) Boltzmann equation. This seems to be the first rigorous result concerning the transition from a stochastic particle system to the corresponding nonlinear kinetic equation in the spatially inhomogeneous case. An earlier attempt to connect the space inhomogeneous master equation and the Boltzmann equation was made in [5].

2.2 Direct simulation Monte Carlo

Stochastic particle models (1.1) turned out to be very fruitful for applications of kinetic theory. Here we sketch some aspects related to numerical simulations of real gas flows. More details can be found, e.g., in [16, Section 3.5].

Bird’s DSMC

Starting from [2], stochastic models (1.1) have been developed in an engineering context for the purpose of numerical calculations (cf. [3]). The independent motion of the particles and their interactions via collisions are decoupled over a sufficiently small time step. The position space is divided into sufficiently small cells. Particles belonging to the same cell perform collisions according to an appropriate random mechanism. It is very easy to incorporate more general interactions (beside elastic collisions), which is important in real applications. The concept and the intention of these algorithms is to perform a “direct simulation of gas flows”, thus the name “direct simulation Monte Carlo (DSMC) method”.

Carlo Cercignani was aware of the great potential of the DSMC method to support theoretical investigations, beside its engineering applications. Over at least a decade

he was involved in corresponding studies concerned with instabilities and turbulence phenomena in rarefied gas flows (cf. [17], [18], [19]).

deviational particles

Many improvements have been incorporated into the original DSMC method in order to make it faster, more accurate and applicable to more complex gas flows. Recently, a new approach has been introduced that goes beyond the idea of "direct simulation". The deviational particle approach developed by Hadjiconstantinou and co-workers (cf. [1], [11]) is based on an appropriately modified kinetic equation that governs the time evolution of the deviation of the actual distribution from a Maxwellian. Stochastic particle systems are designed that approximate the solution of the modified equation. These systems have the form (1.1) but carry in addition a sign ± 1, since the deviation can be positive or negative. The goal is to reduce the fluctuations of the algorithm in order to detect small signals more accurately, which is important for low Mach number flows. The new algorithms have been successfully applied to several simple flow configurations. This approach is related to the "control variates" variance reduction technique known in Monte Carlo theory, but in the kinetic context it is applied to a nonlinear equation.

relation to kinetic equations

DSMC is primarily intended to simulate real gas flows, and not to solve a kinetic equation numerically. Nevertheless, a rigorous proof of convergence (with respect to the number of particles) was given in [20]. Moreover, the approximation order with respect to the splitting time step and the cell size was studied (see, e.g., [14] and references therein). The deviational particle approach was put into the context of Markov jump processes in [21]. On the one hand, this setup provides the background for proving convergence. On the other hand, the tools from Markov process theory helped to generalize the method from hard spheres to the variable hard sphere case, which is often preferred by engineers (see [15] concerning numerical tests). This illustrates that the study of the convergence behaviour of stochastic particle schemes and their relationship with kinetic equations, beside its theoretical interest, can be useful also for practical applications.

2.3 Further applications

Here we consider finite particle systems of the form

$$z_i(t) \qquad i = 1, \ldots, N(t) \qquad t \geq 0\,. \tag{2.4}$$

These models are more general than (1.1) in the sense that the state of each particle is characterized by rather arbitrary properties. In addition to position and velocity, these properties can be mass, size or volume, chemical composition, electrical

charge, and others. There are random interaction mechanisms that change the properties of a certain number of particles. Examples are coagulation, when two particles merge and their sizes are added, or fragmentation, when one particle splits into pieces. In the case of elastic collisions, two particles change their velocities under the restriction of conservation of momentum and energy.

Models (2.4) are often used as "direct simulation" algorithms in applications (e.g., chemical engineering, or semiconductor physics). However, generalized kinetic equations can be derived in analogy with the Boltzmann equation. These equations describe the time evolution of a function $f(t,z)$ that approximately represents the distribution (relative number) of particles with respect to their properties z at time t. More precisely, let $N = N(0)$ be the parameter governing the approximation. Then

$$\int_A f(t,z)\,dz \;=\; \lim_{N\to\infty} \frac{1}{N}\, n_A(t)\,, \tag{2.5}$$

where $n_A(t)$ represents the number of particles with states in the subset A at time t. In the case of one-dimensional properties, (2.5) implies convergence of histograms, when choosing A as intervals.

Note that the quantity at the right-hand side of (2.5) is random and convergence is in probability. In a more abstract setting, the statement is about convergence of the empirical measures of the system (2.4),

$$\mu^{(N)}(t,A) \;=\; \frac{1}{N}\sum_{i=1}^{N(t)} \delta_{z_i(t)}(A)\,, \tag{2.6}$$

where $\delta_z(A) = 1$, if $z \in A$, and $\delta_z(A) = 0$, otherwise. It turns out that convergence of the empirical measures (2.6) to a deterministic limit is equivalent to the factorization property (2.3), where the deterministic limit provides a solution of the corresponding kinetic equation. When studying systems with a variable number of particles, it is more convenient to work with empirical measures and prove the propagation of their convergence. Moreover, the approach via empirical measures does not need any symmetry assumption (invariance of the system with respect to permutations). Further details and references can be found, e.g., in [10] and [16, Chapter 2].

3 Jump processes with a finite number of states

In this section we reproduce some of the results obtained by Leontovich in [13], discuss the assumptions and provide illustrations using the Ehrenfest model [9]. First the results are formulated, while derivations will be given in subsequent subsections.

Consider a system

$$\Big(x_1(t),\ldots,x_N(t)\Big) \qquad t \ge 0\,, \tag{3.1}$$

where N denotes the number of particles and each particle has one of a finite number of states $1,\ldots,L$. The corresponding "particle number process" is

$$\Big(n_1(t),\ldots,n_L(t)\Big) \qquad t \ge 0\,, \tag{3.2}$$

where the components

$$n_v(t) = \sum_{i=1}^{N} \delta_{v,x_i(t)} \qquad v = 1,\ldots,L$$

count the numbers of particles in state v at time t (using the notation $\delta_{v,w} = 1$, if $v = w$, and $\delta_{v,w} = 0$, otherwise). The state spaces of the processes (3.1) and (3.2) are $\{1,\ldots,L\}^N$ and $\{(n_1,\ldots,n_L) \geq 0 : n_1 + \ldots + n_L = N\}$, respectively.

Two types of systems (3.1) will be considered, where particles change their states either independently of each other (mono-molecular processes), or via binary interactions (bi-molecular processes). We will study the asymptotic behaviour (as $N \to \infty$) of

- the vector of the average relative numbers of particles in a given state,

$$f_N(t,v) \quad = \quad \mathbb{E}\,\frac{n_v(t)}{N}\,, \tag{3.3}$$

- the covariance matrix of the vector of relative numbers of particles,

$$g_N(t,v,w) \quad = \quad \mathbb{E}\left(\frac{n_v(t)}{N}\,\frac{n_w(t)}{N}\right) - \mathbb{E}\,\frac{n_v(t)}{N}\,\mathbb{E}\,\frac{n_w(t)}{N} \tag{3.4}$$

- and the matrix

$$\gamma_N(t,v,w) \quad = \quad N\,g_N(t,v,w) - \delta_{v,w}\,f_N(t,v) \tag{3.5}$$

  that is used to characterize the level of fluctuations of the relative numbers of particles around their average values.

