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Analysis of the Closure Approximation for a Class of Stochastic Differential Equations

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Dedicated to Professor Zhenhuan Teng on the occasion of his 80th birthday

Abstract. Motivated by the numerical study of spin-boson dynamics in quantum open systems, we present a convergence analysis of the closure approximation for a class of stochastic differential equations. We show that the naive Monte Carlo simulation of the system by direct temporal discretization is not feasible through variance analysis and numerical experiments. We also show that the Wiener chaos expansion exhibits very slow convergence and high computational cost. Though efficient and accurate, the rationale of the moment closure approach remains mysterious. We rigorously prove that the low moments in the moment closure approximation of the considered model are of exponential convergence to the exact result. It is further extended to more general nonlinear problems and applied to the original spin-boson model with similar structure.

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Key words: Moment closure, spin-boson dynamics, convergence analysis, banded structure.

1. Introduction

In various fields of applied mathematics, the stochastic ordinary differential equations (SODEs) and stochastic partial differential equations (SPDEs) are known to be an effective tool in modeling complicated systems. Examples include chemical reaction networks [11, 16, 19], stochastic hydrodynamics [7, 9, 18], non-equilibrium statistical mechanics [6, 8, 17], and spin-boson dynamics in quantum dissipative systems [15, 20, 24, 25], etc.. Many features of these systems, such as small scale effects and various uncertainties, can be well-described by suitable stochastic dynamics while deterministic modeling either fails or turns out to be too complex. In these systems,

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the statistical quantities such as the mean, variance and high-order moments are of interest.

The Monte Carlo method with suitable temporal discretization is the most direct and popular method in solving these stochastic dynamical systems, but it may encounter great difficulty such as slow convergence and expensive computational cost. In order to achieve a reliable estimate of the interested statistical quantity, a lot of realizations have to be sampled due to the Monte Carlo half order convergence. This situation could be very severe when the interested random variable has extremely large variance. To overcome these difficulties, some approaches are taken to transform the original system into another deterministic system involving the quantities we are interested in. Some representative works include the polynomial chaos expansion or generalized polynomial chaos expansion (gPC), which utilizes the polynomial spectral representation of the random variables in the probability space [10,13,18,22,23], and different kinds of moment closure approach in diverse research fields, such as the hyperbolic moment method for the Boltzmann equation [4,5], moment closure method in stochastic reaction network [12,14], conditional moment closure method in the turbulent combustion problem [1], and flexible random-deterministic method in solving the spin-boson model [24,25], etc.. These methods are effective for certain systems.

The moment closure methods share a similarity that the transformed system is described by an infinite number of differential equations. Truncation of the system is needed for numerical computations. Though efficient and accurate for many systems, the rationale of the moment closure approach remains mysterious for most problems. This can be exemplified by the following simple SODE

$$\mathrm{d}X_t = \mu X_t \mathrm{d}t + X_t(W_t + iV_t)\mathrm{d}t + X_t(\mathrm{d}W_t - i\mathrm{d}V_t), \quad X_0 = 1, \tag{1.1}$$

where W_t and V_t are independent standard Wiener processes with mean $\mathbb{E}W_t = 0$ and covariance $\mathbb{E}W_tW_s = t \wedge s$. If we define the generalised moments $x_n(t) = \mathbb{E}X_t(W_t + iV_t)^n$ and derive the relation among $x_n(t)$ according to Eq. (1.1), we get an infinite ODE system as

$$\frac{\mathrm{d}x_n(t)}{\mathrm{d}t} = \mu x_n(t) + 2n x_{n-1}(t) + x_{n+1}(t), \quad n \in \mathbb{N}, \tag{1.2}$$

by noting the important relation $(\mathrm{d}W_t \pm i\mathrm{d}V_t)^2 = 0$. We will also call (1.2) the moment equations of (1.1) although $x_n(t)$ are not the usual moments in probability theory. The final closure approximations share similar structures in different fields. To obtain an implementable scheme, we make truncation at $n = N$, and thus x_{N+1} in the last equation is abandoned. Theoretically, understanding the effectiveness of this moment closure approach is not clear. Note that x_{N+1} is *not* a small number in general, therefore we actually neglect at least an $\mathcal{O}(1)$ quantity in the Nth moment (for some cases, this may be even worse since x_{N+1} might be $\mathcal{O}(N)$ or bigger). This $\mathcal{O}(1)$ error will propagate to the lower moments and the overall solution might be polluted eventually. It is obvious that we can not hope to get the convergence of the high moments, but what will happen to the low moments? This situation is similar to the computation of the eigenvalues for an unbounded operator [2], in which we only expect to get the convergence of low-lying eigenvalues. This problem, to the best knowledge of the authors, is seldom answered in the previous literature, although there are some related partial results for the BGK model in kinetic theory [3].

In this paper, we are trying to understand the convergence of the moment closure for a class of stochastic differential equations motivated by the numerical study for the spin-boson dynamics in quantum open systems. We start from studying the convergence of a toy model and then extend it to a more general setting, which includes both linear and nonlinear systems. We show that the final convergence estimate for the lowest moment has the form

$$|e_0(t)| \leq \frac{N^\beta e^{CNt}}{(N!)^d}\|x_{N+1}\|_{L^\infty[0,t]},$$

where $e_0(t)$ is the error of the lowest moment between the exact solution and numerical result by moment closure approximation, N is an integer we choose for truncation and $x_{N+1}(t)$ is determined by N and the exact solution. In the analysis we fully take advantage of the special structure of the moment closure system. This exponential convergence estimate perfectly explains the numerical results we did for different model problems.

The rest of the paper is organized as follows. In Section 2, we present the motivating example and give an introduction to different methods. We will show the infeasibility of the direct Monte Carlo simulation, inefficiency of the Wiener chaos expansion for the considered model, and the good performance of moment closure method. In Section 3, we extend our discussion to a general framework and prove its convergence estimate. In Section 4, we generalize our results from linear to non-linear case. In Section 5, numerical examples are listed to confirm our analysis. Then we apply the obtained theorems to the realistic spin-boson model in chemical physics community in Section 6. Finally we draw the conclusion.

