Continued Fraction Solutions of Discrete Master Equations Not Obeying Detailed Balance II*

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In this paper we continue to extend our previous investigation of continued fraction (CF) solutions for the stationary probability of discrete one-variable master equations which generally do not satisfy detailed balance. We derive explicit expressions, directly in terms of the elementary transition rates, for the continued fraction recursion coefficients. Further, we derive several approximate CF-solutions, i.e., we deduce non-systematic and systematic truncation error estimates. The method is applied to two master equations with two-particle jumps for which we derive the exact probability solution and make a comparison with approximate solutions. The investigation is also extended to the case of master equations with multiple birth and death transitions of maximal order R.

1. Introduction

The method of master equations is a generally accepted concept for the modeling of discrete statistical systems [1–3]. In this paper we confine ourselves to a discussion of the stationary solution of discrete master equations of one-variable processes. These master equations occur in many fields, such as in quantum optics, spin-relaxation, chemical reactions or population dynamics when the statistical system under consideration can be assumed to be spatially uniform. The spatial uniformity can arise, for example, because the system is small (e.g., biophysical systems) so that it cannot exhibit any phase boundaries. Alternatively, it can be imposed by external boundary conditions such as thorough stirring in chemical reactions.

In contrast to a one-dimensional Fokker-Planck system, for which the stationary solution is easily obtained by a simple quadrature, the solutions of discrete (number space) master equations are generally of more complicated structure. This is due to the fact that except for the special case of a simple birth and death process (nearest neighbor transitions only) satisfying automatically detailed balance, the master equations with multiple transitions do in general not obey a detailed balance relation.

In a previous paper [4] we derived for a discrete master equation with one-particle and two-particle jumps a continued fraction representation for the stationary solution $P_s(n), n=0,1,2,\ldots$, which in addition is very appropriate for a computer evaluation. In this paper we continue this investigation in more detail. In Sect. 2 we first briefly review the general results for the two-particle jump master equations obtained in [4]. Using the continued fraction representation for the transition function [4, 5] $\xi_n = P_s(n)/P_s(n-1)$, we derive an equivalent *reduced* difference equation for the stationary probability. This reduced form is of major importance because in many cases it allows for an analytic solution (via the method of Laplace [6]). In Sect. 3 we derive exact explicit expressions, directly in terms of the elementary transition rates, for the continued fraction recursion coefficients as well as for the stationary probability itself, if some type of transition rate (1-, 2-

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particle birth or death rate) vanishes identically. We also demonstrate that solutions corresponding to absorbing states as well as an "explosion to infinity" are naturally contained in the continued fraction formulation. In Sect. 4 we elaborate on the important problem of obtaining approximative solutions, i.e., we deduce truncation error estimates for the continued fraction relations. By use of the Lidstone expansion [7, 8], we further develop a systematic approximation procedure. The results in Sect. 3 and 4 are then applied in Sect. 5 to the study of a population-dynamical model and a nonlinear chemical reaction scheme. Finally, in Section 6 we extend the discussion of a continued fraction representation for the stationary solution to the case of multiple birth and death transitions of maximal order $R>2$. Such master equations occur in models for population dynamics [9] and nonlinear chemical reaction schemes.

2. General Stationary Solution of Two-Particle Jump Master Equations

In this section we review the stationary solution of discrete onevariable master equations

$$\dot{P}(n,t)=\sum_m W(n,m)\,P(m,t)-\sum_m W(m,n)\,P(n,t),$$
$$n=0,1,\ldots \tag{2.1}$$

where the transition probabilities $W(n,m)$ are restricted to two-particle jumps only, i.e.,

$$W(i,j)=0 \text{ for } |i-j|>2 \tag{2.2}$$

In the following we use the notation

$$W(n+1,n)=\lambda_n, \qquad n=0,1,\ldots \tag{2.3a}$$

$$W(n-1,n)=\mu_n, \qquad n=1,2,\ldots \tag{2.3b}$$

$$W(n+2,n)=\nu_n, \qquad n=0,1,\ldots \tag{2.3c}$$

$$W(n-2,n)=\omega_n, \qquad n=2,3,\ldots \tag{2.3d}$$

In [4] we derived for the transition function ξ_n of the stationary solution P_s of (2.1)

$$\xi_n=\frac{P_s(n)}{P_s(n-1)} \tag{2.4}$$

the continued fraction representation

$$\xi_n=\frac{a_{n-1}}{b_n+a_{n-2}(\mu_n+\omega_{n+1}\,\xi_{n+1})} \tag{2.5}$$

with

$$a_{-1}=1, \qquad a_0=[0], \qquad a_1=[1]\,[0]-\mu_1\lambda_0 \tag{2.6a}$$

$$[n]=\lambda_n+\nu_n+\mu_n+\omega_n \tag{2.6b}$$

$$b_1=0, b_2=\omega_2\lambda_0 \tag{2.6c}$$

and $\{a_n\}$, $\{b_n\}$ satisfying the coupled recursion relation [4]

$$a_n=[n]\,a_{n-1}-\omega_n\nu_{n-2}\frac{a_{n-1}a_{n-3}}{a_{n-2}}$$
$$-(b_n+\mu_n a_{n-2})\left(\nu_{n-2}\frac{b_{n-1}+\mu_{n-1}a_{n-3}}{a_{n-2}}+\lambda_{n-1}\right) \tag{2.7a}$$

$$b_n=\omega_n(\nu_{n-3}[b_{n-2}+\mu_{n-2}a_{n-4}]+\lambda_{n-2}a_{n-3}). \tag{2.7b}$$

By use of the definition of the transition function ξ_n the continued fraction in (2.5) ultimately yields a *reduced* difference equation for the stationary probability

$$a_{n-2}\,\omega_{n+1}P_s(n+1)+(b_n+a_{n-2}\mu_n)P_s(n)$$
$$-a_{n-1}P_s(n-1)=0 \qquad n=1,2,\ldots. \tag{2.8}$$

Compared with the difference equation given by the master equation (2.1), the difference equation in (2.8) is reduced from order 4 in (2.1) to one of order 2! However, despite the fact that (2.8) is of the form of a difference equation for a simple birth and death process (nearest neighbor transitions) the solution for (2.1) does not generally obey detailed balance. In other words, the coefficients in (2.8) are not transition probabilities corresponding to a stochastic matrix structure and consequently (2.8) should not be looked upon as a master equation.