In the case of a finite number of states, property (2.5) takes the form

$$f(t,v) \quad = \quad \lim_{N\to\infty} \frac{n_v(t)}{N} \qquad v = 1,\ldots,L\,. \tag{3.6}$$

Convergence in probability of uniformly bounded random variables to a deterministic quantity (as in (3.6)) is equivalent to the convergence of the expected values ($f_N \to f$) and the convergence of the variances to zero ($g_N \to 0$). Note that convergence of γ_N implies even $g_N \sim \frac{1}{N}$.

mono-molecular processes

The time evolution of the process (3.1) is defined as follows:

1. The system waits (remains unchanged) a random amount of time that is exponentially distributed with parameter

$$\sum_{i=1}^{N} \lambda_1(x_i)\,, \tag{3.7}$$

   for some non-negative vector λ_1.

2. An index $i = 1, \ldots, N$ is chosen according to the probabilities

$$\frac{\lambda_1(x_i)}{\sum_{j=1}^{N} \lambda_1(x_j)}\,. \tag{3.8}$$

3. A new state $v = 1, \ldots, L$ is chosen according to probabilities $p_1(x_i, v)$.

4. The particle with index i "jumps" into the state v. Go to 1.

Define the quantities

$$\alpha_1(v,w) = \lambda_1(v)\, p_1(v,w) \qquad \text{if} \quad w \neq v \tag{3.9}$$

and

$$\alpha_1(v,v) = -\lambda_1(v) \sum_{w \neq v} p_1(v,w)\,. \tag{3.10}$$

Theorem 3.1 *The quantities (3.3) and (3.5) satisfy*

$$\frac{d}{dt}\, f_N(t,w) = \sum_{v=1}^{L} f_N(t,v)\, \alpha_1(v,w) \tag{3.11}$$

and

$$\frac{d}{dt}\, \gamma_N(t,m,w) \;=\; \sum_{v=1}^{L} \gamma_N(t,w,v)\, \alpha_1(v,m) + \sum_{v=1}^{L} \gamma_N(t,m,v)\, \alpha_1(v,w)\,. \tag{3.12}$$

It follows from (3.11) that the unique solution

$$f_N(t,v) = \exp(t\, \alpha_1')\, f_N(0,v) \tag{3.13}$$

converges provided that the initial value $f_N(0)$ converges. Here α_1' denotes the transposed matrix. According to (3.12), convergence of $\gamma_N(t)$ follows from the convergence of $\gamma_N(0)$.

bi-molecular processes

The time evolution of the process (3.1) is defined as follows:

1. The system waits (remains unchanged) a random amount of time that is exponentially distributed with parameter

$$\frac{1}{2N} \sum_{1 \leq i \neq j \leq N} \lambda_2(x_i, x_j)\,, \tag{3.14}$$

for some non-negative matrix λ_2.

2. A pair of indices i, j is chosen according to the probabilities

$$\frac{\lambda_2(x_i, x_j)}{\sum_{1\le k\ne l\le N} \lambda_2(x_k, x_l)}, \qquad 1 \le i \ne j \le N. \tag{3.15}$$

3. Two new states $v, w = 1, \dots, L$ are chosen according to probabilities $p_2(x_i, x_j, v, w)$.

4. The particles with indices i, j "jump" into the states v and w, respectively. Go to 1.

Define the quantities

$$\alpha_2(v,w,m,z) = \lambda_2(v,w)\, p_2(v,w,m,z) \qquad \text{if} \quad (m,z) \ne (v,w) \tag{3.16}$$

and

$$\alpha_2(v,w,v,w) = -\lambda_2(v,w) \sum_{(m,z)\ne(v,w)} p_2(v,w,m,z). \tag{3.17}$$

Theorem 3.2 *The function (cf. (3.3))*

$$f(t,z) = \lim_{N\to\infty} f_N(t,z) \tag{3.18}$$

satisfies the equation

$$\frac{d}{dt} f(t,z) = \frac{1}{2} \sum_{v,w=1}^{L} f(t,v)\, f(t,w) \sum_{l=1}^{L} \Big[\alpha_2(v,w,l,z) + \alpha_2(v,w,z,l)\Big]. \tag{3.19}$$

The function (cf. (3.5))

$$\gamma(t,w,v) = \lim_{N\to\infty} \gamma_N(t,w,v) \tag{3.20}$$

satisfies the equation

$$\begin{aligned} \frac{d}{dt}\gamma(t,y,z) = & \qquad (3.21)\\ & \frac{1}{2} \sum_{v,w=1}^{L} \Big(\gamma(t,z,v)\, f(t,w) + f(t,v)\, \gamma(t,z,w)\Big) \sum_{l=1}^{L} \Big[\alpha_2(v,w,l,y) + \alpha_2(v,w,y,l)\Big] + \\ & \frac{1}{2} \sum_{v,w=1}^{L} \Big(\gamma(t,y,v)\, f(t,w) + f(t,v)\, \gamma(t,y,w)\Big) \sum_{l=1}^{L} \Big[\alpha_2(v,w,l,z) + \alpha_2(v,w,z,l)\Big] + \\ & \frac{1}{2} \sum_{v,w=1}^{L} f(t,v)\, f(t,w) \Big[\alpha_2(v,w,y,z) + \alpha_2(v,w,z,y)\Big]. \end{aligned}$$

weak equations

Equivalent weak forms of equations (3.11) and (3.19) are obtained via the transformations

$$\begin{aligned}
&\frac{d}{dt}\sum_{w=1}^{L}\varphi(w)\,f(t,w) = \\
&= \sum_{w=1}^{L}\varphi(w)\sum_{v=1}^{L}f_N(t,v)\,\alpha_1(v,w) = \sum_{v=1}^{L}f_N(t,v)\sum_{w=1}^{L}\varphi(w)\,\alpha_1(v,w) \\
&= \sum_{v=1}^{L}f_N(t,v)\left[\sum_{w\neq v}\varphi(w)\,\alpha_1(v,w)+\varphi(v)\,\alpha_1(v,v)\right] \\
&= \sum_{v=1}^{L}f_N(t,v)\sum_{w\neq v}\Big[\varphi(w)-\varphi(v)\Big]\alpha_1(v,w) = \sum_{v=1}^{L}f_N(t,v)\sum_{w=1}^{L}\Big[\varphi(w)-\varphi(v)\Big]\alpha_1(v,w) \\
&= \sum_{v=1}^{L}f_N(t,v)\sum_{w=1}^{L}\Big[\varphi(w)-\varphi(v)\Big]\lambda_1(v)\,p_1(v,w) \qquad (3.22)
\end{aligned}$$

and

$$\begin{aligned}
&\frac{d}{dt}\sum_{z=1}^{L}\varphi(z)\,f(t,z) = \qquad (3.23)\\
&\qquad \frac{1}{2}\sum_{v,w=1}^{L}f(t,v)\,f(t,w)\sum_{l,z=1}^{L}\varphi(z)\Big[\alpha_2(v,w,l,z)+\alpha_2(v,w,z,l)\Big] \\
&= \frac{1}{2}\sum_{v,w=1}^{L}f(t,v)\,f(t,w)\sum_{l,z=1}^{L}\Big[\varphi(z)+\varphi(l)\Big]\alpha_2(v,w,l,z) \\
&= \frac{1}{2}\sum_{v,w=1}^{L}f(t,v)\,f(t,w)\left\{\sum_{l,z\neq v,w}\Big[\varphi(z)+\varphi(l)\Big]\alpha_2(v,w,l,z)\right. \\
&\qquad \left.-\Big[\varphi(w)+\varphi(v)\Big]\sum_{l,z\neq v,w}\alpha_2(v,w,l,z)\right\} \\
&= \frac{1}{2}\sum_{v,w=1}^{L}f(t,v)\,f(t,w)\sum_{l,z=1}^{L}\Big[\varphi(z)+\varphi(l)-\varphi(w)-\varphi(v)\Big]\alpha_2(v,w,l,z) \\
&= \frac{1}{2}\sum_{v,w=1}^{L}f(t,v)\,f(t,w)\sum_{l,z=1}^{L}\Big[\varphi(z)+\varphi(l)-\varphi(w)-\varphi(v)\Big]q_2(v,w)\,p_2(v,w,l,z)\,,
\end{aligned}$$