2. Motivating example and comparison of methods

2.1. Stochastic description of spin-boson model

The spin-boson model is a quantum dissipative system of fundamental importance [20, 24, 25]. It is comprised of two parts: a two-state system to be observed and a bath of infinite harmonic oscillators coupled to the two state system. When only the reduced density matrix of the system is interested, the effect of the harmonic oscillator bath can be fully described by the spectral density function and we will arrive at an SDE:

$$\begin{aligned} i\mathrm{d}\rho_s = [H_s + \bar{g}(t) f_s, \rho_s]\mathrm{d}t + \frac{1}{2}[f_s, \rho_s](\mathrm{d}W_1(t) + i\mathrm{d}W_4(t)) \\ + \frac{i}{2}\{f_s, \rho_s\}(\mathrm{d}W_2(t) - i\mathrm{d}W_3(t)), \end{aligned} \tag{2.1}$$

where i is the imaginary unit, ρ_s is the 2×2 density matrix for the spin variable,

$$H_s=-\frac{1}{2}\sigma_x=-\frac{1}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad f_s=\frac{1}{2}\sigma_z=\frac{1}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix},$$

are the Hamiltonian of the system and the matrix for the spin component in the spin-boson interaction energy, respectively. W_j for $j=1,2,3,4$ are independent standard Wiener processes. $[A,B]=AB-BA$ and $\{A,B\}=AB+BA$ are commutator and anti-commutator operator, respectively. We have already set the Planck constant $\hbar$ and other constants as 1 in the above formulation. Here $\bar{g}(t)$ completely captures the influence of the environment and can be called the bath-induced mean field. It can be described by a kernel function $\alpha(t)$ as

$$\begin{aligned}\bar{g}(t)=&\frac{1}{2}\bigg(\int_0^t\alpha(t-s)(\mathrm{d}W_1(s)-i\mathrm{d}W_4(s)-i\mathrm{d}W_2(s)+\mathrm{d}W_3(s))\\&\qquad+\alpha^*(t-s)(\mathrm{d}W_1(s)-i\mathrm{d}W_4(s)+i\mathrm{d}W_2(s)-\mathrm{d}W_3(s))\bigg)\\\equiv&\frac{1}{2}(g_1(t)+h_1(t)),\end{aligned}\tag{2.2}$$

where $\alpha^*(t)$ is the conjugate of $\alpha(t)$.

It turns out that the direct Monte Carlo simulation with temporal discretization is not feasible for this model. The critical issue is that the variance of ρ_s increases very fast as time increases, which will be further analyzed in the next subsection. This property makes the necessary number of realizations in Monte Carlo sampling grows too rapidly in time to afford in practical computations. To overcome this issue, a hierarchical approach is proposed for this system by Shao and his co-workers [24]. Specifically, let us assume that the kernel function α can be written as a sum of exponentials. In the simplest case, there is only one exponential

$$\alpha(t)=\gamma e^{-\Omega t},$$

where γ is real and Ω is assumed to be a complex number with positive real part. The differential equations for the two components of $\bar{g}(t)$ can be derived as

$$\mathrm{d}g_1(t)=-\Omega g_1(t)\mathrm{d}t+\frac{\gamma}{2}(\mathrm{d}W_1(t)-i\mathrm{d}W_4(t)-i\mathrm{d}W_2(t)+\mathrm{d}W_3(t)),\tag{2.3a}$$

$$\mathrm{d}h_1(t)=-\Omega^* h_1(t)\mathrm{d}t+\frac{\gamma}{2}(\mathrm{d}W_1(t)-i\mathrm{d}W_4(t)+i\mathrm{d}W_2(t)-\mathrm{d}W_3(t)).\tag{2.3b}$$

Define auxiliary matrices

$$\rho_{mn}(t)=\mathbb{E}(g_1^m(t)h_1^n(t)\rho_s(t)),\quad m,n\in\mathbb{N}.\tag{2.4}$$

We get the following hierarchical equations by using Itô's formula and Eqs. (2.3a)-(2.3b)

$$\begin{aligned}\frac{\mathrm{d}\rho_{mn}}{\mathrm{d}t} =& - i[H_s, \rho_{mn}] - i[f_s, \rho_{m+1,n} + \rho_{m,n+1}] \\ &+ i\gamma(n\rho_{m,n-1}f_s - mf_s\rho_{m-1,n}) - (m\Omega + n\Omega^*)\rho_{mn}. \end{aligned} \tag{2.5}$$

These equations are not closed without further treatment as long as a finite number of terms are concerned. To numerically solve it, a truncation where all terms ρ_{mn} with $m + n > N$ are set to zero forms a closed set of differential equations. The numerical results show this method is powerful for the considered system [24, 25]. After considering suitably simplified model at first, we will give rationales and theorems why this closure approximation is effective in Section 6.

2.2. A toy model

To better understand the hierarchical approach, let us take a look at a toy model at first. Let X_t be an one dimensional stochastic process described by the following stochastic differential equation

$$\mathrm{d}X_t = \mu X_t \mathrm{d}t + X_t W_t \mathrm{d}t + X_t \mathrm{d}W_t, \quad X_0 = 1, \tag{2.6}$$

where W_t is a standard Wiener process and μ is a real constant. This equation can be essentially understood as a simplified scalar variant of Eq. (2.1) with $\alpha(t) = 1$. We are interested in the mean value of X_t. Of course this SDE is quite easy and can be solved analytically:

$$X_t = \exp\left(\left(\mu - \frac{1}{2}\right)t + \int_0^t W_s \mathrm{d}s + W_t\right). \tag{2.7}$$

A direct calculation gives the mean and variance of X_t:

$$\begin{aligned}\mathbb{E}X_t &= \exp\left(\mu t + \frac{t^3}{6} + \frac{t^2}{2}\right), \\ \mathrm{Var}(X_t) &= \exp\left(\left(\mu + \frac{3}{2}\right)t + \frac{2t^3}{3} + 2t^2\right). \end{aligned}$$