In terms of the transition function ξ_n the stationary solution of (2.1) is written as

$$P_s(n)=P_s(0)\prod_{i=1}^{n}\xi_i \tag{2.9}$$

with $P_s(0)$ determined by the normalization. The product solution in (2.9) can be recast in the form of a continued fraction [4]

$$P_s(n)=P_s(0)\frac{a_0\ldots a_{n-1}}{d_n+d_{n-1}a_{n-2}\,\omega_{n+1}\,\xi_{n+1}} \tag{2.10}$$

with $\{d_n\}$ satisfying the recursion relation

$$d_n=(b_n+a_{n-2}\mu_n)d_{n-1}+\omega_n a_{n-1}a_{n-3}d_{n-2}. \tag{2.11}$$

and

$$d_0=1, \qquad d_1=\mu_1. \tag{2.12}$$

3. Exact Solutions for Special Cases

In this section we study the simplifications which arise from the exact solutions of the recursion relations of the continued fraction expressions and of the stationary probability (2.10) if some of the transition rates vanish identically.

a) Transition Rates $v_n \equiv 0$

For the special case where all the two-particle jump birth rates v_n vanish, the recursion relation for a_n (2.7a) simplifies considerably, giving

$$a_n = (\lambda_n + \mu_n + \omega_n) a_{n-1} - \lambda_{n-1} \lambda_{n-2} \omega_n a_{n-3} - \mu_n \lambda_{n-1} a_{n-2} \tag{3.1}$$

with b_n given by

$$b_n = \omega_n \lambda_{n-2} a_{n-3}. \tag{3.2}$$

By virtue of $a_{-1}=1$, we easily verify that the solutions of (3.1) and (3.2) are given by

$$a_n = \prod_{i=0}^{n} \lambda_i, \quad n=0,1\ldots \tag{3.3}$$

$$b_n = \omega_n \prod_{i=0}^{n-2} \lambda_i, \quad n=2,3,\ldots. \tag{3.4}$$

As a consequence we obtain from (2.5) for the transition function ξ_n the explicit result

$$\xi_n = \frac{\lambda_{n-1}}{(\omega_n + \mu_n) + \omega_{n+1} \xi_{n+1}} \tag{3.5}$$

as, equivalently, for the reduced difference equation for $P_s(n)$

$$\omega_{n+1} P_s(n+1) + (\omega_n + \mu_n) P_s(n) - \lambda_{n-1} P_s(n-1) = 0$$
$$n=1,2,\ldots. \tag{3.6}$$

This reduced difference equation can be solved advantageously by use of the method of Laplace [6] (see Sect. 5).
By virtue of (3.5), we obtain for the stationary solution (2.10)

$$P_s(n) = P_s(0) \frac{\lambda_0 \ldots \lambda_{n-1}}{c_n + c_{n-1} \omega_{n+1} \xi_{n+1}}, \tag{3.7a}$$

where

$$c_n = (\mu_n + \omega_n) c_{n-1} + c_{n-2} \lambda_{n-1} \omega_n,$$
$$c_0 = 1, \quad c_1 = \mu_1. \tag{3.7b}$$

If $\lambda_n = 0$ we obtain from (3.5) $\xi_{n+1} = 0$ yielding $P_s(i) = 0$ for all $i > n$. In particular, if $\lambda_0 = 0$ the stationary solution is

$$P_s(i) = \delta_{0,i} \tag{3.8}$$

i.e., the state $n=0$ is an absorbing state. Further, if with $v_n \equiv 0$ there are also no two-particle jump death rates present, i.e., $\omega_n \equiv 0, n \geqq 2$, we immediately find from (3.5) the well-known detailed balance result

$$\xi_n = \frac{\lambda_{n-1}}{\mu_n} \tag{3.9a}$$

$$P_s(n) = P_s(0) \prod_{i=1}^{n} \frac{\lambda_{i-1}}{\mu_i}. \tag{3.9b}$$

b) Transition Rates $\omega_n \equiv 0$

In the case of identically vanishing two-particle jump death rates $\omega_n \equiv 0$ the continued fraction coefficient b_n in (2.7b) is zero and the recursion relation for $\{d_n\}$ simplies to

$$d_n = \mu_n a_{n-2} d_{n-1}, \tag{3.10}$$

yielding in virtue of (2.12)

$$d_n = \mu_1 \ldots \mu_n a_0 \ldots a_{n-2}. \tag{3.11}$$

As a consequence, we obtain for the stationary solution $P_s(n)$ the explicit result

$$P_s(n) = P_s(0) \frac{a_{n-1}}{\mu_1 \ldots \mu_n}, \quad n=1,2,\ldots \tag{3.12}$$

and

$$\xi_n = \frac{a_{n-1}}{\mu_n a_{n-2}}. \tag{3.13}$$

The evaluation of the stationary probability is reduced to the calculation of the $(n-1)$-th order continued fraction coefficient a_{n-1} which obeys from (2.7a) the recursion

$$a_n = (\lambda_n + \mu_n + v_n) a_{n-1} - \mu_n \mu_{n-1} v_{n-2} a_{n-3} - \mu_n \lambda_{n-1} a_{n-2}. \tag{3.14}$$

Using the transformation f_n

$$a_n = f_n \prod_{i=1}^{n} \mu_i \tag{3.15}$$

(3.14) can be recast in the form

$$f_n - f_{n-1} = \left(\frac{\lambda_n}{\mu_n} + \frac{v_n}{\mu_n}\right) f_{n-1} - \frac{\lambda_{n-1}}{\mu_{n-1}} f_{n-2} - \frac{v_{n-2}}{\mu_{n-2}} f_{n-3} \tag{3.16}$$

with

$$f_{-3} = f_{-2} = 0, \quad f_{-1} = 1, \quad f_0 = v_0 + \lambda_0. \tag{3.17}$$

Summation of the relation in (3.16) from $n=0$ to $n=i$ equals

$$f_i = (\alpha_i + \beta_i) f_{i-1} + \beta_{i-1} f_{i-2} \tag{3.18}$$

where

$$\alpha_i=\frac{\lambda_i}{\mu_i}, \quad \beta_i=\frac{\nu_i}{\mu_i}. \tag{3.19}$$

The recursion relation in (3.18) written in terms of the coefficients $\{a_n\}$ yields for (3.14) the considerably simplified recursion

$$a_n=(\lambda_n+\nu_n)\,a_{n-1}+\mu_n\,\nu_{n-1}\,a_{n-2} \qquad n=1,\ldots. \tag{3.20}$$

An analytical solution of this recursion relation is advantageously investigated by using the more simple relation in (3.18).

