A Contracted Path Integral Solution of the Discrete Master Equation

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Abstract

A new representation of the exact time dependent solution of the discrete master equation is derived. This representation can be considered as contraction of the path integral solution of HAKEN. It allows the calculation of the probability distribution of the occurence time for each path and is suitable as basis of new computational solution methods.

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INTRODUCTION

The master equation [1–4] plays a very important role in the description of stochastically behaving systems. In statistical physics it arises in the MARKOFFian limit [5] of the *generalized master equation* [5]. The generalized master equation is obtained as a special representation of the NAKAJIMA-ZWANZIG equation, which results by projection of the VON NEUMANN equation for the *statistical operator* [6] on the relevant variables of the considered system [7,8]. Applications of the master equation reach from nonequilibrium thermodynamics [9–11], over chemistry [9,12] and biology [13] to the social sciences [14–18].

In most cases a concrete master equation is only numerically soluble. For a small number of possible system states computer programs for the solution of a linear system of first order ordinary differential equations can be used. However, in many situations *Monte Carlo simulations* [19] have to be applied, yielding only approximate results. An alternative approach is the *path integral solution* discussed below. It provides an *exact* expression for the *time dependent* solution even of the *generalized* master equation, for which very few solution methods exist up to now. This expression is a suitable starting point for the development of new *computational* solution methods. It also allows the calculation of the probability that a system takes a 'desired' or a 'catastrophic' path, which is very important for technical and other applications.

THE PATH INTEGRAL SOLUTION

Let $p(x,t)$ with $0 \leq p(x,t) \leq 1$ and $\sum_x p(x,t) = 1$ denote the *probability* of the considered system to be in *state* x at time t. Further, for $x' \neq x$ let

$$w(x'|x;t) = \lim_{\Delta t \to 0} \frac{p(x', t + \Delta t | x, t)}{\Delta t} \tag{1}$$

be the *transition rate* (i.e., the *transition probability* $p(x', t + \Delta t | x, t)$ per time unit Δt) from state x to state x'. Then, the *master equation* for the temporal development of the probability distribution of the system reads

$$\frac{dp(x,t)}{dt} = \sum_{x'(\neq x)} \left[w(x|x';t)p(x',t) - w(x'|x;t)p(x,t) \right]. \tag{2}$$

Having the limit $\Delta t \to 0$ in mind, this equation can be written in the form

$$p(x, t+\Delta t) = p(x,t) + \Delta t \sum_{x'(\neq x)} w(x|x';t)p(x',t) - \Delta t \sum_{x'(\neq x)} w(x'|x;t)p(x,t)$$

$$= \sum_{x'} p(x, t+\Delta t|x', t)p(x', t) \tag{3}$$

with

$$p(x, t+\Delta t|x', t) = \delta_{xx'} + \Delta t \sum_{x''(\neq x)} \left[w(x|x'';t)\delta_{x'x''} \right] - \delta_{xx'}\Delta t \sum_{x''(\neq x)} w(x''|x;t), \tag{4}$$

which is also called a *propagator*, and the Kronecker function

$$\delta_{xx'} := \begin{cases} 1 & \text{if } x = x' \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

The solution of the master equation (2) is, therefore,

$$p(x,t) = \lim_{N \to \infty} \sum_{x_{N-1}} \sum_{x_{N-2}} \cdots \sum_{x_0} \left[\prod_{i=1}^{N} p(x_i, t_i | x_{i-1}, t_{i-1}) \right] p(x_0, t_0), \tag{6}$$

where $x_N := x$, $t_i := t_0 + i\Delta t$, and $\Delta t := (t - t_0)/N$. This representation is a consequence of the Chapman-Kolmogorov equation [2], and it is the basis of Haken's approximate path integral solution of the master equation [20].