2.3. Difficulty of the Monte Carlo method

Although the toy model can be solved analytically, we can still get some insight from it. As we know the convergence order of the Monte Carlo method is $\mathcal{O}(N^{-\frac{1}{2}})$ where N is the sampling size. Therefore if we expect the relative error obtained by Monte Carlo simulation is less than one percent, we should ask

$$N^{-\frac{1}{2}} \frac{\sigma(X_t)}{\mathbb{E}X_t} \leq 0.01,$$

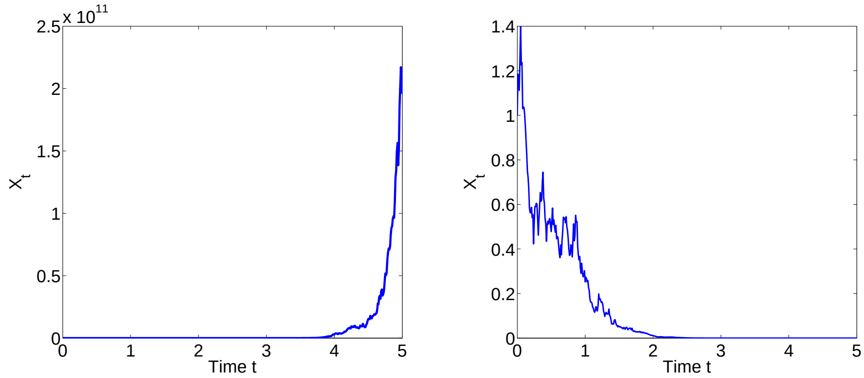


Figure 1: Two sample paths of toy model drawn from stochastic simulation. Euler-Maruyama method is used to solve this stochastic differential equation with fixed time step size $\Delta t = 1e - 5$. These two paths vary great in magnitudes, which brings severe numerical roundoff error in averaging.

where $\sigma(X_t) = \sqrt{\text{Var}(X_t)}$ is the standard deviation of X_t. This requires

$$N \approx \text{Var}(X_t)/(0.01\mathbb{E}X_t)^2.$$

Take $\mu = 1$ and $t = 2$ for example, this number would be about 2.14×10^7. When the time increases, this number grows exponentially. The huge number of paths makes the direct Monte Carlo method impractical.

Another issue by direct Monte Carlo simulation associated with the near divergence behavior of the variance is the numerical roundoff error. In taking the average among different sampling trajectories we will encounter the sum of numbers with very different magnitudes. This is explicitly shown in Fig. 1 for two typical trajectories. The range in which the paths vary is so wide that the numerical roundoff error will completely deteriorate the results.

2.4. Moment closure method

Using the idea in the hierarchical approach, we define $x_n(t) = \mathbb{E}(X_t W_t^n)$. Applying Itô's formula to $X_t W_t^n$ $(n \geq 2)$ gives

$$\begin{aligned} \mathrm{d}X_t W_t^n =& X_t \mathrm{d}W_t^n + W_t^n \mathrm{d}X_t + \mathrm{d}X_t \mathrm{d}W_t^n \\ =& nX_t W_t^{n-1}\mathrm{d}W_t + \frac{1}{2}n(n-1)X_t W_t^{n-2}\mathrm{d}t + \mu X_t W_t^n \mathrm{d}t \\ &+ X_t W_t^{n+1}\mathrm{d}t + X_t W_t^n \mathrm{d}W_t + nX_t W_t^{n-1}\mathrm{d}t. \end{aligned} \tag{2.8}$$

Writing this equation into an integral form and taking expectation we get

$$\begin{aligned} \mathbb{E}X_t W_t^n =& \mathbb{E}\Big(X_0 W_0^t + n\int_0^t X_s W_s^{n-1}\mathrm{d}s + \frac{1}{2}n(n-1)\int_0^t X_s W_s^{n-2}\mathrm{d}s \\ &+ \mu\int_0^t X_s W_s^n \mathrm{d}s + \int_0^t X_s W_s^{n+1}\mathrm{d}s\Big). \end{aligned} \tag{2.9}$$

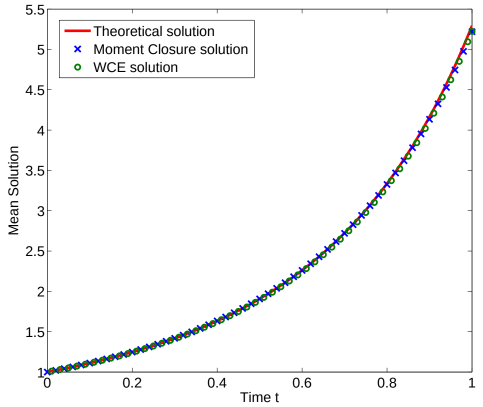


Figure 2: Efficiency comparison of Moment Closure method and WCE method for toy model. Red line is the theoretical solution, blue $\times$ is the solution of moment closure method and green $\circ$ is the solution of WCE method. The computation cost is compared under similar accuracy. Moment closure method takes only 1.64 seconds to achieve 1.4% relative error of $X(1)$ while WCE method takes 24,461 seconds (about 6.8 hours) to achieve 1.3% relative error. The ODE solver is Runge-Kutta 4-th order with time step size 10^{-5}. For the WCE truncation, we choose $N = K = 8$. For the moment closure truncation we choose $N = 3$.

With the notation $x_n(t) = \mathbb{E}X_t W_t^n$ we have

$$\frac{\mathrm{d}x_n(t)}{\mathrm{d}t} = nx_{n-1}(t) + \frac{1}{2}n(n-1)x_{n-2}(t) + \mu x_n(t) + x_{n+1}(t), \tag{2.10a}$$

$$x_n(0) = 0, \qquad n \geq 2. \tag{2.10b}$$

For $n = 0$ and $n = 1$, an easy calculation gives

$$\frac{\mathrm{d}x_0(t)}{\mathrm{d}t} = \mu x_0(t) + x_1(t), \tag{2.11a}$$

$$\frac{\mathrm{d}x_1(t)}{\mathrm{d}t} = x_0(t) + \mu x_1(t) + x_2(t). \tag{2.11b}$$

Define $x_{-2}(t) = x_{-1}(t) = 0$, we have that Eqs. (2.11a) and (2.11b) can be included in Eq. (2.10) with a uniform expression. For the numerical solution, we will choose a suitably large integer N and set the terms $x_n(t)$ to be zero for $n > N$. The numerical result is shown in Fig. 2, which demonstrates the effectiveness of the moment closure approach.