Finally, let us assume that the birth rates μ_i are not all strictly positive. Then for $\mu_i=0, i\in\mathbb{N}$, we have from (3.13) an undefined transition rate ξ_i

$$\xi_i=\frac{P_s(i)}{P_s(i-1)}=\infty \tag{3.21}$$

which indicates that $P_s(i-1)$ equals zero and subsequently

$$P_s(i-2)=P_s(i-1)/\xi_{i-1}=0, \text{etc.}$$

$$P_s(j)=0, \quad j=0,\ldots i-1. \tag{3.22}$$

Clearly, for $\mu_i\equiv 0, i=0,1,\ldots$ the system undergoes an explosion to the infinity state.

c) *No One-Particle Jumps*, $\mu_i\equiv 0, \lambda_i\equiv 0$

Where there are only two-particle jump birth and death transitions present (for example, the stochastic modeling of a two-photon laser [10]), the recursion relation for $\{a_n\}$ can be solved explicitly, yielding

$$a_n=\prod_{i=0}^{n}\nu_i \qquad n=0,1,\ldots \tag{3.23}$$

and recursively

$$b_n=0 \qquad n=1,2,\ldots. \tag{3.24}$$

The transition factor ξ_n reads

$$\xi_n=\frac{\nu_{n-1}}{\omega_{n+1}\,\xi_{n+1}} \tag{3.25}$$

which consequently has the product representation

$$\xi_n=\frac{\nu_{n-1}\,\omega_{n+2}\,\nu_{n+1}\cdots}{\omega_{n+1}\,\nu_n\,\omega_{n+3}\cdots}. \tag{3.26}$$

The continued fraction coefficients $\{d_n\}$ are from (2.12) calculated to be

$$d_{2n+1}=0 \tag{3.27a}$$

$$d_{2n}=\left(\prod_{i=2}^{2n}\omega_i\right)a_0^2\,a_1^2\ldots a_{2n-3}^2\,a_{2n-1}. \tag{3.27b}$$

By virtue of (2.9) and (2.10), we find for the stationary solution $P_s(n)$

$$P_s(2n)=P_s(0)\prod_{i=1}^{n}\frac{\nu_{2i-2}}{\omega_{2i}} \tag{3.28}$$

$$P_s(2n+1)=P_s(1)\prod_{i=1}^{n}\frac{\nu_{2i-1}}{\omega_{2i+1}}. \tag{3.29}$$

These explicit solutions exhibit a detailed balance structure which holds separately for the even sub-lattice $\{n=0,2,4,\ldots\}$ and the odd sub-lattice $\{n=1,3,5,\ldots\}$. First we note that for a finite number N of states, the ratio

$$\xi_1=\frac{P_s(1)}{P_s(0)}=\frac{\nu_0\,\omega_3\ldots\nu_{N-1}}{\omega_2\,\nu_1\ldots\omega_{N+1}\,\xi_{N+1}} \tag{3.30}$$

remains *undefined* because the value of ξ_{N+1} is not defined. This behavior exhibits the fact that for any *finite* stochastic matrix introducing only two-particle jump transitions the even and odd subb-lattices do not couple. This is reflected in a degenerate zero-eigenvalue of the corresponding stochastic matrix. The *infinite many* stationary solutions are characterized by the two parameters occurring in (3.28–3.29) where with one *arbitrary* parameter $0\leqq P_s(i)\leqq 1$, $i=0$ or 1, the remaining parameter is fixed by the normalization.

4. Approximation Methods

Although expressions for the stationary solution described in the previous sections are already in a very appropriate form for a computer evaluation, analytical solutions of the continued fraction solutions generally cannot be obtained (except in special cases). The investigation of approximative solutions is valuable because of the interest in obtaining analytical approximative results as well as because of interest in solutions requiring a minimum of computer time.

A first method of approximatively evaluating the expression for the stationary probability in (2.10) is based on the observation that the transition factor ξ_n varies generally on a slower scale than the probabilities themselves [4, 5, 11]. Assuming ξ_n to be slowly varying we may set in (2.5) $\xi_n\approx\xi_{n+1}$ yielding

$$\xi_n\approx\frac{b_n+a_{n-2}\,\mu_n}{2a_{n-2}\,\omega_{n+1}}\left\{\sqrt{1+\frac{4\omega_{n+1}\,a_{n-1}\,a_{n-2}}{(b_n+a_{n-2}\,\mu_n)^2}}-1\right\}. \tag{4.1}$$

Noting $\xi_n\geqq 0$, we have hereby chosen in (4.1) for the solution of the quadratic equation the $(+)$ sign for the square root expression.

With ξ_n given in (4.1), we obtain from (2.10) the approximative solution

$$P_s(n) \approx P_s(0) \cdot \frac{a_0 \dots a_{n-1}}{d_n + \frac{d_{n-1}}{2}\left[(b_n + a_{n-2}\mu_n)\left\{\sqrt{1 + \frac{4\omega_{n+1} a_{n-1} a_{n-2}}{(b_n + a_{n-2}\mu_n)^2}} - 1\right\}\right]} \tag{4.2}$$

Moreover, the extrema values $\{\bar{n}\}$ of the probability solution are approximately given by setting $\xi_{\bar{n}} = 1$ and solving for $\bar{n}$, i.e., an approximate extrema value $\bar{n}$ obeys

$$a_{\bar{n}-2}\,\omega_{\bar{n}+1} + (b_{\bar{n}} + a_{\bar{n}-2}\,\mu_{\bar{n}}) - a_{\bar{n}-1} = 0. \tag{4.3}$$