where φ is an arbitrary vector and the properties

$$\sum_{w=1}^{L}\alpha_1(v,w)=0 \qquad \text{and} \qquad \sum_{m,z=1}^{L}\alpha_2(v,w,m,z)=0 \qquad (3.24)$$

were used. The weak equations make the analogy with corresponding (linear and nonlinear) Boltzmann equations more evident. Moreover, the transformations (3.22)

and (3.23) clarify the relationships (3.9), (3.10), (3.16), (3.17) between the parameters λ, p (determining the evolution of the system) and α (occurring in the kinetic equation).

3.1 General properties

We first recall several properties that will be used both for mono-molecular and bi-molecular processes.

representations of the quantities (3.3) and (3.5)

The *generating function* of the process (3.2) is defined as

$$\Phi^{(N)}(t,u_1,\dots,u_L) = \mathbb{E}\, u_1^{n_1(t)}\dots u_L^{n_L(t)} = \sum_{n_1+\dots+n_L=N} u_1^{n_1}\dots u_L^{n_L} V(t,n_1,\dots,n_L)\,, \qquad (3.25)$$

where V denotes the distribution of the process. Using the identity

$$u_1^{n_1}\dots u_L^{n_L} = u_{x_1}\dots u_{x_N} \qquad (3.26)$$

one obtains from (3.25)

$$\Phi^{(N)}(t,u_1,\dots,u_L) = \sum_{x_1,\dots,x_N=1}^{L} u_{x_1}\dots u_{x_N} W(t,x_1,\dots,x_N)\,, \qquad (3.27)$$

where W denotes the distribution of the process (3.1). It follows from (3.27) that

$$\begin{aligned}\frac{\partial}{\partial u_v}\Phi^{(N)}(t,u_1,\dots,u_L) &= \sum_{x_1,\dots,x_N=1}^{L}\sum_{i=1}^{N}\left(\left(\frac{\partial}{\partial u_v}u_{x_i}\right)\prod_{\substack{k=1\\k\neq i}}^{N}u_{x_k}\right)W(t,x)\\ &= \sum_{i=1}^{N}\sum_{\substack{x_1,\dots,x_N=1\\x_i=v}}^{L}\left(\prod_{\substack{k=1\\k\neq i}}^{N}u_{x_k}\right)W(t,x) \qquad (3.28)\end{aligned}$$

and

$$\begin{aligned}&\frac{\partial^2}{\partial u_v\,\partial u_w}\Phi^{(N)}(t,u_1,\dots,u_L) =\\ &\qquad \sum_{x_1,\dots,x_N=1}^{L}\sum_{1\le i\neq j\le N}\left(\left(\frac{\partial}{\partial u_v}u_{x_i}\right)\left(\frac{\partial}{\partial u_w}u_{x_j}\right)\prod_{\substack{k=1\\k\neq i,j}}^{N}u_{x_k}\right)W(t,x)\\ &= \sum_{1\le i\neq j\le N}\sum_{\substack{x_1,\dots,x_N=1\\x_i=v,x_j=w}}^{L}\left(\prod_{\substack{k=1\\k\neq i,j}}^{N}u_{x_k}\right)W(t,x)\,. \qquad (3.29)\end{aligned}$$

On the other hand, the generating function (3.25) satisfies

$$\frac{\partial}{\partial u_v}\Phi^{(N)}(t,u_1,\ldots,u_L)\bigg|_{u=1} = \mathbb{E}\, n_v(t) \tag{3.30}$$

and

$$\frac{\partial^2}{\partial u_v\,\partial u_w}\Phi^{(N)}(t,u_1,\ldots,u_L)\bigg|_{u=1} = \mathbb{E}\,[n_v(t)\,n_w(t)] - \delta_{v,w}\,\mathbb{E}\, n_v(t)\,. \tag{3.31}$$

Representing it in the form

$$\Phi^{(N)}(t,u_1,\ldots,u_L) = \exp\Big(N\,\varphi^{(N)}(t,u_1,\ldots,u_L)\Big) \tag{3.32}$$

one obtains

$$\frac{\partial}{\partial t}\,\Phi^{(N)}(t,u_1,\ldots,u_L) = \Phi^{(N)}(t,u_1,\ldots,u_L)\,N\,\frac{\partial}{\partial t}\varphi^{(N)}(t,u_1,\ldots,u_L) \tag{3.33}$$

and

$$\frac{\partial}{\partial u_v}\Phi^{(N)}(t,u_1,\ldots,u_L) = \Phi^{(N)}(t,u_1,\ldots,u_L)\,N\,\frac{\partial}{\partial u_v}\varphi^{(N)}(t,u_1,\ldots,u_L) \tag{3.34}$$

and

$$\begin{aligned}\frac{\partial^2}{\partial u_w\,\partial u_v}\Phi^{(N)}(t,u_1,\ldots,u_L) = \\ \Phi^{(N)}(t,u_1,\ldots,u_L)\,N\,\frac{\partial}{\partial u_w}\varphi^{(N)}(t,u_1,\ldots,u_L)\,N\,\frac{\partial}{\partial u_v}\varphi^{(N)}(t,u_1,\ldots,u_L) + \\ \Phi^{(N)}(t,u_1,\ldots,u_L)\,N\,\frac{\partial^2}{\partial u_w\,\partial u_v}\varphi^{(N)}(t,u_1,\ldots,u_L)\,.\end{aligned} \tag{3.35}$$

It follows from (3.30), (3.31), (3.34) and (3.35) that (cf. (3.3))

$$\frac{\partial}{\partial u_v}\varphi^{(N)}(t,u_1,\ldots,u_L)\bigg|_{u=1} = \frac{1}{N}\,\frac{\partial}{\partial u_v}\Phi^{(N)}(t,u_1,\ldots,u_L)\bigg|_{u=1} = f_N(t,v) \tag{3.36}$$

and (cf. (3.4), (3.5))

$$\begin{aligned}\frac{\partial^2}{\partial u_w\,\partial u_v}\varphi^{(N)}(t,u_1,\ldots,u_L)\bigg|_{u=1} = \\ \frac{1}{N}\,\frac{\partial^2}{\partial u_w\,\partial u_v}\Phi^{(N)}(t,u_1,\ldots,u_L)\bigg|_{u=1} - \\ N\,\frac{\partial}{\partial u_w}\varphi^{(N)}(t,u_1,\ldots,u_L)\bigg|_{u=1}\,\frac{\partial}{\partial u_v}\varphi^{(N)}(t,u_1,\ldots,u_L)\bigg|_{u=1} \\ = \frac{1}{N}\Big[\mathbb{E}\,(n_w(t)\,n_v(t)) - \delta_{w,v}\,\mathbb{E}\, n_w(t)\Big] - N\,f_N(t,w)\,f_N(t,v) \\ = N\,g_N(t,w,v) - \delta_{w,v}\,f_N(t,w) = \gamma_N(t,w,v)\,.\end{aligned} \tag{3.37}$$

Kolmogorov's forward equation

Consider a Markov jump process $Z(t)$ with a finite state space. Its time evolution is defined as follows:

1. The process stays in state z for an exponentially distributed time with parameter $\lambda(z)$, for some non-negative vector λ.
2. The process jumps into state y distributed according to probabilities $p(z,y)$. Go to 1.