2.5. Inefficiency of the Wiener chaos expansion

The Wiener chaos expansion (WCE) has been utilized in solving SPDEs in stochastic hydrodynamics [13, 18]. The basic idea is to represent the Wiener functional X_t through Hermite polynomial spectral expansions, which is a general method to solve the SDEs driven by Wiener processes.

For any orthonormal basis $\{m_j(s),\ j=1,2,\cdots\}$ in $L^2([0,T])$, define

$$\xi_j=\int_0^T m_j(s)\mathrm{d}W_s,\quad j=1,2,\cdots. \tag{2.12}$$

It is easy to show that ξ_j are independently identically distributed standard Gaussian random variables and

$$W_s=\int_0^T 1_{[0,s]}(\tau)\mathrm{d}W_\tau=\sum_{j=1}^\infty \xi_j\int_0^s m_j(\tau)\mathrm{d}\tau, \tag{2.13}$$

where $1_{[0,s]}(\tau)$ is the characteristic function of interval $[0,s]$. As a result, one can view the solution X_t as a function of time t and the infinite random vector $\boldsymbol{\xi}=(\xi_1,\xi_2,\cdots)$.

Denote the set of multi-indices with finite number of non-zero components as

$$\mathcal{I}=\left\{\boldsymbol{\alpha}=(\alpha_j)_{j\geq 1},\ \alpha_j\in\{0,1,2,\cdots\},\ |\boldsymbol{\alpha}|=\sum_{j=1}^\infty \alpha_j<\infty\right\} \tag{2.14}$$

and define the Wick polynomial

$$T_{\boldsymbol{\alpha}}(\boldsymbol{\xi})=\prod_{j=1}^\infty H_{\alpha_j}(\xi_j),\quad \boldsymbol{\alpha}\in\mathcal{I}, \tag{2.15}$$

where

$$H_n(\xi)=(-1)^n\frac{1}{\sqrt{n!}}e^{\frac{\xi^2}{2}}\frac{\mathrm{d}^n}{\mathrm{d}\xi^n}e^{-\frac{\xi^2}{2}}$$

is the normalized nth order Hermite polynomial. We have that the solution X_s of the SDEs driven by Wiener process has the representation

$$X_s=\sum_{\boldsymbol{\alpha}\in\mathcal{I}} x_{\boldsymbol{\alpha}}(s)T_{\boldsymbol{\alpha}},\quad x_{\boldsymbol{\alpha}}(s)=\mathbb{E}(X_sT_{\boldsymbol{\alpha}}),\quad s\leq T, \tag{2.16}$$

if $\mathbb{E}|X_s|^2<\infty$. The validity of the above assertion is ensured by Cameron-Martin theorem [13]. Furthermore, the first two statistical moments of X_s can be given by

$$\mathbb{E}X_s=x_0(s),\quad \mathbb{E}X_s^2=\sum_{\boldsymbol{\alpha}\in\mathcal{I}}|x_{\boldsymbol{\alpha}}(s)|^2. \tag{2.17}$$

With this idea, we can establish the equations for the WCE coefficients $x_{\boldsymbol{\alpha}}(t)$ for Eq. (2.6) as

$$\frac{\mathrm{d}x_{\boldsymbol{\alpha}}}{\mathrm{d}t}=\mu x_{\boldsymbol{\alpha}}+\sum_{j=1}^\infty\left(\sqrt{\alpha_j+1}x_{\boldsymbol{\alpha}_j^+}+\sqrt{\alpha_j}x_{\boldsymbol{\alpha}_j^-}\right)M_j(t)+\sum_{j=1}^\infty\sqrt{\alpha_j}x_{\boldsymbol{\alpha}_j^-}m_j(t), \tag{2.18}$$

where $\boldsymbol{\alpha}_j^+=(\cdots,\alpha_{j-1},\alpha_j+1,\alpha_{j+1},\cdots)$, $\boldsymbol{\alpha}_j^-=(\cdots,\alpha_{j-1},\alpha_j-1,\alpha_{j+1},\cdots)$, $m_j(t)$ is the orthonormal basis mentioned above and $M_j(t)=\int_0^t m_j(s)\mathrm{d}s$. We remark here that to establish Eq. (2.18) we should take the Wick product between the WCE of X_t and $\mathrm{d}W_t$ since the stochastic integral is assumed in Itô sense.

The numerical implementation requires the truncation in both $\boldsymbol{\xi}$ and $\boldsymbol{\alpha}$. Suppose we want to keep only K Gaussian random variables and Wick polynomials up to Nth order. Define the truncated index set

$$\mathcal{I}_{K,N} = \{\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_K),\ |\boldsymbol{\alpha}| \le N\},$$

then the resulting approximation has $\sum_{n=0}^{K} \binom{K+n-1}{n}$ terms altogether.

Now we compare the efficiency of WCE with the moment closure method. We apply both methods to the toy model (2.6) to get the mean value of X_t at $t=1$. For the truncated ordinary differential equations (ODEs), we use the fourth order Runge-Kutta method to solve with fixed time stepsize $\Delta t = 10^{-5}$. We compare the time cost with the same target accuracy: 1% relative error for $X_{t=1}$. To achieve this goal, we need to set $N=K=8$ in WCE and only $N=3$ in moment closure method. The numerical results are shown in Fig. 2. The relative error by moment closure method and WCE method is 1.4% and 1.3%, respectively. The accuracy of both methods are close to each other while the computational cost is quite different. We only need to solve a 4 dimensional ODEs in moment closure method compared with a 12,870 dimensional ODEs in WCE method. Also the ODEs in moment closure method are much simpler and easier for implementation. The time cost clearly shows the efficiency of moment closure method. The WCE takes about 24,461 seconds (about 6.8 hours) while moment closure method only takes 1.64 seconds.

This difference becomes more apparent when the system involves multiple Wiener processes. To achieve a good accuracy of the spin-boson dynamics (2.1), similar cutoff $(N=K=8)$ is needed for WCE method. However the SDEs (2.1) has 4 Wiener processes which means it will lead to a $12870^4 \ge 10^{16}$ dimensional ODE system. We even do not know whether we would encounter stiffness issue which is common for large ODE systems. The huge computational cost makes that the WCE is not appropriate for this problem.

3. Convergence of moment closure method

3.1. Simple case

Although the toy model (2.6) looks to be easy, detailed analysis is not so simple. To understand the convergence of moment closure method in a more accessible way, we consider the model (1.1) proposed in the introduction.