Assuming $\bar{n}$ to be an extremal value, we may expand ξ_n around $\bar{n}$

$$\xi_n \approx 1 + \left(\frac{\partial \xi_n}{\partial n}\right)_{\bar{n}} (n - \bar{n}) + \dots \tag{4.4a}$$

such that with (2.9) and by use of the Euler MacLaurin summation formula we have in lowest order the Gaussian approximation of (4.2)

$$P_s(n) \approx P_s(\bar{n}) \exp -\frac{(n-\bar{n})^2}{2\sigma}, \tag{4.4b}$$

where

$$\sigma = -\left[\left.\frac{\partial \xi_n}{\partial n}\right|_{n=\bar{n}}\right]^{-1} \tag{4.5}$$

$$= \frac{2a_{\bar{n}-2}\,\omega_{\bar{n}+1} + a_{\bar{n}-2}\,\mu_{\bar{n}} + b_{\bar{n}}}{\frac{\partial}{\partial n}(a_{n-2}\,\omega_{n+1} + a_{n-2}\,\mu_n + b_n - a_{n-1})|_{n=\bar{n}}}. \tag{4.6}$$

For example, if $v_n \equiv 0$ (Sect. 3a), we obtain the simplified relations

$$2\omega_{\bar{n}} + \mu_{\bar{n}} - \lambda_{\bar{n}} = 0 \tag{4.7}$$

$$\sigma = \frac{3\omega_{\bar{n}} + \mu_{\bar{n}}}{\frac{\partial}{\partial n}(2\omega_n + \mu_n - \lambda_n)|_{n=\bar{n}}} \tag{4.8}$$

and if $\omega_n \equiv 0$ (Sect. 3b)

$$\mu_{\bar{n}} - \lambda_{\bar{n}} - 2v_{\bar{n}} = 0 \tag{4.9}$$

$$\sigma = \frac{\mu_{\bar{n}} + v_{\bar{n}}}{\frac{\partial}{\partial n}(\mu_n - \lambda_n - 2v_n)|_{n=\bar{n}}}. \tag{4.10}$$

This Gaussian approximation is known to give very satisfactory results when the transition rates correspond to a large system size [12, 13].

We further note from Sect. 3 that if either the transition rates $\omega_n \equiv 0$ or $v_n \equiv 0$, the calculation of the transition factor ξ_n is reduced to the evaluation of the explicit expressions in (3.5), (3.13). We may utilize this fact in developing an approximation scheme in terms of a parameter θ; we write (2.5) in terms of the new rates

$$\hat{v}_n = 2\theta v_n, \; 0 \leq \theta \leq 1 \tag{4.11}$$

$$\hat{\omega}_n = 2(1-\theta)\,\omega_n = 2\theta'\,\omega_n \tag{4.12}$$

and denote the resulting continued fraction by $\hat{\xi}_n(\theta, \theta')$. Clearly for $\theta = 0$, i.e., $\hat{v}_n \equiv 0$, $\hat{\omega}_n = 2\omega_n$, we can make use of the results in Sect. 3a and for $\theta = 1$, i.e., $\hat{\omega}_n = 0$, $\hat{v}_n = 2v_n$ of those in Sect. 3b. The solution in (2.5) is obtained by setting $\theta = \theta' = \frac{1}{2}$. Thus, by evaluating $\hat{\xi}_n$ at $\theta = 0$ and $\theta = 1$, we may construct an approximative interpolation solution for $\xi_n = \hat{\xi}_n(\frac{1}{2}, \frac{1}{2})$. By virtue of the Lidstone expansion [7, 8], we can write for the value of the fraction $\hat{\xi}_n(\theta, \theta')$ at an intermediate point θ

$$\hat{\xi}_n(\theta, \theta') = \hat{\xi}_n(1,0)\,\theta + \hat{\xi}_n(0,1)(1-\theta) + \sum_{i=1}^{\infty} \{c_i(\theta)\,\hat{\xi}_n^{(2i)}(1,0) + c_i(1-\theta)\,\hat{\xi}_n^{(2i)}(0,1)\}. \tag{4.13}$$

In (4.13) $\hat{\xi}^{(2i)}(1,0)$ denotes the $2i$-th derivative $\left.\frac{\partial^{2i}}{\partial\theta^{2i}}\hat{\xi}_n\right|_{\theta=1}$ and $\hat{\xi}_n^{(2i)}(0,1)$ the derivative $\left.\frac{\partial^{2i}}{\partial\theta^{2i}}\hat{\xi}_n\right|_{\theta=0}$ and the coefficient c_n is given by

$$c_n(\theta) = \frac{1}{2n!}\left[\frac{d^{2n}}{dx^{2n}}\frac{\sinh\theta x}{\sinh x}\right]\Bigg|_{x=0} \tag{4.14}$$

$$= \frac{2^{2n+1}}{(2n+1)!}\,\Phi_{2n+1}\left(\frac{1+\theta}{2}\right), \; n \geq 1 \tag{4.14b}$$

where Φ_n is the Bernoulli polynomial of order n [14]. For example, we find for $\theta = \frac{1}{2}$

$$c_0(\tfrac{1}{2}) = \tfrac{1}{2} \text{ (Linear interpolation)} \tag{4.15}$$

$$c_1(\tfrac{1}{2}) = -1/16 \tag{4.16}$$

$$c_2(\tfrac{1}{2}) = 5/678. \tag{4.17}$$

In contrast to the Taylor expansion, there occur no odd derivatives in (4.13). This is because, unlike the Taylor series, we evaluate the derivatives of $\hat{\xi}_n(\theta, \theta')$ at the *two* points $\theta = 0$. $\theta' = 0$. In the lowest order (linear interpolation) we obtain the approximation

$$\xi_n \approx \frac{1}{2}\frac{\lambda_{n-1}}{(2\omega_n + \mu_n) + \frac{2\omega_{n+1}\lambda_n}{(2\omega_{n+1} + \mu_{n+1}) + \frac{2\omega_{n+2}\lambda_{n+1}}{\ddots}}} + \frac{1}{2}\frac{\hat{a}_{n-1}}{\mu_n \hat{a}_{n-2}} \tag{4.18}$$

with $\hat{a}_n$ satisfying

$$\hat{a}_{-1}=1, \hat{a}_0=\lambda_0+2\nu_0$$
$$\hat{a}_n=(\lambda_n+2\nu_n)\hat{a}_{n-1}+2\mu_n\nu_{n-1}\hat{a}_{n-2}. \tag{4.19}$$

With (4.1) we may write further

$$\xi_n\approx\frac{1}{2}\frac{\lambda_{n-1}}{2\omega_n+\mu_n+\frac{1}{2}\left(-1+\sqrt{1+\frac{8\lambda_n\omega_{n+1}}{(2\omega_{n+1}+\mu_{n+1})^2}}\right)}+\frac{1}{2}\frac{\hat{a}_{n-1}}{\mu_n\hat{a}_{n-2}}. \tag{4.20}$$

Substitution of (4.18) or (4.20) in (2.10) yields a closed simple approximation solution for $P_s(n)$. In contrast to the approximation in (4.1), the approximative solution in (4.18) can be successively improved by calculating (e.g., by numerical computer evaluation) some of the even derivatives of $\xi_n(\theta, 1-\theta)$ at $\theta=0$ and $\theta=1$. There exist, of course, other possibilities of applying the Lidstone expansion. For example, the Lidstone method has been used to obtain time-dependent solutions of nearest neighbor master equations describing vibrational relaxation and intramolecular decay [15].