The distribution of the process

$$W(t,y) \;=\; \mathbb{P}(Z(t)=y)$$

satisfies *Kolmogorov's forward equation*

$$\frac{\partial}{\partial t}W(t,y) = \sum_z W(t,z)\,\lambda(z)\,p(z,y) - W(t,y)\,\lambda(y)\,. \tag{3.38}$$

3.2 Mono-molecular processes

According to the definition of mono-molecular processes (cf. (3.7), (3.8)), we introduce

$$\lambda(x) = \sum_{i=1}^{N} \lambda_1(x_i) \qquad\qquad x=(x_1,\ldots,x_N)$$

and

$$p(x,y) = \frac{1}{\lambda(x)} \sum_{i=1}^{N} \lambda_1(x_i) \sum_{v=1}^{L} p_1(x_i,v)\,\delta_{T_1(x,i,v),y}\,,$$

where the transformation $T_1(x,i,v)$ replaces the i-th component of x by v. Equation (3.38) implies (cf. (3.9), (3.10))

$$\begin{aligned}
\frac{\partial}{\partial t}W(t,x) &= \sum_y W(t,y) \sum_{i=1}^{N} \lambda_1(y_i) \sum_{v=1}^{L} p_1(y_i,v)\,\delta_{T_1(y,i,v),x} - W(t,x)\,\lambda(x) \\
&= \sum_{i=1}^{N} \sum_{v=1}^{L} \sum_{y:\,T_1(y,i,v)=x} W(t,y)\,\lambda_1(y_i)\,p_1(y_i,v) - W(t,x)\,\lambda(x) \\
&= \sum_{i=1}^{N} \sum_{w=1}^{L} W(t,T_1(x,i,w))\,\lambda_1(w)\,p_1(w,x_i) - W(t,x) \sum_{i=1}^{N} \lambda_1(x_i) \sum_{w=1}^{L} p_1(x_i,w) \\
&= \sum_{i=1}^{N} \sum_{w\neq x_i} W(t,T_1(x,i,w))\,\lambda_1(w)\,p_1(w,x_i) - W(t,x) \sum_{i=1}^{N} \lambda_1(x_i) \sum_{w\neq x_i} p_1(x_i,w) \\
&= \sum_{i=1}^{N} \sum_{w\neq x_i} W(t,T_1(x,i,w))\,\alpha_1(w,x_i) + W(t,x) \sum_{i=1}^{N} \alpha_1(x_i,x_i) \\
&= \sum_{i=1}^{N} \sum_{w=1}^{L} W(t,T_1(x,i,w))\,\alpha_1(w,x_i)\,.
\end{aligned} \tag{3.39}$$

It follows from (3.27) and (3.39) that

$$\begin{aligned}
\frac{\partial}{\partial t}\Phi^{(N)}(t,u_1,\dots,u_L) &= \sum_{x_1,\dots,x_N=1}^{L} u_{x_1}\dots u_{x_N}\sum_{i=1}^{N}\sum_{v=1}^{L} W(t,T_1(x,i,v))\,\alpha_1(v,x_i)\\
&= \sum_{v=1}^{L}\sum_{i=1}^{N}\sum_{l=1}^{L}\sum_{\substack{x_1,\dots,x_N=1\\ x_i=l}}^{L} u_{x_1}\dots u_{x_N}\,W(t,T_1(x,i,v))\,\alpha_1(v,x_i)\\
&= \sum_{v=1}^{L}\sum_{i=1}^{N}\sum_{l=1}^{L}\alpha_1(v,l)\,u_l\sum_{\substack{x_1,\dots,x_N=1\\ x_i=l}}^{L}\left(\prod_{\substack{k=1\\ k\neq i}}^{N}u_{x_k}\right)W(t,T_1(x,i,v))\\
&= \sum_{v=1}^{L}\sum_{l=1}^{L}\alpha_1(v,l)\,u_l\sum_{i=1}^{N}\sum_{\substack{x_1,\dots,x_N=1\\ x_i=v}}^{L}\left(\prod_{\substack{k=1\\ k\neq i}}^{N}u_{x_k}\right)W(t,x)\,. \qquad (3.40)
\end{aligned}$$

One obtains, according to (3.28) and (3.40),

$$\frac{\partial}{\partial t}\Phi^{(N)}(t,u_1,\dots,u_L)=\sum_{v=1}^{L}\frac{\partial}{\partial u_v}\Phi^{(N)}(t,u_1,\dots,u_L)\sum_{l=1}^{L}\alpha_1(v,l)\,u_l$$

and, according to (3.32)-(3.34),

$$\frac{\partial}{\partial t}\varphi^{(N)}(t,u_1,\dots,u_L)=\sum_{v=1}^{L}\frac{\partial}{\partial u_v}\varphi^{(N)}(t,u_1,\dots,u_L)\sum_{l=1}^{L}\alpha_1(v,l)\,u_l\,. \qquad (3.41)$$

Equation (3.41) implies

$$\begin{aligned}
\frac{\partial}{\partial t}\frac{\partial}{\partial u_w}\varphi^{(N)}(t,u_1,\dots,u_L) &= \sum_{v=1}^{L}\frac{\partial^2}{\partial u_w\,\partial u_v}\varphi^{(N)}(t,u_1,\dots,u_L)\sum_{l=1}^{L}\alpha_1(v,l)\,u_l+\\
&\quad\sum_{v=1}^{L}\left(\frac{\partial}{\partial u_v}\varphi^{(N)}(t,u_1,\dots,u_L)\right)\alpha_1(v,w)
\end{aligned}$$

so that (cf. (3.24))

$$\frac{d}{dt}\left(\frac{\partial}{\partial u_w}\varphi^{(N)}(t,u_1,\dots,u_L)\bigg|_{u=1}\right)=\sum_{v=1}^{L}\frac{\partial}{\partial u_v}\varphi^{(N)}(t,u_1,\dots,u_L)\bigg|_{u=1}\alpha_1(v,w) \qquad (3.42)$$

and

$$\begin{aligned}
&\frac{d}{dt}\left(\frac{\partial^2}{\partial u_m\,\partial u_w}\varphi^{(N)}(t,u_1,\dots,u_L)\bigg|_{u=1}\right)= \qquad (3.43)\\
&\quad\sum_{v=1}^{L}\frac{\partial^2}{\partial u_w\,\partial u_v}\varphi^{(N)}(t,u_1,\dots,u_L)\bigg|_{u=1}\alpha_1(v,m)+\\
&\quad\sum_{v=1}^{L}\frac{\partial^2}{\partial u_m\,\partial u_v}\varphi^{(N)}(t,u_1,\dots,u_L)\bigg|_{u=1}\alpha_1(v,w)\,.
\end{aligned}$$

According to (3.3), (3.5), (3.36) and (3.37), equations (3.42) and (3.43) take the form (3.11) and (3.12), respectively.