In the following, we will restrict our considerations to time independent transition rates $w(x'|x;t) \equiv w(x'|x)$ and derive a contracted form of expression (6). In order to achieve this simplification we utilize the fact that the system will normally not change the state x_i over many time periods Δt. That means, within the time interval $\tau := t - t_0$ the system will usually have changed its state x_i a finite number of times only. Let $x_0, x_1, \ldots, x_n$ be the sequence of states the system shows between times t_0 and t. Then,

$$\mathcal{C}_n := x_0 \to x_1 \to \ldots \to x_n \tag{7}$$

with $x_n := x$ shall be called the *path* of the system, and

$$p(\mathcal{C}_n, \tau) \equiv p(x_0 \to \ldots \to x_n, \tau) \tag{8}$$

shall denote the probability that the system takes the path $\mathcal{C}_n$ during the time interval τ. This implies the relation

$$p(x, t) = p(x, t_0 + \tau) = \sum_{n=0}^{\infty} \sum_{\mathcal{C}_n} p(\mathcal{C}_n, \tau)$$

$$\equiv \sum_{n=0}^{\infty} \sum_{x_{n-1}(\neq x_n)} \sum_{x_{n-2}(\neq x_{n-1})} \ldots \sum_{x_0(\neq x_1)} p(x_0 \to \ldots \to x_n, \tau) \,. \tag{9}$$

The representation (9) of the solution of the master equation (2) is the desired contraction of formula (6) and has been suggested by EMPACHER [21]. In order to derive the explicit form of the *path probabilities* $p(\mathcal{C}_n, \tau)$, we will extend an idea of WEIDLICH [22]. For this purpose we rewrite the master equation (2) in vectorial form

$$\frac{d\boldsymbol{p}(t)}{dt} = (W - D)\boldsymbol{p}(t) \tag{10}$$

with

$$\boldsymbol{p}(t) := (p(1, t), \ldots, p(x, t), \ldots)^{\mathrm{tr}} \tag{11}$$

and the matrices

$$W \equiv \left(W_{xx'}\right) := \left(w(x|x')\right),$$
$$D \equiv \left(D_{xx'}\right) := \left(w_x \delta_{xx'}\right), \tag{12}$$

where

$$W_{xx} \equiv w(x|x) := 0 \,,$$
$$w_x := \sum_{x'(\neq x)} w(x'|x) \,. \tag{13}$$

w_x is the total rate of transitions from state x to all other states.

Applying the LAPLACE transformation

$$\tilde{f}(u) := \int_{t_0}^{\infty} dt \, \mathrm{e}^{-u(t-t_0)} f(t) \tag{14}$$

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with a function, vector or matrix f to equation (10) we obtain

$$u\tilde{\boldsymbol{p}}(u) - \boldsymbol{p}(t_0) = (W - D)\tilde{\boldsymbol{p}}(u)\,, \tag{15}$$

that means,

$$\tilde{\boldsymbol{p}}(u) = (uE - W + D)^{-1}\boldsymbol{p}(t_0)\,, \tag{16}$$

where $E \equiv \left(\delta_{xx'}\right)$ is the unity matrix and M^{-1} denotes the inverse of a matrix M. The desired solution of the master equation (10) is, finally, found by inverse LAPLACE transformation

$$f(u) = \frac{1}{2\pi \mathrm{i}} \int\limits_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} du\ \mathrm{e}^{u(t-t_0)}\,\tilde{f}(u) \tag{17}$$

of $\tilde{\boldsymbol{p}}(u)$. It yields

$$\begin{aligned}
\boldsymbol{p}(t) &= \frac{1}{2\pi \mathrm{i}} \int\limits_{-c-\mathrm{i}\infty}^{-c+\mathrm{i}\infty} du\ \mathrm{e}^{-u(t-t_0)}(D - uE - W)^{-1}\boldsymbol{p}(t_0) \\
&= \frac{1}{2\pi \mathrm{i}} \int\limits_{-c-\mathrm{i}\infty}^{-c+\mathrm{i}\infty} du\ \mathrm{e}^{-u(t-t_0)}[E - (D - uE)^{-1}W]^{-1}(D - uE)^{-1}\boldsymbol{p}(t_0)\,.
\end{aligned} \tag{18}$$