5. Applications

As a first example, we investigate a population dynamical model with constant simple birth rates $\lambda_n=\lambda$. $n=0, 1, \ldots$ and simple linear death rates $\mu_n=an, n=1, 2, \ldots$ The transition factor for this nearest neighbor process is from (3.9a) given by

$$\xi_n=\frac{\lambda}{a\cdot n}=\frac{\alpha}{n}, \alpha=\frac{\lambda}{a}. \tag{5.1}$$

The stationary probability is easily evaluated to be a Poissonian

$$P_s(n)=P_s(0)\frac{\alpha^n}{n!} \tag{5.2}$$

$$=\frac{\alpha^n}{n!}e^{-\alpha}. \tag{5.3}$$

The statistical mean value $\langle n\rangle$ is calculated to be

$$\langle n\rangle=\alpha \tag{5.4}$$

and the variance σ is given by

$$\sigma=\alpha. \tag{5.5}$$

We observe that for this example the Gaussian approximation in (4.3) and (4.5) for the mean and variance coincide with the exact values in (5.4) and (5.5).

Next we investigate the process obtained by substituting for the simple death rate a *two-particle* death mechanism with linear transition rates ω_n given by

$$\omega_n=\frac{a}{2}n, \quad n=2, 3, \ldots. \tag{5.6}$$

Clearly the process with $\lambda_n\equiv\lambda$, $\omega_n=\frac{a}{2}n$, $\mu_n\equiv 0$, $\nu_n\equiv 0$ does not satisfy detailed balance. However, it is interesting to investigate whether the Poissonian form is conserved with the linear transition rates in (5.6). By use of (3.5) we find for the stationary transition factor

$$\xi_1=\frac{\lambda}{a\xi_2}=\alpha\xi_2^{-1} \tag{5.7}$$

$$\xi_n=\frac{\beta}{n+(n+1)\xi_{n+1}}, \quad \beta=2\alpha$$
$$=\frac{1}{n}\cdot\frac{n\beta}{n+}\frac{(n+1)\beta}{(n+1)+}\cdots \quad n=2, 3, \ldots. \tag{5.8}$$

Setting

$$\xi_n=\frac{1}{n}\frac{u(n+1)}{u(n)} \tag{5.9}$$

$u(n)$ satisfies the difference equation

$$u(n+2)+n\,u(n+1)-\beta n\,u(n)=0. \tag{5.10}$$

We find the solution to this difference equation by using a method originated by Laplace [6]. With a continuation to complex variables $n\to z$, we set for the unknown function $u(z)$ the transformation

$$u(z)=\int_q^p t^{z-1}f(t)\,dt \tag{5.11}$$

with $\{q, p\}$ being parameters determined below. Inserting (5.11) in (5.10) we obtain with a partial integration

$$\int_q^p t^{z-1}\left[t^2 f(t)-t\,d\frac{(f(t)(t-\beta))}{dt}\right]dt$$
$$=-[t^z f(t)(t-\beta)]_q^p. \tag{5.12}$$

The integration limits $\{q, p\}$ are now fixed by imposing

$$[t^z f(t)(t-\beta)]_q^p=0. \tag{5.13}$$

The integrand on the left-hand side of (5.12) [first order differential equation for $f(t)$] is then integrated to give (up to a multiplication constant $A \equiv 1$)

$$f(t)=\left(\frac{\beta-t}{\beta}\right)^{(\beta-1)} e^t, \quad \beta>0. \tag{5.14}$$

As a consequence we find for the parameters $\{q, p\}$ from (5.13), (5.14)

$$q=0, \quad p=\beta. \tag{5.15}$$

The unique solution in (5.11) for $z \in \mathbb{N}$ is then written in the form

$$u(n)=\int_0^\beta t^{n-1}\left(\frac{\beta-t}{\beta}\right)^{(\beta-1)} e^t\, dt \tag{5.16a}$$

$$=\beta^n \int_0^1 s^{(n-1)}(1-s)^{(\beta-1)} e^{\beta s}\, ds, \quad s=\frac{t}{\beta} \tag{5.16b}$$

$$=\beta^n B(\beta, n)\, M(n, \beta+n, \beta), \quad n=2, \ldots. \tag{5.16c}$$

Hereby, $B(\beta, n) \equiv B(n, \beta)$ denotes Euler's Beta-function

$$B(\beta, n)=\int_0^1 s^{n-1}(1-s)^{(\beta-1)}\, ds=\frac{\Gamma(n)\,\Gamma(\beta)}{\Gamma(n+\beta)} \tag{5.17}$$

where $\Gamma(n)$ is the Gamma function and $M(n, \beta+n, \beta)$ denotes Kummer's confluent hypergeometric function [16]. Insertion of the solution in (5.16c) into (5.10) yields the well-known recursion for the confluent hypergeometric function [16].

The stationary transition function ξ_n is from (5.9) given by

$$\xi_n=\frac{\beta}{\beta+n}\,\frac{M(n+1, \beta+n+1, \beta)}{M(n, \beta+n, \beta)}; \quad n=2, 3, \ldots \tag{5.18}$$

and in virtue of (5.7)

$$\xi_1=\frac{\beta+2}{2}\,\frac{M(2, \beta+2, \beta)}{M(3, \beta+3, \beta)}. \tag{5.19}$$

For the stationary probability (2.9) we obtain in terms of the parameter c

$$c=P_s(0)\frac{\beta}{2}[M(3, \beta+3, \beta)]^{-1} \tag{5.20}$$

$$P_s(n)=c\,\beta^{n-2}\frac{\Gamma(\beta+3)}{\Gamma(\beta+n+1)} M(n+1, \beta+n+1, \beta)$$
$$n=1, 2, \ldots. \tag{5.21}$$

The constant c is being determined by the normalization condition

$$c=\left\{\frac{2}{\beta} M(3, \beta+3, \beta)+\Gamma(\beta+3)\right.$$
$$\left.\cdot \sum_{n=1}^{\infty} \frac{\beta^{n-2}}{\Gamma(\beta+n+1)} M(n+1, \beta+n+1, \beta)\right\}^{-1}. \tag{5.22}$$

The exact solution in (5.21) is *not* of Poissonian form. However, in the Gaussian approximation, we find that the statistical mean value remains unchanged. The approximate variance σ is from (4.8) given by

$$\sigma=\tfrac{3}{2}\alpha \tag{5.23}$$

which is seen to be broadened by a factor 1.5.