Though Eq. (1.1) involves two independent Wiener processes, the relation $(\mathrm{d}W_t \pm i\mathrm{d}V_t)^2 = 0$ makes the moment system simpler. Define $x_n(t) = \mathbb{E}X_t(W_t + iV_t)^n$ and take moments we get the system (1.2) by defining $x_{-1}(t) = 0$ for an unified expression. The initial value of the ODE system is $x_0(0) = 1,\ x_n(0) = 0,\ n \ge 1$. Truncate to a finite N

we obtain

$$\frac{\mathrm{d}\boldsymbol{y}(t)}{\mathrm{d}t} = A_N \boldsymbol{y}(t), \qquad A_N = \begin{pmatrix} \mu & 1 & & & & \\ 2 & \mu & 1 & & & \\ & 4 & \mu & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & 1 \\ & & & & 2N & \mu \end{pmatrix} \in \mathbb{R}^{(N+1)\times(N+1)}, \tag{3.1}$$

where $\boldsymbol{y}(t) = (y_0(t), \cdots, y_N(t))^T$. We now show the exponential convergence of the closure system in this simple case.

Theorem 3.1. *The lowest moment $y_0(t)$ in the solution of ODEs* (3.1) *converges to $x_0(t)$ as N goes to infinity, and the error estimate has the form*

$$|x_0(t) - y_0(t)| \leq \frac{e^{(|\mu|+1+2N)t}}{N!2^N} \|x_{N+1}\|_{L^\infty[0,t]}. \tag{3.2}$$

Proof. From now on, we fix N and simplify the notation A_N as A. To see why the moment closure works, let us focus on the difference between the truncated variable $\boldsymbol{y}(t)$ and the original one $\boldsymbol{x}(t) = (x_0(t), \cdots, x_N(t))^T$. Define $\boldsymbol{e}(t) = \boldsymbol{x}(t) - \boldsymbol{y}(t)$ and the ODEs for $\boldsymbol{e}(t)$ is

$$\frac{\mathrm{d}\boldsymbol{e}(t)}{\mathrm{d}t} = A\boldsymbol{e}(t) + \boldsymbol{g}(t), \tag{3.3}$$

where $\boldsymbol{g}(t) = (0, \cdots, 0, x_{N+1})^T$ is determined by the original SDE.

The ODE (3.3) can be solved as

$$\boldsymbol{e}(t) = \int_0^t e^{A(t-s)} \boldsymbol{g}(s) \mathrm{d}s$$

and we are interested in $e_0(t)$. Now we analyze the convergence by sufficiently utilizing the special structure of A. Take $D = \mathrm{diag}\{d_0, \cdots, d_N\}$ where $d_k = k!2^k$. It can be easily shown that the matrix $D^{-1}AD = A^T$. With this observation, we obtain

$$\begin{aligned} |e_0(t)| =& \Big| \Big(\int_0^t e^{A(t-s)} \boldsymbol{g}(s) \mathrm{d}s \Big)_0 \Big| = \Big| \Big(\int_0^t D e^{A^T(t-s)} D^{-1} \boldsymbol{g}(s) \mathrm{d}s \Big)_0 \Big| \\ \leq& \int_0^t d_0 \Big| \Big(e^{A^T(t-s)} \Big)_{0N} \Big| \frac{1}{d_N} |x_{N+1}(s)| \mathrm{d}s \\ \leq& \int_0^t \frac{d_0}{d_N} e^{\|A^T\|_\infty (t-s)} |x_{N+1}(s)| \mathrm{d}s \\ \leq& \int_0^t \frac{e^{\|A^T\|_\infty (t-s)}}{N!2^N} |x_{N+1}(s)| \mathrm{d}s, \end{aligned} \tag{3.4}$$

where $\|A\|_\infty$ is the L^∞-norm of the matrix A. It is obvious that $\|A^T\|_\infty = |\mu| + 1 + 2N$. Thus we get (3.2). ☐

Although the above analysis heavily depends on the tridiagonal structure of the coefficient matrix A, the convergence estimate (3.2) provides us many insights about the moment closure method. The following points are indeed general for more complicated problems to be considered later:

(1). For given t, the convergence is exponential as $N \to \infty$. Taking advantage of Stirling's formula, we have that the leading order behavior of the error estimate is

$$\exp\left(-N\ln N - N\ln 2 + N + 2Nt\right). \tag{3.5}$$

The convergence is exponential as long as the relation $\ln N + \ln 2 > 1 + 2t$ holds and N gets large.

(2). For given N, the convergence deteriorates when the time t increases. This fact is straightforward from Eq. (3.5). Note the deterioration rate may be fast.

(3). The error estimate depends on the growth of truncated terms. In general, if the truncated term x_{N+1} mildly grows, the final convergence is obviously true due to the factorial term in the denominator. However, one can show that the terms like $\mathbb{E}X_tW_t^n$ for Eq. (2.6) or $|\mathbb{E}X_t(W_t+iV_t)^N|$ for Eq. (1.1) indeed grow in a factorial fashion. Thus the rigorous proof for different examples should be checked case by case. In the above example we have

$$\left|\frac{1}{N!}\mathbb{E}X_t(W_t+iV_t)^N\right| \le (\mathbb{E}|X_t|^2)^{\frac{1}{2}}\left(\frac{1}{(N!)^2}\mathbb{E}|W_t+iV_t|^{2N}\right)^{\frac{1}{2}}, \tag{3.6a}$$

$$\mathbb{E}|X_t|^2 \le e^{(2\mathrm{Re}(\mu)+2)t+\frac{2}{3}t^3}\mathbb{E}|X_0|^2, \tag{3.6b}$$

$$\frac{1}{(N!)^2}\mathbb{E}|W_t+iV_t|^{2N} \le \frac{1}{(N!)^2}\sqrt{\frac{\pi}{2}}t^{2N}\mathbb{E}|Y|^{2N+1} \le \frac{1}{(N!)^2}t^{2N}(2N)!! \le \frac{2^Nt^{2N}}{N!}, \tag{3.6c}$$

where Re(μ) is the real part of μ, Y is a standard Gaussian random variable with mean 0 and variance 1, and the proof of (3.6a) is shown in Appendix A. This establishes the estimate on $|x_{N+1}(t)|$ and thus the exponential convergence of the closure approximation. Similar arguments hold at least for most of the later examples.