3.3 Bi-molecular processes

According to the definition of bi-molecular processes (cf. (3.14), (3.15)), we introduce

$$\lambda(x) = \frac{1}{2N} \sum_{1\le i\ne j\le N} \lambda_2(x_i, x_j) \qquad x = (x_1, \ldots, x_N)$$

and

$$p(x,y) = \frac{1}{2N\,\lambda(x)} \sum_{1\le i\ne j\le N} \lambda_2(x_i, x_j) \sum_{v,w=1}^{L} p_2(x_i, x_j, v, w)\, \delta_{T_2(x,i,j,v,w),y}\,,$$

where the transformation $T_2(x,i,j,v,w)$ replaces the i-th and j-th components of x by v and w, respectively. One obtains

$$\begin{aligned}
&\sum_y W(t,y)\,\lambda(y)\,p(y,x) = \\
&\qquad \frac{1}{2N} \sum_y W(t,y) \sum_{1\le i\ne j\le N} \lambda_2(y_i,y_j) \sum_{v,w=1}^{L} p_2(y_i,y_j,v,w)\, \delta_{T_2(y,i,j,v,w),x} \\
&= \frac{1}{2N} \sum_{1\le i\ne j\le N} \sum_{v,w=1}^{L} \sum_{y:\, T_2(y,i,j,v,w)=x} W(t,y)\,\lambda_2(y_i,y_j)\,p_2(y_i,y_j,v,w) \\
&= \frac{1}{2N} \sum_{1\le i\ne j\le N} \sum_{l,m=1}^{L} W(t, T_2(x,i,j,l,m))\,\lambda_2(l,m)\,p_2(l,m,x_i,x_j)
\end{aligned}$$

so that equation (3.38) implies (cf. (3.16), (3.17))

$$\begin{aligned}
\frac{\partial}{\partial t} W(t,x) &= \frac{1}{2N} \sum_{1\le i\ne j\le N} \sum_{l,m=1}^{L} W(t, T_2(x,i,j,l,m))\,\lambda_2(l,m)\,p_2(l,m,x_i,x_j) - \\
&\qquad \frac{1}{2N} W(t,x) \sum_{1\le i\ne j\le N} \lambda_2(x_i,x_j) \sum_{l,m=1}^{L} p_2(x_i,x_j,l,m) \\
&= \frac{1}{2N} \sum_{1\le i\ne j\le N} \sum_{(l,m)\ne(x_i,x_j)} W(t, T_2(x,i,j,l,m))\,\lambda_2(l,m)\,p_2(l,m,x_i,x_j) - \\
&\qquad \frac{1}{2N} W(t,x) \sum_{1\le i\ne j\le N} \lambda_2(x_i,x_j) \sum_{(l,m)\ne(x_i,x_j)} p_2(x_i,x_j,l,m) \\
&= \frac{1}{2N} \sum_{1\le i\ne j\le N} \sum_{(l,m)\ne(x_i,x_j)} W(t, T_2(x,i,j,l,m))\,\alpha_2(l,m,x_i,x_j) + \\
&\qquad \frac{1}{2N} W(t,x) \sum_{1\le i\ne j\le N} \alpha_2(x_i,x_j,x_i,x_j) \\
&= \frac{1}{2N} \sum_{1\le i\ne j\le N} \sum_{l,m=1}^{L} W(t, T_2(x,i,j,l,m))\,\alpha_2(l,m,x_i,x_j)\,. \qquad (3.44)
\end{aligned}$$

It follows from (3.27) and (3.44) that

$$\begin{aligned}
\frac{\partial}{\partial t}\Phi^{(N)}(t,u_1,\dots,u_L) = \\
&\frac{1}{2N}\sum_{x_1,\dots,x_N=1}^{L} u_{x_1}\dots u_{x_N}\sum_{1\le i\ne j\le N}\sum_{v,w=1}^{L} W\big(t,T_2(x,i,j,v,w)\big)\,\alpha_2(v,w,x_i,x_j)\\
=\;&\frac{1}{2N}\sum_{v,w=1}^{L}\sum_{1\le i\ne j\le N}\sum_{x_1,\dots,x_N=1}^{L} u_{x_1}\dots u_{x_N} W\big(t,T_2(x,i,j,v,w)\big)\,\alpha_2(v,w,x_i,x_j)\\
=\;&\frac{1}{2N}\sum_{v,w=1}^{L}\sum_{1\le i\ne j\le N}\sum_{l,m=1}^{L}\sum_{\substack{x_1,\dots,x_N=1\\ x_i=l,x_j=m}}^{L} u_{x_1}\dots u_{x_N} W\big(t,T_2(x,i,j,v,w)\big)\,\alpha_2(v,w,x_i,x_j)\\
=\;&\frac{1}{2N}\sum_{v,w=1}^{L}\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m\times\\
&\sum_{1\le i\ne j\le N}\sum_{\substack{x_1,\dots,x_N=1\\ x_i=l,x_j=m}}^{L}\left(\prod_{\substack{k=1\\ k\ne i,j}}^{N} u_{x_k}\right) W\big(t,T_2(x,i,j,v,w)\big)\\
=\;&\frac{1}{2N}\sum_{v,w=1}^{L}\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m\sum_{1\le i\ne j\le N}\sum_{\substack{x_1,\dots,x_N=1\\ x_i=v,x_j=w}}^{L}\left(\prod_{\substack{k=1\\ k\ne i,j}}^{N} u_{x_k}\right) W(t,x)\,. \qquad (3.45)
\end{aligned}$$

One obtains, according to (3.29) and (3.45),

$$\frac{\partial}{\partial t}\Phi^{(N)}(t,u_1,\dots,u_L) = \frac{1}{2N}\sum_{v,w=1}^{L}\frac{\partial^2}{\partial u_v\,\partial u_w}\Phi^{(N)}(t,u_1,\dots,u_L)\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m$$

and, according to (3.32), (3.33), (3.35),

$$\begin{aligned}
&\frac{\partial}{\partial t}\varphi^{(N)}(t,u_1,\dots,u_L) = \qquad (3.46)\\
&\quad\frac{1}{2}\sum_{v,w=1}^{L}\left[\left(\frac{\partial}{\partial u_v}\varphi^{(N)}\right)\left(\frac{\partial}{\partial u_w}\varphi^{(N)}\right)+\frac{1}{N}\,\frac{\partial^2}{\partial u_v\,\partial u_w}\varphi^{(N)}\right]\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m\,.
\end{aligned}$$

Remark 3.3 *It is assumed that a solution of the "basic equation" (3.46) can be constructed in the form*

$$\varphi^{(N)}(t) = \varphi_0(t)+\frac{1}{N}\,\varphi_1(t)+\frac{1}{N^2}\,\varphi_2(t)+\dots, \qquad (3.47)$$

where the functions $\varphi_0,\varphi_1,\dots$ do not depend on N, and that

$$\lim_{N\to\infty}\left(\frac{\partial}{\partial u_v}\varphi^{(N)}(t,u_1,\dots,u_L)\Big|_{u=1}\right) = \frac{\partial}{\partial u_v}\varphi_0(t,u_1,\dots,u_L)\Big|_{u=1} \qquad (3.48)$$

and

$$\lim_{N\to\infty}\left(\frac{\partial^2}{\partial u_w\,\partial u_v}\varphi^{(N)}(t,u_1,\dots,u_L)\Big|_{u=1}\right) = \frac{\partial^2}{\partial u_w\,\partial u_v}\varphi_0(t,u_1,\dots,u_L)\Big|_{u=1}, \qquad (3.49)$$

where the right-hand sides in (3.48), (3.49) are finite.