In the second example, we consider the nonlinear chemical reaction scheme originated by Nicolis [17] for the variable X

$$A \xrightarrow{k_1} X, \quad 2X \xrightarrow{k_2} A.$$

By use of the combinatorial mass-action kinetics, we obtain the master equation

$$\dot{P}(0)=2k_2 P(2)-k_1 N_A P(0) \tag{5.24a}$$

$$\dot{P}(n)=k_1 N_A P(n-1)+k_2(n+1)(n+2) P(n+2)$$
$$-(k_1 N_A+k_2 n(n-1)) P(n), n=1, 2, \ldots. \tag{5.24b}$$

N_A denotes the number of A-molecules which are held constant. With the notation

$$a=\frac{k_1 N_A}{k_2} \tag{5.25}$$

we recast (5.24) for the stationary solution in the form

$$0=2P_s(2)-aP_s(0) \tag{5.26a}$$

$$0=aP_s(n-1)+(n+1)(n+2)P_s(n+2)$$
$$-(a+n(n-1))P_s(n), n=1, \ldots. \tag{5.26b}$$

The stationary transition factor ξ_n is then from (3.5) given by

$$\xi_n=\frac{a}{n(n-1)+n(n+1)\,\xi_{n+1}} \quad n=1, 2, \ldots. \tag{5.27}$$

In contrast to (5.8) the relation in (5.27) also holds "naturally" for $n=1$. As before in (5.9) we write

$$\xi_n=\frac{1}{n}\cdot\frac{a}{(n-1)+}\,\frac{a}{n+}\cdots \equiv \frac{1}{n}\cdot\frac{u(n+1)}{u(n)} \tag{5.28}$$

where the quantity $u(n)$ obeys the difference equation $(n \to z)$

$$u(z+2)+z\,u(z+1)-a\,u(z)=0, \quad a>0. \tag{5.29}$$

Setting for $u(z)$ the (Laplace)-transformation

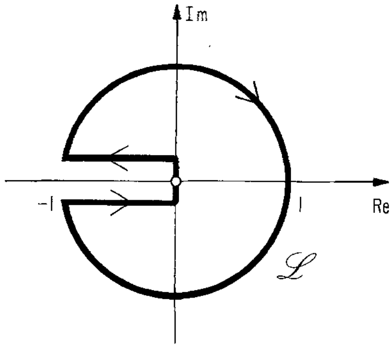

Fig. 1. Path of integration for (5.35)

$$u(z)=\int_q^p t^{z-1} f(t)\,dt \tag{5.30}$$

we obtain

$$\int_q^p t^{z-1}\left[f(t)(t^2-a)-t\frac{d(f(t)t)}{dt}\right]dt=-K(t)\Big|_q^p \tag{5.31}$$

where

$$K(t)=t^{z+1}f(t). \tag{5.32}$$

Setting the integrand on the left-hand side equal to zero and solving for $f(t)$, we find

$$f(t)=\frac{1}{t}\exp\left(t+\frac{a}{t}\right). \tag{5.33}$$

For $t=0$, the factor $\exp\left(t+\frac{a}{t}\right)$ possesses an essential singularity. However, noting that

$$\lim_{t\uparrow 0} K(t)=\lim_{t\uparrow 0} t^z \exp\left(t+\frac{a}{t}\right) \tag{5.34}$$

for t negative and real, we can choose the point $z=0$ as an integration limit. Denoting the integration path by $\mathscr{L}$ (see Fig. 1), we can write for the solution in (5.30)

$$u(z)=\int_{\mathscr{L}} t^{z-2}\exp\left(t+\frac{a}{t}\right)dt. \tag{5.35}$$

By use of the transformation $t=i\sqrt{a}\,s$ and the relation for the generating function of the Bessel function [18]

$$\exp\left\{i\sqrt{a}\left(s-\frac{1}{s}\right)\right\}=\sum_{n=-\infty}^{\infty}\mathfrak{J}_n(2i\sqrt{a})\,s^n \tag{5.36}$$

we obtain for the solution $u(n)$ the result

$$u(n)=(-2\pi)\,i^n a^{\frac{n-1}{2}}\,\mathfrak{J}_{-(n-1)}(2i\sqrt{a}). \tag{5.37}$$

With the relations $\mathfrak{J}_{-n}(z)=(-1)^n\mathfrak{J}_n(z)$ and $I_{-n}(z)=I_n(z)=(i)^{-n}\mathfrak{J}_n(iz)$ with $I_n(z)$ denoting the first modified Bessel function, we recast (5.37) in the form

$$u(n)=-2\pi i\,a^{\frac{n-1}{2}}\,I_{n-1}(2\sqrt{a}). \tag{5.38}$$

The stationary transition factor ξ_n is with (5.28) given by

$$\xi_n=\frac{\sqrt{a}}{n}\,\frac{I_{n-1}(2\sqrt{a})}{I_{n-2}(2\sqrt{a})};\qquad n=1,2,\ldots. \tag{5.39}$$

Setting $a=2X_0^2$ (X_0: deterministic stationary state [17]), the stationary probability $P_s(n)$ reads

$$P_s(n)=P_s(0)\frac{2^{\frac{n}{2}}X_0^n}{n!}\,\frac{I_{n-1}(2\sqrt{2}X_0)}{I_1(2\sqrt{2}X_0)}\qquad n=0,1,\ldots \tag{5.40}$$

where $P_s(0)$ is determined by the normalization

$$\frac{1}{P_s(0)}=\sum_{n=0}^{\infty}\frac{2^{\frac{n}{2}}}{n!}X_0^n\,\frac{I_{n-1}(2\sqrt{2}X_0)}{I_1(2\sqrt{2}X_0)}. \tag{5.41}$$