The above points on the nature of the considered closure approximation will be clearly demonstrated in Section 5 for numerical computations.

Remark 3.1. The estimate (3.2) can be similarly obtained if one takes the diagonal matrix $D = \mathrm{diag}\{d_0,\cdots,d_N\}$ where $d_k = \sqrt{k!}2^{k/2}$. With such choice we get a symmetric tridiagonal matrix $B = D^{-1}AD$ with off-diagonal entries $\sqrt{2k}$. This will result in the error estimate

$$|x_0(t) - y_0(t)| \le \frac{e^{(|\mu|+2\sqrt{2N})t}}{\sqrt{N!}2^{N/2}}\|x_{N+1}\|_{L^\infty[0,t]}. \tag{3.7}$$

Here we see a trade-off between the growth in the exponential function in the nominator and the growth in the factorial term in the denominator. The choice $d_k = \sqrt{k!}2^{k/2}$ gives slower growth speed $\sqrt{N!}$ in the denominator but sharper estimate $\sqrt{N}$ on the eigenvalues (the careful readers may find that the eigen-polynomials of A_N satisfy similar recursive relations for Hermite polynomials [21]). However, the bad growth condition on the remainder term $\|x_{N+1}\|_{L^\infty[0,t]}$ in this example requires $N!$ in the denominator, which is utilized in the theorem. Such trade-off is also clearly demonstrated in the general Theoerem 3.2.

3.2. Main result

Our analysis is not limited to the scalar case. Assume there is an infinite ODE system for variable $\boldsymbol{x}^T = (\boldsymbol{x}_1^T, \boldsymbol{x}_2^T, \cdots)$ as

$$
\begin{aligned}
&\frac{\mathrm{d}\boldsymbol{x}_1}{\mathrm{d}t} = L_{11}\boldsymbol{x}_1 + U_{12}\boldsymbol{x}_2 + \cdots + U_{1p}\boldsymbol{x}_p,\\
&\frac{\mathrm{d}\boldsymbol{x}_2}{\mathrm{d}t} = L_{21}\boldsymbol{x}_1 + L_{22}\boldsymbol{x}_2 + U_{23}\boldsymbol{x}_3 + \cdots + U_{2,p+1}\boldsymbol{x}_{p+1},\\
&\cdots\\
&\frac{\mathrm{d}\boldsymbol{x}_j}{\mathrm{d}t} = L_{j1}\boldsymbol{x}_1 + \cdots + L_{jj}\boldsymbol{x}_j + U_{j,j+1}\boldsymbol{x}_{j+1} + \cdots + U_{j,j+p-1}\boldsymbol{x}_{j+p-1}, \quad \cdots
\end{aligned}
$$

where $\boldsymbol{x}_j \in \mathbb{R}^{m_j}$, $L_{jk} \in \mathbb{R}^{m_j\times m_k}$, $U_{jk} \in \mathbb{R}^{m_j\times m_k}$. To get an approximation to this system, we choose an integer N and only keep the terms whose subscript is not bigger than N. The ODEs after truncation read

$$
\begin{aligned}
&\frac{\mathrm{d}\boldsymbol{y}_1}{\mathrm{d}t} = L_{11}\boldsymbol{y}_1 + U_{12}\boldsymbol{y}_2 + \cdots + U_{1p}\boldsymbol{y}_p,\\
&\frac{\mathrm{d}\boldsymbol{y}_2}{\mathrm{d}t} = L_{21}\boldsymbol{y}_1 + L_{22}\boldsymbol{y}_2 + U_{23}\boldsymbol{y}_3 + \cdots + U_{2,p+1}\boldsymbol{y}_{p+1},\\
&\cdots\\
&\frac{\mathrm{d}\boldsymbol{y}_N}{\mathrm{d}t} = L_{N1}\boldsymbol{y}_1 + \cdots + L_{N,N-1}\boldsymbol{y}_{N-1} + L_{N,N}\boldsymbol{y}_N.
\end{aligned}
$$

It is a linear ODE system which can be written in matrix form

$$
\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = A\boldsymbol{y}, \tag{3.8}
$$

where

$$
A = \begin{pmatrix}
L_{11} & \cdots & U_{1p} & 0 & & \\
L_{21} & \ddots & \ddots & U_{2,p+1} & \ddots & \\
\vdots & \vdots & \ddots & \ddots & \ddots & 0\\
\cdots & \cdots & \cdots & \ddots & \ddots & U_{N-p+1,N}\\
\cdots & \cdots & \cdots & \cdots & \ddots & \vdots\\
\cdots & \cdots & \cdots & \cdots & L_{N-1,N} & L_{N,N}
\end{pmatrix}, \tag{3.9}
$$

and A consists of many sub-matrices. A is a block lower Hessenberg matrix with upper bandwidth p, hereafter matrix in such form is referred to as a p-LH matrix. We need to put some restrictions on these sub-matrices. To simplify the exposition, we first define the notation $\lesssim$ as

Notation 3.1. *We say a matrix $B \lesssim b$ where b is a positive number if $|B_{jk}| \leq Kb$ for some positive $K \sim \mathcal{O}(1)$ and all j, k.*

For each partitioned matrix A as above, we have the decomposition $A = L + U$, where L is its lower triangular part and U is its upper triangular part excluding the diagonals. Furthermore, we decompose L into two parts $L = \hat{L} + \tilde{L}$ where $\hat{L}$ represents the part which has $\mathcal{O}(1)$ entries independent of truncation number N, i.e., $\hat{L}_{jk} \sim \mathcal{O}(1)$, while the entries in the other part $\tilde{L}$ may depend on the truncation number N.

We make the following reasonable assumptions on the partitioned matrix A:

(A1) The non-zero elements in $\tilde{L}$ is located in the sub-matrices $\tilde{L}_{j,j-k}$ for $k = 0 : q$ and $L_{j,j-k} \lesssim j^{\alpha_k}$;

(A2) The non-zero elements in U is located in the sub-matrices $U_{j,j+k}$ for $k = 1 : p-1$ and $U_{j,j+k} \lesssim j^{\beta_k}$;

(A3) The number of the non-zero elements in each row of A is $\mathcal{O}(1)$.