The geometric series

$$[E - (D - uE)^{-1}W]^{-1} = \sum_{n=0}^{\infty}[(D - uE)^{-1}W]^n \tag{19}$$

converges, if the constant c is chosen sufficiently large. Taking into account

$$[(D - uE)^{-1}W]_{xx'} = \sum_{x''}(w_x - u)^{-1}\delta_{xx''}w(x''|x') = \frac{w(x|x')}{w_x - u} \tag{20}$$

and (13) we obtain

$$\begin{aligned}
&\sum_{n=0}^{\infty}\sum_{x_0}\{[(D - uE)^{-1}W]^n(D - uE)^{-1}\}_{x_n x_0}p(x_0, t_0) \\
&= \sum_{n=0}^{\infty}\sum_{x_{n-1}(\neq x_n)}\cdots\sum_{x_0(\neq x_1)}\frac{w(\mathcal{C}_n)}{\prod\limits_{j=0}^{n}(w_{x_j} - u)}p(x_0, t_0)
\end{aligned} \tag{21}$$

with

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$$w(\mathcal{C}_n) \equiv w(x_0 \to \ldots \to x_n) := \begin{cases} \delta_{xx_0} & \text{if } n = 0 \\ \prod\limits_{j=1}^{n} w(x_j|x_{j-1}) & \text{if } n \geq 1. \end{cases} \tag{22}$$

Now, evaluating (18) by means of (21) and comparing the result with (9) leads to the explicit expression for the path probabilities $p(\mathcal{C}_n, \tau)$. It reads [16]

$$p(\mathcal{C}_n, \tau) = \frac{1}{2\pi i} \int\limits_{-c-i\infty}^{-c+i\infty} du \, \frac{e^{-u\tau} w(\mathcal{C}_n)}{\prod\limits_{j=0}^{n} (w_{x_j} - u)} p(x_0, t_0) \,. \tag{23}$$

This important result is in accordance with a detailed heuristic derivation of Empacher [21]. By application of the residue theorem integral (23) can easily be evaluated. For example, if all total rates w_x are identical (i.e., $w_x \equiv w$), we get [16]

$$p(\mathcal{C}_n, \tau) = \frac{\tau^n}{n!} e^{-w\tau} w(\mathcal{C}_n) p(x_0, t_0) \,, \tag{24}$$

whereas we obtain

$$p(\mathcal{C}_n, \tau) = \sum_{i=0}^{n} \frac{e^{-w_{x_i}\tau} w(\mathcal{C}_n)}{\prod\limits_{\substack{j=0 \\ (j \neq i)}}^{n} (w_{x_j} - w_{x_i})} p(x_0, t_0) \,, \tag{25}$$

if the total rates w_x are all different from each other. Expressions (24) and (25) are polynomially increasing functions in τ for $\tau \approx 0$ and exponentially decreasing functions for $\tau \to \infty$.

Note that for some cases the 'path integral' (9), (23) can be analytically evaluated [21]. Moreover, a similar relation exists for the *generalized* master equation

$$\frac{d\boldsymbol{p}(t)}{dt} = \int\limits_{t_0}^{t} dt' \, [W(t - t') - D(t - t')]\boldsymbol{p}(t') \tag{26}$$

with

$$W_{xx'}(t - t') := \begin{cases} w(x|x'; t - t') & \text{if } x' \neq x \\ 0 & \text{otherwise,} \end{cases} \tag{27}$$

since a Laplace transformation of (26) leads to [5]

$$u\tilde{\boldsymbol{p}}(u) - \boldsymbol{p}(t_0) = [\tilde{W}(u) - \tilde{D}(u)]\tilde{\boldsymbol{p}}(u) \,. \tag{28}$$

In (22) and (23) one has, therefore, only to replace $w(x'|x)$ by $\tilde{w}(x'|x; u)$ and w_x by $\tilde{w}_x(u) :=$ $\sum_{x'(\neq x)} \tilde{w}(x'|x; u)$.