It is a consequence of (3.46) and (3.47) that the function φ_0 satisfies the equation

$$\frac{\partial}{\partial t}\varphi_0(t,u_1,\dots,u_L) = \tag{3.50}$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\left(\frac{\partial}{\partial u_v}\varphi_0(t,u_1,\dots,u_L)\right)\left(\frac{\partial}{\partial u_w}\varphi_0(t,u_1,\dots,u_L)\right)\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m\,,$$

which implies

$$\frac{\partial}{\partial u_z}\frac{\partial}{\partial t}\varphi_0(t,u_1,\dots,u_L) =$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\frac{\partial}{\partial u_z}\left[\left(\frac{\partial}{\partial u_v}\varphi_0\right)\left(\frac{\partial}{\partial u_w}\varphi_0\right)\right]\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m +$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\left(\frac{\partial}{\partial u_v}\varphi_0\right)\left(\frac{\partial}{\partial u_w}\varphi_0\right)\frac{\partial}{\partial u_z}\left(\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m\right)$$

and

$$\frac{\partial^2}{\partial u_y\,\partial u_z}\frac{\partial}{\partial t}\varphi_0(t,u_1,\dots,u_L) =$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\frac{\partial^2}{\partial u_y\,\partial u_z}\left[\left(\frac{\partial}{\partial u_v}\varphi_0\right)\left(\frac{\partial}{\partial u_w}\varphi_0\right)\right]\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m +$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\frac{\partial}{\partial u_z}\left[\left(\frac{\partial}{\partial u_v}\varphi_0\right)\left(\frac{\partial}{\partial u_w}\varphi_0\right)\right]\frac{\partial}{\partial u_y}\left(\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m\right) +$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\frac{\partial}{\partial u_y}\left[\left(\frac{\partial}{\partial u_v}\varphi_0\right)\left(\frac{\partial}{\partial u_w}\varphi_0\right)\right]\frac{\partial}{\partial u_z}\left(\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m\right) +$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\left(\frac{\partial}{\partial u_v}\varphi_0\right)\left(\frac{\partial}{\partial u_w}\varphi_0\right)\frac{\partial^2}{\partial u_y\,\partial u_z}\left(\sum_{l,m=1}^{L}\alpha_2(v,w,l,m)\,u_l\,u_m\right)$$

so that (cf. (3.24))

$$\frac{d}{dt}\left(\frac{\partial}{\partial u_z}\varphi_0(t,u_1,\dots,u_L)\Big|_{u=1}\right) = \tag{3.51}$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\left\{\frac{\partial}{\partial u_v}\varphi_0(t,u_1,\dots,u_L)\Big|_{u=1}\frac{\partial}{\partial u_w}\varphi_0(t,u_1,\dots,u_L)\Big|_{u=1}\right\}\times$$
$$\sum_{l=1}^{L}\Big[\alpha_2(v,w,l,z)+\alpha_2(v,w,z,l)\Big]$$

and

$$\frac{d}{dt}\left(\frac{\partial^2}{\partial u_y\,\partial u_z}\varphi_0(t,u_1,\dots,u_L)\Big|_{u=1}\right) = \tag{3.52}$$

$$\frac{1}{2}\sum_{v,w=1}^{L}\frac{\partial}{\partial u_z}\left[\left(\frac{\partial}{\partial u_v}\varphi_0\right)\left(\frac{\partial}{\partial u_w}\varphi_0\right)\right]_{u=1}\sum_{l=1}^{L}\Big[\alpha_2(v,w,l,y)+\alpha_2(v,w,y,l)\Big]+$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\frac{\partial}{\partial u_y}\left[\left(\frac{\partial}{\partial u_v}\varphi_0\right)\left(\frac{\partial}{\partial u_w}\varphi_0\right)\right]_{u=1}\sum_{l=1}^{L}\Big[\alpha_2(v,w,l,z)+\alpha_2(v,w,z,l)\Big]+$$
$$\frac{1}{2}\sum_{v,w=1}^{L}\frac{\partial}{\partial u_v}\varphi_0\Big|_{u=1}\frac{\partial}{\partial u_w}\varphi_0\Big|_{u=1}\Big[\alpha_2(v,w,y,z)+\alpha_2(v,w,z,y)\Big].$$

It follows from (3.36), (3.48) and (3.51) that the function (3.18) exists and satisfies equation (3.19), and from (3.37), (3.49) and (3.52) that the function (3.20) exists and satisfies equation (3.21).

We have reproduced the derivation of equations (3.19), (3.21) given by Leontovich in [13]. Some more effort would have to be spent in order to fill the remaining gaps, that is, to prove the assumptions collected in Remark 3.3. It follows from (3.46) (by comparing terms having the same order with respect to N) that φ_0 satisfies the non-linear equation (3.50) and $\varphi_1,\varphi_2,\ldots$ satisfy linear equations as, for example,

$$\frac{\partial}{\partial t}\varphi_1(t,u_1,\ldots,u_L)=$$
$$\frac{1}{2}\sum_{v,w}\left[\frac{\partial}{\partial u_v}\varphi_1\,\frac{\partial}{\partial u_w}\varphi_0+\frac{\partial}{\partial u_v}\varphi_0\,\frac{\partial}{\partial u_w}\varphi_1+\frac{\partial^2}{\partial u_v\,\partial u_w}\varphi_0\right]\sum_{l,m}\alpha_2(v,w,l,m)\,u_l\,u_m\,.$$

Properties of these solutions have to be studied in order to justify the assumptions concerning convergence of the series representation (3.47) and its regularity properties (3.48), (3.49). However, Leontovich's approach via generating functions is restricted to the finite state space. More general results have been obtained by other methods. For example, [10, Theorem 2.3] implies (3.6) for all $t>0$ provided that it holds for $t=0$.

3.4 Examples

We consider several examples, where explicit calculations are possible. First we study various initial states of the system (3.1) and illustrate their convergence properties. Then we introduce a classical example of a mono-molecular process and study both transient and steady state behaviour.

3.4.1 Initial states

Here we check the assumptions from Remark 3.3 in terms of the initial state of the particle system. Conditions (3.47)-(3.49) take the form (cf. (3.36), (3.37))

$$\varphi^{(N)}(0)=\varphi_0(0)+\frac{1}{N}\,\varphi_1(0)+\frac{1}{N^2}\,\varphi_2(0)+\ldots, \tag{3.53}$$

$$\lim_{N\to\infty} f_N(0,v) = \frac{\partial}{\partial u_v}\,\varphi_0(0,u_1,\ldots,u_L)\bigg|_{u=1} \tag{3.54}$$

and

$$\lim_{N\to\infty} \gamma_N(0,w,v) = \frac{\partial^2}{\partial u_w\,\partial u_v}\,\varphi_0(0,u_1,\ldots,u_L)\bigg|_{u=1}. \tag{3.55}$$

Recall (cf. (3.25), (3.26))

$$\Phi^{(N)}(0,u_1,\ldots,u_L) \;=\; \mathbb{E}\,u_{x_1(0)}\ldots u_{x_N(0)} \tag{3.56}$$

and (cf. (3.32))

$$\varphi^{(N)}(0,u_1,\ldots,u_L) = \frac{1}{N}\log\Phi^{(N)}(0,u_1,\ldots,u_L)\,. \tag{3.57}$$