Here we employed the conventional notation $j = n_1 : n_2$ in matrix analysis, which means $j = n_1, n_1+1, \cdots, n_2$ for natural numbers $n_1 \leq n_2$.

Let us illustrate these assumptions through the following concrete example. Take

$$P = \begin{pmatrix} 1^2 & 1^1 & 1^3 & 0 & 0 \\ 2^{1.5}+1 & 2^2 & 2^1 & 2^3 & 0 \\ 1 & 3^{1.5} & 3^2 & 3^1 & 3^3 \\ 1 & 1 & 4^{1.5}+1 & 4^2 & 4^1 \\ 2 & 1 & 1 & 5^{1.5} & 5^2 \end{pmatrix}.$$

We naturally define the matrices

$$U = \begin{pmatrix} 0 & 1^1 & 1^3 & 0 & 0 \\ 0 & 0 & 2^1 & 2^3 & 0 \\ 0 & 0 & 0 & 3^1 & 3^3 \\ 0 & 0 & 0 & 0 & 4^1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \tilde{L} = \begin{pmatrix} 1^2 & 0 & 0 & 0 & 0 \\ 2^{1.5} & 2^2 & 0 & 0 & 0 \\ 0 & 3^{1.5} & 3^2 & 0 & 0 \\ 0 & 0 & 4^{1.5} & 4^2 & 0 \\ 0 & 0 & 0 & 5^{1.5} & 5^2 \end{pmatrix},$$

and $\hat{L} = P - \tilde{L} - U$. The corresponding parameters in Assumptions (A1)-(A3) are $p = 3$, $\beta_1 = 1$, $\beta_2 = 3$ and $q = 1$, $\alpha_0 = 2$, $\alpha_1 = 1.5$.

Now we state the main theorem in this paper.

Theorem 3.2. *For an infinite linear ODEs with a p-LH coefficient matrix, if the Assumptions (A1)-(A3) are satisfied, and there exists a positive real number d such that*

$$d \leq \frac{1-\beta_j}{j}, \qquad j = 1 : p-1, \tag{3.10a}$$

$$d \geq \frac{\alpha_j - 1}{j}, \qquad j = 0 : q, \tag{3.10b}$$

then the lowest moments $\boldsymbol{y}_1$ in the solution of the truncated equations converge to the original lowest moments $\boldsymbol{x}_1$ as N goes to infinity. We have the error estimate

$$\|\boldsymbol{x}_1-\boldsymbol{y}_1\|_\infty \lesssim \frac{N^\beta e^{CNt}}{((N-p+2)!)^d}\max_{j=N+1:N+p-1}\|\boldsymbol{x}_j\|_\infty, \tag{3.11}$$

where $\|\boldsymbol{x}\|_\infty$ is the $L^\infty[0,t]$ norm of $|\boldsymbol{x}(\cdot)|$, C is a positive constant independent of N and t and $\beta=\max_{j=1:p-1}\beta_j$.

Proof. Define the difference between the original variables $\boldsymbol{x}(t)$ and truncated variables $\boldsymbol{y}(t)$ as $\boldsymbol{e}_j(t)=\boldsymbol{x}_j(t)-\boldsymbol{y}_j(t)\in\mathbb{R}^{m_j}$. We have

$$\frac{\mathrm{d}\boldsymbol{e}(t)}{\mathrm{d}t}=A\boldsymbol{e}(t)+\boldsymbol{g}(t),\quad \boldsymbol{e}(0)=0. \tag{3.12}$$

Here $\boldsymbol{g}(t)=(0,\cdots,0,\boldsymbol{g}_{N-p+2}(t),\cdots,\boldsymbol{g}_N(t))$ and $\boldsymbol{g}_j(t)=\sum_{k=1}^{j-N+p-1}U_{j,N+k}\boldsymbol{x}_{N+k}(t)$ is only decided by the original system, thus

$$\|\boldsymbol{g}\|_\infty\lesssim N^\beta\max_{j=N+1:N+p-1}\|\boldsymbol{x}_j\|_\infty.$$

Solving (3.12) we have

$$\boldsymbol{e}(t)=\int_0^t e^{A(t-s)}\boldsymbol{g}(s)\mathrm{d}s. \tag{3.13}$$

Define the block diagonal matrix $D=\mathrm{diag}\{D_1,\cdots,D_N\}$ where $D_j\in\mathbb{R}^{m_j\times m_j}$ are diagonal matrices defined as $D_j=\mathrm{diag}\{(j!)^d,\cdots,(j!)^d\}$. Taking similarity transformation $B=D^{-1}AD$, we get

$$\boldsymbol{e}(t)=\int_0^t De^{B(t-s)}D^{-1}\boldsymbol{g}(s)\mathrm{d}s. \tag{3.14}$$

From condition (3.10a), we have the block upper triangular part of B

$$B_{j,j+k}=D_j^{-1}U_{j,j+k}D_{j+k}\lesssim j^{kd+\beta_k}\le j. \tag{3.15}$$

For the block lower triangular part of B induced by $\tilde{L}$ and $\hat{L}$, we have

$$\begin{aligned}&D_j^{-1}\tilde{L}_{j,j-k}D_{j-k}\lesssim j^{\alpha_k-kd}\le j,\\&D_j^{-1}\hat{L}_{j,j-k}D_{j-k}\lesssim j^{-kd}.\end{aligned}$$

Using Assumption (A3) that the number of non-zero elements in each row is $\mathcal{O}(1)$, we get

$$\|B\|_\infty\lesssim N+\max_{j=1:N}\sum_{k=1}^{j}j^{-kd}\lesssim N.$$

Defining matrix $\hat{B}(s)=e^{B(t-s)}$, we have

$$\|\hat{B}\|_\infty\le e^{\|B\|_\infty(t-s)}\le e^{CN(t-s)}.$$

Simple calculation shows

$$\boldsymbol{e}_1(t)=\int_0^t \frac{\hat{B}(s)_{1,N-p+2}\boldsymbol{g}_{N-p+2}(s)}{((N-p+2)!)^d}+\cdots+\frac{\hat{B}(s)_{1,N}\boldsymbol{g}_N}{(N!)^d}\mathrm{d}s. \tag{3.16}$$