PATH OCCURENCE TIMES AND COMPUTATIONAL METHODS

In numerical evaluations of formula (9), one can, of course, not sum up an infinite number of different paths. One will rather restrict the summation to the paths which give the most important contributions. In order to find out which paths are negligible, we will calculate the probability distribution

$$p(\tau|\mathcal{C}_n) := \frac{p(\mathcal{C}_n, \tau)}{p(\mathcal{C}_n)} \tag{29}$$

of the occurence time τ of a path $\mathcal{C}_n$ given that this path is traversed. Here, we have introduced the normalization factor

$$p(\mathcal{C}_n) := \int_0^\infty d\tau \; p(\mathcal{C}_n, \tau) \,. \tag{30}$$

We expect, that $p(\tau|\mathcal{C}_n)$ is maximal for a certain time $\hat{\tau}(\mathcal{C}_n)$. On the one hand, for $\tau \ll \hat{\tau}(\mathcal{C}_n)$ there is not enough time for the n transitions $x_{i-1} \to x_i$ to occur. On the other hand, for $\tau \gg \hat{\tau}(\mathcal{C}_n)$ the likelihood of further transitions

$$x_n \to x_{n+1} \to \ldots \to x_{n+l} \tag{31}$$

with $l \geq 1$ is great. In order to determine the mean $\langle\tau\rangle_{\mathcal{C}_n}$ of the *path occurence time* τ and its variance

$$\theta_{\mathcal{C}_n} := \langle(\tau - \langle\tau\rangle_{\mathcal{C}_n})^2\rangle_{\mathcal{C}_n} = \langle\tau^2\rangle_{\mathcal{C}_n} - (\langle\tau\rangle_{\mathcal{C}_n})^2 \tag{32}$$

we need the quantities

$$\langle\tau^k\rangle_{\mathcal{C}_n} := \int_0^\infty d\tau \; \tau^k p(\tau|\mathcal{C}_n) \,. \tag{33}$$

By means of the residue theorem one obtains [16]

$$
\begin{aligned}
\langle \tau^k \rangle_{\mathcal{C}_n} &= \frac{1}{2\pi i} \int\limits_{-c-i\infty}^{-c+i\infty} du \, \frac{w(\mathcal{C}_n)}{p(\mathcal{C}_n) \prod\limits_{i=0}^{n}(w_{x_i} - u)} p(x_0, t_0) \left(-\frac{d}{du} \right)^k \int\limits_{0}^{\infty} d\tau \, e^{-u\tau} \\
&= \frac{w(\mathcal{C}_n)}{p(\mathcal{C}_n)} \frac{k!}{2\pi i} \int\limits_{-c-i\infty}^{-c+i\infty} du \, \frac{p(x_0, t_0)}{u^{k+1} \prod\limits_{i=0}^{n}(w_{x_i} - u)} \\
&= p(x_0, t_0) \frac{w(\mathcal{C}_n)}{p(\mathcal{C}_n)} \left(\frac{d}{du} \right)^k \prod\limits_{i=0}^{n} \frac{1}{(w_{x_i} - u)} \Bigg|_{u=0} .
\end{aligned}
\tag{34}
$$

From this we can derive

$$
p(\mathcal{C}_n) = p(x_0, t_0) w(\mathcal{C}_n) \prod_{i=0}^{n} \frac{1}{w_{x_i}} , \tag{35}
$$

$$
\langle \tau \rangle_{\mathcal{C}_n} = \sum_{i=0}^{n} \frac{1}{w_{x_i}} , \tag{36}
$$

and

$$
\theta_{\mathcal{C}_n} = \sum_{i=0}^{n} \frac{1}{(w_{x_i})^2} . \tag{37}
$$

In order to get an approximate solution of $p(x, t) = p(x, t_0 + \tau)$, we have only to sum up the path probabilities $p(\mathcal{C}_n, \tau)$ of paths $\mathcal{C}_n$, for which

$$
|\tau - \langle \tau \rangle_{\mathcal{C}_n}| \leq a\sqrt{\theta_{\mathcal{C}_n}} \tag{38}
$$

holds. The parameter a depends on the desired accuracy of the approximation.