Noting the relation [19]

$$I_j(4X_0)=2^{\frac{-j}{2}}\sum_{i=0}^{\infty}\frac{2^{\frac{i}{2}}X_0^i}{i!}\,I_{i-j}(2\sqrt{2}X_0) \tag{5.42}$$

the sum in (5.41) can be evaluated explicitly to give

$$P_s(0)=\frac{I_1(2\sqrt{2}X_0)}{\sqrt{2}\,I_1(4X_0)}. \tag{5.43}$$

The normalized stationary probability is consequently given by

$$P_s(n)=2^{\frac{n-1}{2}}\frac{X_0^n}{n!}\,\frac{I_{n-1}(2\sqrt{2}X_0)}{I_1(4X_0)},\qquad n=0,1,2,\ldots. \tag{5.44}$$

The probability in (5.44) is *not* a Poissonian although the transition probabilities in (5.26) obey combinatorial mass-action law kinetics [see also the result for the variance σ in (5.49)].
The factorial moments $\langle n^j\rangle_f$

$$\langle n^j\rangle_f=\langle n(n-1)\ldots(n-j+1)\rangle \tag{5.45}$$

are from (5.42) and (5.44) easily calculated to be

$$\langle n^j\rangle_f=X_0^j\,\frac{I_{j-1}(4X_0)}{I_1(4X_0)}. \tag{5.46}$$

The exact statistical mean value $\langle n\rangle$ is consequently given by

$$\langle n\rangle=X_0\frac{I_0(4X_0)}{I_1(4X_1)}=X_0\left(1+\frac{1}{8X_0}+0(X_0^{-2})\right). \tag{5.47}$$

The result in (5.47) compares with the Gaussian approximation (4.7)

$$\bar{n}=\frac{1+\sqrt{1+2a}}{2}\approx X_0\left(1+\frac{1}{2X_0}+\dots\right). \quad (5.48)$$

The variance σ is exactly given by

$$\sigma=X_0\frac{I_0(4X_0)}{I_1(4X_0)}\left(1-X_0\frac{I_0(4X_0)}{I_1(4X_0)}\right)+X_0^2$$
$$=\tfrac{3}{4}X_0+X_0\left(\frac{1}{16X_0}+O(X_0^{-2})\right) \quad (5.49)$$

which coincides up to order 0(1) with the Gaussian approximation in (4.8). The exact values in (5.48), (5.49) are identical to those calculated by Mazo [20], who used the technique of the generating function. In this context, it is worthwhile emphasizing the following: A numerical or even analytical evaluation of the stationary probability in terms of the continued fraction relations is straightforward in all those cases for which either all or a finite set of transition rates do not obey an analytical relation of the form in (5.6), (5.26). For example, explicit results of the form in (5.18) can be obtained for an arbitrary two-particle death rate $\omega_2>0$. In contrast, the generating function for such a case (non-analytical rates) can almost never be evaluated explicitly and a corresponding numerical evaluation is rather cumbersome.

6. Exact Solutions of One-Variable Master Equations with Many-Particle Jumps

In this section we extend the discussion of exact stationary solutions to the case of many-particle jumps of order j, i.e., to transition probabilities $W(n \pm j, n)$ with $1\leqq j\leqq R$.

a) Simple Death Rates Only

The simple solutions in (3.12), (3.13) with *no* multiple deaths of order $j\geqq 2$ suppose a generalization for the case of multiple births v_n^j

$$v_n^j=W(n+j,n);j=1,2,\dots R. \quad (6.1)$$

With n varying between $0\leqq n<\infty$, the stationary probability $P_s(n)$ obeys the set of equations

$$-[0]\,P_s(0)+\mu_1\,P_s(1) \qquad =0 \quad (6.2\text{a})$$
$$\vdots$$
$$-[1]\,P_s(1)+\mu_2\,P_s(2)+v_0^1\,P_s(0) \qquad =0 \quad (6.2\text{b})$$
$$\vdots$$
$$-[R]\,P_s(R)+\mu_{R+1}\,P_s(R+1)+\sum_{\substack{i=0\\ j=R-i}}^{R-1} v_i^j\,P_s(i)=0 \quad (6.2\text{c})$$
$$\vdots$$
$$+[n]\,P_s(n)+\mu_{n+1}\,P_s(n+1)+\sum_{\substack{i=n-R\\ j=n-i}}^{n-1} v_i^j\,P_s(i) \quad =0,$$
$$n=R,\dots \quad (6.2\text{d})$$

where

$$[0]=\sum_{i=1}^{R} v_0^i\,;\,[n]=\sum_{i=1}^{R} v_n^i+\mu_n, \qquad n=1,2,\dots. \quad (6.3)$$

Solving equations (6.2a), (6.2b) for the stationary transition factor yields explicitly

$$\xi_1=\frac{[0]}{\mu_1}, \quad (6.4)$$

$$\xi_2=\frac{[1]\,[0]-v_0^1\,\mu_1}{\mu_2\,[0]}. \quad (6.5)$$

Observing (3.13) we try the ansatz

$$\xi_n=\frac{a_{n-1}}{\mu_n\,a_{n-2}} \quad (6.6)$$

with the coefficients $\{a_n\}$ satisfying the recursion relation

$$a_n=[n]\,a_{n-1}-v_{n-1}^1\,\mu_n\,a_{n-2}-v_{n-2}^2\,\mu_n\,\mu_{n-1}\,a_{n-3}-\dots$$
$$-v_{n-R}^R\,\mu_n\,\dots\,\mu_{n-R+1}\,a_{n-R+1} \quad (6.7)$$

$$a_{-1}=1,\,a_0=[0],\,a_1=[1]\,[0]-v_0^1\,\mu_1. \quad (6.8)$$

The result in (6.3) is easily proved by induction on n. The generalization of (3.12) to multiple birth rates v_n^i, $i=1,\dots R$ is from (6.6) given by

$$P_s(n)=P_s(0)\frac{a_{n-1}}{\mu_1\dots\mu_n}, \qquad n=1,2,\dots \quad (6.9)$$

with $\{a_n\}$ satisfying the recursion relation (6.7). Within the Gaussian approximation we obtain for the variance σ the result

$$\sigma=\frac{\frac{1}{2}\sum_{i=1}^{R} i(i+1)\,v_{\bar{n}}^i}{\frac{\partial}{\partial n}\left(-\sum_{i=1}^{R} i\,v_n^i+\mu_n\right)\Big|_{\bar{n}}}. \quad (6.10)$$

with $\bar{n}$ satisfying

$$\mu_{\bar{n}}=\sum_{i=1}^{R} i\,v_{\bar{n}}^i=0. \quad (6.10\text{b})$$

The simplicity of the solution in (6.9) is reflected in the structure of the master equation for $P_s(n)$. The relation (6.2) introduces, via a successive solution from $n=0$ up to n, only one further unknown quantity $P_s(n+1)$ characterized by the simple death rate μ_{n+1}. In other words, the explicit consideration of the boundary conditions in (6.2) for $n=0,\dots R$ enables the explicit form in (6.9).