Example 3.4 *Consider* **independent** *initial particles, with* **identical** *distribution*

$$\mathbb{P}(x_1(0)=l) = p_l\,, \qquad l=1,\ldots,L\,. \tag{3.58}$$

One obtains

$$\Phi^{(N)}(0,u_1,\ldots,u_L) = \left(\mathbb{E}\,u_{x_1(0)}\right)^N = \left(\sum_{l=1}^{L} u_l\,p_l\right)^N = \exp\left(N\log\sum_{l=1}^{L} u_l\,p_l\right)$$

and

$$\varphi^{(N)}(0,u_1,\ldots,u_L) = \log\sum_{l=1}^{L} u_l\,p_l \tag{3.59}$$

so that

$$f_N(0,v) \;=\; \frac{\partial}{\partial u_v}\,\varphi^{(N)}(0,u_1,\ldots,u_L)\bigg|_{u=1} = \frac{p_v}{\sum_{l=1}^{L} u_l\,p_l}\bigg|_{u=1} = p_v \tag{3.60}$$

and

$$\gamma_N(0,w,v) = \frac{\partial^2}{\partial u_w\,\partial u_v}\,\varphi^{(N)}(0,u_1,\ldots,u_L)\bigg|_{u=1} = -\frac{p_v\,p_w}{\left(\sum_{l=1}^{L} u_l\,p_l\right)^2}\bigg|_{u=1} = -p_v\,p_w\,. \tag{3.61}$$

It follows from (3.59)-(3.61) that conditions (3.53)-(3.55) are fulfilled.

Example 3.5 *Consider* **deterministic** *initial particles,* $n_l(0)$ *of them located in state* l*, where*

$$\lim_{N\to\infty}\frac{n_l(0)}{N} = f(0,l)\,, \qquad l=1,\ldots,L\,. \tag{3.62}$$

One obtains (cf. (3.56))

$$\Phi^{(N)}(0,u_1,\ldots,u_L) = u_1^{n_1(0)} \ldots u_L^{n_L(0)}$$

and (cf. (3.57))

$$\varphi^{(N)}(0,u_1,\ldots,u_L) = \frac{1}{N}\sum_{l=1}^{L} n_l(0)\log u_l \tag{3.63}$$

so that

$$f_N(0,v) \;=\; \frac{\partial}{\partial u_v}\,\varphi^{(N)}(0,u_1,\ldots,u_L)\Big|_{u=1} = \frac{n_v(0)}{N}$$

and

$$\gamma_N(0,w,v) = \frac{\partial^2}{\partial u_w\,\partial u_v}\,\varphi^{(N)}(0,u_1,\ldots,u_L)\Big|_{u=1} = -\delta_{w,v}\,\frac{n_v(0)}{N}\,. \tag{3.64}$$

It follows from (3.62) and (3.63) that

$$\lim_{N\to\infty}\varphi^{(N)}(0,u_1,\ldots,u_L) = \sum_{l=1}^{L} f(0,l)\log u_l =: \varphi_0(0,u_1,\ldots,u_L)\,. \tag{3.65}$$

However, the series representation (3.53) does not hold. Indeed, it would imply

$$\varphi_1(0) = \lim_{N\to\infty} N\Big[\varphi^{(N)}(0) - \varphi_0(0)\Big] = \lim_{N\to\infty}\sum_{l=1}^{L}\Big[n_l(0) - N\,f(0,l)\Big]\log u_l\,. \tag{3.66}$$

Consider $L=2$ *and* $n_1(0) = \mathrm{Int}[N/2]$ *(integer part) so that* $f(0,1) = f(0,2) = \frac{1}{2}$. *Then*

$$n_1(0) - N\,f(0,1) \;=\; \begin{cases} 0 \;, & \textit{if } N \textit{ is even}\,,\\ -0.5\,, & \textit{otherwise}\end{cases}$$

so that (3.66) does not exist. Conditions (3.54), (3.55) are fulfilled with φ_0 *defined in (3.65).*

Example 3.6 *Consider* **identical** *initial particles, with distribution (3.58). This means that initially all particles are in the same state, which is random. One obtains (cf. (3.56))*

$$\Phi^{(N)}(0,u_1,\ldots,u_L) = \mathbb{E}\left(u_{x_1(0)}\right)^N = \sum_{l=1}^{L} u_l^N\,p_l$$

and (cf. (3.57))

$$\varphi^{(N)}(0,u_1,\ldots,u_L) = \frac{1}{N}\log\sum_{l=1}^{L} u_l^N\,p_l\,, \tag{3.67}$$

which implies

$$\frac{\partial}{\partial u_v}\,\varphi^{(N)}(0,u_1,\ldots,u_L)=\frac{u_v^{N-1}\,p_v}{\sum_{l=1}^{L}u_l^N\,p_l}$$

and

$$\frac{\partial^2}{\partial u_w\,\partial u_v}\,\varphi^{(N)}(0,u_1,\ldots,u_L)= \\ \frac{\delta_{v,w}\,(N-1)\,u_v^{N-2}\,p_v\sum_{l=1}^{L}u_l^N\,p_l-u_v^{N-1}\,p_v\,N\,u_w^{N-1}\,p_w}{\left(\sum_{l=1}^{L}u_l^N\,p_l\right)^2}$$

so that

$$f_N(0,v)=\frac{\partial}{\partial u_v}\,\varphi^{(N)}(0,u_1,\ldots,u_L)\bigg|_{u=1}=p_v$$

and

$$\gamma_N(0,w,v)=\frac{\partial^2}{\partial u_w\,\partial u_v}\,\varphi^{(N)}(0,u_1,\ldots,u_L)\bigg|_{u=1}=\delta_{v,w}\,(N-1)\,p_v-p_v\,N\,p_w\,. \qquad (3.68)$$

It follows from (3.67) that (weighted l_q-norm)

$$\begin{aligned}\lim_{N\to\infty}\varphi^{(N)}(0,u_1,\ldots,u_L) &= \lim_{N\to\infty}\log\left(\sum_{l=1}^{L}u_l^N\,p_l\right)^{\frac{1}{N}} \\ &= \log\left(\max_{l=1,\ldots,L}u_l\right)=:\varphi_0(0,u_1,\ldots,u_L)\,. \qquad (3.69)\end{aligned}$$

However, the series representation (3.53) does not hold. Indeed, consider $L=2$, $p_1=p_2=\frac{1}{2}$, $u_1=1$, $u_2=\frac{1}{2}$ so that

$$\varphi^{(N)}(0,u_1,u_2)=\frac{1}{N}\log\left(\frac{1}{2}\left[1+\frac{1}{2^N}\right]\right)=\frac{1}{N}\left[\log\frac{1}{2}+\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k!}\left(\frac{1}{2^N}\right)^k\right]$$

and $\varphi_0(0,u_1,u_2)=0$. Condition (3.53) would imply

$$\varphi_1(0)=\lim_{N\to\infty}N\Big[\varphi^{(N)}(0)-\varphi_0(0)\Big]=\log\frac{1}{2}$$

and

$$\begin{aligned}\varphi_k(0) &= \lim_{N\to\infty}N^k\left[\varphi^{(N)}(0)-\frac{1}{N}\,\varphi_1(0)\right]=\lim_{N\to\infty}N^{k-1}\log\left(1+\frac{1}{2^N}\right) \\ &= 0 \qquad \forall k\geq 2\,.\end{aligned}$$

As to conditions (3.54), (3.55), we note that expression (3.68) does not converge, except in the deterministic case $p_1=1$. The function φ_0 defined in (3.69) does not have a continuous first derivative so that the second derivative does not exist.