In the following the computational solution method shall be explained in more detail. Let us assume to have chosen $a = 3$ for the accuracy parameter. Then, about 99 percent of the distribution function $p(\tau | \mathcal{C}_n)$ are found between $\tau_1 := \langle \tau \rangle_{\mathcal{C}_n} - a\sqrt{\theta_{\mathcal{C}_n}}$ and $\tau_2 := \langle \tau \rangle_{\mathcal{C}_n} + a\sqrt{\theta_{\mathcal{C}_n}}$. This implies that for every given τ the paths $\mathcal{C}_n$ which fulfil condition (38) will reconstruct about 99 percent of the distribution function $p(x, t_0 + \tau)$ defined by (9). Therefore, one possible method of numerically calculating the distribution function $p(x, t_0 + \tau)$ is the following:

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1. For every x set $p(x, t_0 + \tau) := 0$ and calculate w_x from $w(x'|x)$ according to (13).

2. Let $n = 0$ and generate all paths $\mathcal{C}_0 := x_0$ of length $n = 0$. Define the *relevance status* of each path $\mathcal{C}_0$ by setting $s(\mathcal{C}_0) := 1$. Calculate $\langle \tau \rangle_{\mathcal{C}_0} := 1/w_{x_0}$ and $\theta_{\mathcal{C}_0} := 1/(w_{x_0})^2$ for every path $\mathcal{C}_0$. If condition (38) is fulfilled, then add $\exp(-w_{x_0}\tau)p(x_0, t_0)$ to $p(x_0, t_0+\tau)$.

3. Let $n := n + 1$ and generate all paths $\mathcal{C}_n := \mathcal{C}_{n-1} \to x_n$ for which the subpath $\mathcal{C}_n$ is relevant, that means, $s(\mathcal{C}_n) = 1$. Calculate $\langle \tau \rangle_{\mathcal{C}_n} := \langle \tau \rangle_{\mathcal{C}_{n-1}} + 1/w_{x_n}$ and $\theta_{\mathcal{C}_n} := \theta_{\mathcal{C}_{n-1}} + 1/(w_{x_n})^2$ for every generated path $\mathcal{C}_n$.

4. If condition (38) is satisfied, then calculate $p(\mathcal{C}_n, \tau)$ according to (25) (or the corresponding explicit formula of (23)) and add $p(\mathcal{C}_n, \tau)$ to $p(x_n, t_0+\tau)$. If $\tau < \langle \tau \rangle_{\mathcal{C}_n} - a\sqrt{\theta_{\mathcal{C}_n}}$ is fulfilled, then cancel the relevance of $\mathcal{C}_n$ by setting $s(\mathcal{C}_n) := 0$.

5. If there are no relevant paths $\mathcal{C}_n$ with $s(\mathcal{C}_n) = 1$ left, then stop the procedure. Otherwise procede with 3.

More refined, but more complicated algorithms can be developed for computers with little memory.

CONCLUSIONS AND OUTLOOK

We have derived a contracted and explicit path integral solution for the discrete master equation. The result is also applicable to the generalized master equation, and it allows the development of numerical methods of solution.

The advantage of the path integral solution with respect to other solution methods is that one can calculate the probability of a system to take 'desired' paths or 'catastrophic' paths consisting of sequences of *selected* states only. This is of interest for prognoses (e.g., szenario techniques) or the (technical) control of a system's temporal evolution, especially if the probability distribution develops several maxima.

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[22] See Ref. [15], section 7.1.