b) Simple Birth Rates Only

Dealing with no multiple birth rates of order $j\geqq 2$, we find in terms of the multiple death transitions μ_n^j

$$\mu_n^j = W(n-j, n); \quad j=1,2,\dots R, n-j \geqq 0 \tag{6.11}$$

for $P_s(n)$ the set of equations

$$0 = -[0]\,P_s(0) + \sum_{\substack{i=1\\ j=i}}^{R} \mu_i^j P_s(i), \tag{6.12a}$$

$$0 = -[1]\,P_s(1) + \sum_{\substack{i=2\\ j=i-1}}^{R+1} \mu_i^j P_s(i) + \lambda_0 P_s(0) \tag{6.12b}$$

$$\vdots \qquad\qquad \vdots$$

$$0 = -[n]\,P_s(n) + \sum_{\substack{i=n+1\\ j=i-n}}^{R+n} \mu_i^j P_s(i) + \lambda_{n-1} P_s(n-1) \tag{6.12c}$$

with

$$[0] = \lambda_0, \ [1] = \lambda_1 + \mu_1^1 \tag{6.12d}$$

$$[n] = \begin{cases} \lambda_n + \sum_{i=1}^{n} \mu_n^i, & 1 \leqq n \leqq R \\ \lambda_n + \sum_{i=1}^{R} \mu_n^i, & n = R, R+1, \dots . \end{cases} \tag{6.12e}$$

As before, we calculate first the transition factors $\xi_n = P_s(n)/P_s(n-1)$ giving

$$\xi_1 = \frac{\lambda_0}{\mu_1^1 + \xi_2[\mu_2^2 + \xi_3[\mu_3^3 + \dots \xi_R \mu_R^R]\dots]}. \tag{6.13}$$

For ξ_2 we obtain by virtue of (6.13)

$$\xi_2 = \frac{\lambda_1}{(\mu_1^2 + \mu_2^2) + \xi_3[\mu_3^2 + \mu_3^3 + \xi_4[\mu_4^3 + \mu_4^4 + \dots + \xi_R[\mu_R^{R-1} + \mu_R^R + \xi_{R+1}\mu_{R+1}^R]\dots]} \tag{6.14}$$

Because of the results in (6.13), (6.14) we suggest for ξ_n the ansatz

$$\xi_n = \frac{\lambda_{n-1}}{\sum_{i=1}^{N_1} \mu_n^i + \xi_{n+1}\left[\sum_{i=2}^{N_2} \mu_{n+1}^i + \xi_{n+2}\left[\sum_{i=3}^{N_3} \mu_{n+2}^i + \dots + \xi_{n+R-1}\mu_{n+R-1}^R\right]\dots\right]} \tag{6.15}$$

where

$$N_j = \begin{cases} n+j-1, & \text{if } n+j-1 \leqq R \\ R, & \text{if } n+j-1 > R. \end{cases} \tag{6.16}$$

The ansatz (6.15), (6.16) is verified by a somewhat cumbersome but straight-forward calculation. In particular, we render for $R=2$ the results in Sect. 3.a and for $R=3$ we have

$$\xi_1 = \frac{\lambda_0}{\mu_1^1 + \xi_2[\mu_2^2 + \xi_3 \mu_3^3]} \tag{6.17}$$

$$\xi_2 = \frac{\lambda_1}{\mu_2^1 + \mu_2^2 + \xi_3[\mu_3^2 + \mu_3^3 + \xi_4 \mu_4^3]} \tag{6.18}$$

$$\xi_n = \frac{\lambda_{n-1}}{\mu_n^1 + \mu_n^2 + \mu_n^3 + \xi_{n+1}[\mu_{n+1}^2 + \mu_{n+1}^3 + \xi_{n+2}\mu_{n+2}^3]}; \quad n = 3, 4, \dots . \tag{6.19}$$

The continued fraction expression in (6.15) is equivalently recast in the form of a reduced difference equation

$$-\lambda_{n-1} P_s(n-1) + \sum_{i=1}^{N_1} \mu_n^i P_s(n) + \dots \sum_{i=j}^{N_j} \mu_{n+j}^i P_s(n+j) + \dots + \mu_{n+R}^R P_s(n+R-1) = 0. \tag{6.20}$$

Moreover, the approximation methods in Sect. 5 can be extended straightforwardly to the case with multiple births or deaths. In particular, we find within the Gaussian approximation for the variance σ from (6.15)

$$\sigma = -\left[\frac{\partial \xi}{\partial n}\bigg|_{\bar{n}}\right]^{-1} = \frac{\frac{1}{2}\sum_{i=1}^{R} i(i+1)\mu_{\bar{n}}^i}{\frac{\partial}{\partial n}\left(\sum_{i=1}^{R} i\mu_n^i - \lambda_n\right)\bigg|_{\bar{n}}} \tag{6.21}$$

with $\bar{n}$ satisfying

$$\lambda_{\bar{n}} - \sum_{i=1}^{R} i\mu_{\bar{n}}^i = 0. \tag{6.22}$$

For example, setting $\lambda_n \equiv \lambda, \mu_n^i = \frac{\mu}{R} n \delta_{i,R}$ we obtain from (6.22)

$$\bar{n} = \frac{\lambda}{\mu}, \tag{6.23}$$

and

$$\sigma = \frac{(R+1)\lambda}{2\mu}. \tag{6.24}$$

Consequently, the stationary probability $P_s(n)$ broadens with increasing multiple death transitions $n \to n-R$, $R = 1, 2, \dots$.

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