3.4.2 Ehrenfest model

The Ehrenfest model [9] is a special mono-molecular process. There are two states 1 and 2 indicating the number of the box, where the particle is located. Particles are chosen at random and then moved into the other box.

mean values

Equation (3.11) takes the form

$$\begin{aligned} \frac{d}{dt} f_N(t,1) &= -a\, f_N(t,1) + b\, f_N(t,2) \\ \frac{d}{dt} f_N(t,2) &= a\, f_N(t,1) - b\, f_N(t,2)\,, \end{aligned}$$

where $a = \lambda_1(1)$ and $b = \lambda_1(2)$. The transposed matrix

$$\alpha_1' = \begin{pmatrix} -a & b \\ a & -b \end{pmatrix}$$

satisfies

$$(\alpha_1')^k = [-(a+b)]^{k-1}\, \alpha_1', \qquad k \geq 1\,,$$

so that

$$\begin{aligned} \exp(t\,\alpha_1') &= \sum_{k=0}^{\infty} \frac{(t\,\alpha_1')^k}{k!} = I + \alpha_1' \sum_{k=1}^{\infty} \frac{[-(a+b)]^{k-1} t^k}{k!} = I - \frac{1}{a+b}\, \alpha_1' \sum_{k=1}^{\infty} \frac{[-(a+b)\,t]^k}{k!} \\ &= I - \frac{\exp(-(a+b)\,t) - 1}{a+b}\, \alpha_1'\,. \end{aligned} \tag{3.70}$$

Thus, the solution (3.13) takes the form

$$f_N(t) = f_N(0) - \frac{\exp(-(a+b)\,t) - 1}{a+b}\, \alpha_1'\, f_N(0)\,. \tag{3.71}$$

It follows from (3.71) that

$$f_N(\infty) = \left(I + \frac{1}{a+b}\, \alpha_1' \right) f_N(0)$$

so that

$$f_N(\infty,1) = \frac{b}{a+b} \qquad \text{and} \qquad f_N(\infty,2) = \frac{a}{a+b}\,.$$

fluctuations

Consider the standard case $a = b = 1$. Since γ_N is symmetric, equation (3.12) reduces to the system

$$\begin{aligned}
\frac{d}{dt}\gamma_N(t,1,1) &= 2\,\gamma_N(t,1,1)\,\alpha_1(1,1) + 2\,\gamma_N(t,1,2)\,\alpha_1(2,1) \\
&= -2\,\gamma_N(t,1,1) + 2\,\gamma_N(t,1,2) \\
\frac{d}{dt}\gamma_N(t,1,2) &= \gamma_N(t,2,1)\,\alpha_1(1,1) + \gamma_N(t,2,2)\,\alpha_1(2,1) + \\
&\quad \gamma_N(t,1,1)\,\alpha_1(1,2) + \gamma_N(t,1,2)\,\alpha_1(2,2) \\
&= -2\,\gamma_N(t,1,2) + \gamma_N(t,1,1) + \gamma_N(t,2,2) \qquad (3.72) \\
\frac{d}{dt}\gamma_N(t,2,2) &= 2\,\gamma_N(t,2,1)\,\alpha_1(1,2) + 2\,\gamma_N(t,2,2)\,\alpha_1(2,2) \\
&= -2\,\gamma_N(t,2,2) + 2\,\gamma_N(t,1,2)\,.
\end{aligned}$$

Assume

$$\gamma_N(0) = \begin{pmatrix} c & d \\ d & c \end{pmatrix} \qquad (3.73)$$

so that $\gamma_N(0)$ commutes with α_1. Then a solution of (3.72) is obtained in the form (cf. (3.12), (3.70))

$$\begin{aligned}
\gamma_N(t) &= \exp(2t\,\alpha_1)\,\gamma_N(0) = \left(I + \frac{1}{2}\,\alpha_1\right)\gamma_N(0) - \frac{1}{2}\exp(-4t)\,\alpha_1\,\gamma_N(0) \\
&= \frac{c+d}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \frac{c-d}{2}\exp(-4t)\,\alpha_1\,. \qquad (3.74)
\end{aligned}$$

initial states

In Example 3.4, condition (3.73) holds with $c = d = -\frac{1}{4}$ provided that (cf. (3.58), (3.61))

$$p_1 = p_2 = \frac{1}{2}\,. \qquad (3.75)$$

One obtains (cf. (3.71))

$$f_N(t,1) = f_N(t,2)) = \frac{1}{2} \qquad \forall t \geq 0 \qquad (3.76)$$

and (cf. (3.5), (3.74))

$$g_N(t) = \frac{1}{N}\left(\gamma_N(t) + \frac{1}{2}I\right) = -\frac{1}{4N}\,\alpha_1 \qquad \forall t \geq 0\,. \qquad (3.77)$$

In this case, the system starts already in the steady state.

In Example 3.5, condition (3.73) holds with $c = -\frac{1}{2}$ and $d = 0$ provided that (cf. (3.62), (3.64))

$$n_1(0) = n_2(0)\,.$$

One obtains constant expected values (3.76) and the covariance matrix (cf. (3.5), (3.74))

$$g_N(t) = -\frac{1}{4N}\Big[1 - \exp(-4t)\Big]\,\alpha_1$$

so that (cf. (3.77))

$$g_N(0) = 0 \qquad \text{and} \qquad g_N(\infty) = -\frac{1}{4N}\,\alpha_1\,. \tag{3.78}$$

In this case, the norm of the covariance matrix is monotonically increasing in time.

In Example 3.6, condition (3.73) is satisfied with (cf. (3.68))

$$c = \frac{N}{4} - \frac{1}{2}\,, \qquad d = -\frac{N}{4}$$

provided that (3.75) holds. One obtains constant expected values (3.76) and the covariance matrix (cf. (3.5), (3.74))

$$g_N(t) = -\frac{1}{4N}\Big[1 + (N-1)\,\exp(-4t)\Big]\,\alpha_1$$

so that (cf. (3.77), (3.78))

$$g_N(0) = -\frac{1}{4}\,\alpha_1 \qquad \text{and} \qquad g_N(\infty) = -\frac{1}{4N}\,\alpha_1\,.$$

In this case, the norm of the covariance matrix is monotonically decreasing in time. Moreover, $g_N(t)$ does not converge to zero with $N \to \infty$, for any $t \geq 0$, but $g_N(\infty)$ does. This means that the system is not "chaotic" for any $t > 0$, but its steady state is.

Acknowledgements

It was at the Workshop "Direct Simulation Monte Carlo: The Past 40 Years and the Future" (Politecnico di Milano, June 02-05, 2003), when I first talked to Carlo Cercignani about the old Leontovich paper [13]. At that time I was collecting material for the historical part of the book [16]. I was curious whether Carlo can provide some more details about Kac's attitude to the Leontovich approach. During our conversation Carlo suggested that it might be useful to produce an english translation of the Leontovich paper in order to make access to it easier. I hesitated to take the effort of translating the whole paper [13], since it contains quite a few misprints and making a correct and precise translation would be a hard job. On the other hand, though not all

conclusions are completely rigorous, the paper is very rich of ideas. The main contents of § 4 of [13] was discussed in [16, Section 2.3.3]. A considerable part of the remaining material has been reproduced in Section 3 of the present paper.

Beside his extraordinary scientific excellence and rare productivity, Carlo Cercignani was a man of intelligent and concise humor. Among many of his jokes and funny remarks during talks and conferences I remember one episode related to the topic of this paper. During a panel discussion at the "Third International Congress on Industrial and Applied Mathematics" (Hamburg, July 03-07, 1995) there was a dispute about the direct simulation Monte Carlo method. After an exchange of thoughts about the importance of this numerical tool, Carlo made the concluding remark "I would like the method even if it was called Monte Helmut" (referring to the first name of one particularly active panel member).

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