For each term inside the integral we have

$$\left\|\frac{\hat{B}(s)_{1,j}\boldsymbol{g}_j(s)}{(j!)^d}\right\|_\infty \le \frac{\|\hat{B}(s)_{1,j}\|_\infty\|\boldsymbol{g}_j(s)\|_\infty}{(j!)^d}\lesssim \frac{N^\beta e^{CN(t-s)}\max_{j=N+1:N+p-1}\|\boldsymbol{x}_j\|_\infty}{((N-p+2)!)^d}.$$

Substituting this into (3.16) we have

$$\begin{aligned}\|\boldsymbol{e}_1\|_\infty &\lesssim \int_0^t \frac{N^\beta e^{CN(t-s)}\max_{j=N+1:N+p-1}\|\boldsymbol{x}_j(s)\|_\infty}{((N-p+2)!)^d}\mathrm{d}s\\ &\lesssim \frac{N^\beta e^{CNt}}{((N-p+2)!)^d}\max_{j=N+1:N+p-1}\|\boldsymbol{x}_j\|_\infty. \end{aligned}\tag{3.17}$$

The proof is completed. □

From the final estimate and the whole proof procedure we can learn the following important points and make possible extensions.

(1). The observation made in Section 3.1 for the simple case still holds in this general situation. They are natural and will be verified by the numerical results in Section 5.

(2). When t is fixed, the convergence rate is dominated by

$$\begin{aligned}&\frac{N^\beta e^{CNt}}{((N-p+2)!)^d}\\ &\sim\exp\left(-d(N-p+2)\ln(N-p+2)+d(N-p+2)+\beta\ln N+CNt\right)\\ &\sim\exp\left(-dN\ln N+dN+\beta\ln N+CNt\right).\end{aligned}$$

Of course we need the truncated terms $\max_{j=N+1:N+p-1}\|\boldsymbol{x}_j\|_\infty$ grow slower than exponential function as in the toy model case.

(3). Our general theorem is not limited to the moment closure for the considered class of stochastic differential equations. No matter where the infinite ODEs come from, as long as it satisfies the assumptions of the theorem, we will obtain the final estimate. This extends the applicable range of our analysis.

(4). The convergence is not only correct for the lowest moments $\boldsymbol{x}_1(t)$. Similar proof can show that the lower moments $\boldsymbol{x}_i$ also converge if i is independent of N.

(5) It is not difficult to find that all of the arguments above hold true if the absolute value is replaced with the complex modulus when the coefficients L, U and the solution $\boldsymbol{x}$ are complex variables. This enables the application to our motivating spin-boson model in Section 6.

Remark 3.2. For some problems, it is possible that the admissible d required by (3.10a)-(3.10b) is negative or in an empty set. In such case, the current framework will be invalid and we have to resort to other ideas.

Now we will demonstrate our restrictions on the growth of elements in coefficient matrix are essential through counterexamples. Let us consider the ODEs

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = j^{2+\alpha} x_{j-1} + x_{j+1}, \quad j \geq 1, \tag{3.18}$$

where $x_0 \equiv 0$ is defined to get a uniform expression and $\alpha > 0$ is a strictly positive number. This ODEs violate the criterion in our theorem, i.e., no positive number d exists such that $d \leq 1$ and $d \geq 2+\alpha-1 = 1+\alpha$ are satisfied at the same time. Make truncation to order N we get

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = A\boldsymbol{y}, \qquad A = \begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & \cdots \\ 2^{2+\alpha} & 0 & 1 & \cdots & \cdots & \cdots \\ 0 & 3^{2+\alpha} & 0 & 1 & 0 & \cdots \\ \vdots & \ddots & \ddots & \cdots & \cdots & 1 \\ 0 & \cdots & \cdots & \cdots & N^{2+\alpha} & 0 \end{pmatrix}.$$

We will show the truncated system does *not* converge to the original system in general.

Lemma 3.1. *We have the error estimate between the truncated variable $\boldsymbol{y}$ and the original variable $\boldsymbol{x}$:*

$$|x_1(t) - y_1(t)| \gtrsim \frac{N^{(2+\alpha)cN}}{(N+2cN)!} \int_0^t (t-s)^{N+2cN} x_{N+1}(s)\mathrm{d}s,$$

where $c > 1/\alpha$ is a positive constant.

Proof. Define $\boldsymbol{e}(t) = \boldsymbol{x}(t) - \boldsymbol{y}(t)$ and the dynamics of $\boldsymbol{e}(t)$ can be derived as

$$\frac{\mathrm{d}\boldsymbol{e}(t)}{\mathrm{d}t} = A\boldsymbol{e}(t) + \boldsymbol{g}(t),$$

where $\boldsymbol{g}(t) = (0, \cdots, 0, x_{N+1}(t))^T$ and $\boldsymbol{e}(0) = 0$. Simiarly we have the analytical solution

$$\boldsymbol{e}(t) = \int_0^t e^{A(t-s)} \boldsymbol{g}(s)\mathrm{d}s.$$

Thus

$$\boldsymbol{e}_1(t) = \int_0^t e^{A(t-s)}(1, N) x_{N+1}(s)\mathrm{d}s,$$

where the notation $e^{A(t-s)}(1, N)$ denotes the $(1, N)$-element of matrix $e^{A(t-s)}$. From now on, we will mix the notation Q_{jk} or $Q(j, k)$ in denoting the (j, k)-element of matrix Q. Let us focus on the analysis of $e^{A(t-s)}(1, N)$. We decompose A as $A = L + U$ where L and U are lower and upper triangular part of A.

For any given integer k, $(LU)^k U^{N-1}$ is one term in the expansion of $(L+U)^{N+2k-1}$. Note that all elements in L and U are positive, we have

$$(L+U)^{N+2k-1}(1,N) \geq (LU)^k U^{N-1}(1,N) = N^{(2+\alpha)k}(t-s)^{N+2k-1}.$$

Using the expansion $e^{A(t-s)} = \sum_{k=0}^{\infty} \frac{A^k(t-s)^k}{k!}$, we have

$$e^{A(t-s)}(1,N) \geq \sum_{k=0}^{\infty} \frac{N^{(2+\alpha)k}(t-s)^{N+2k-1}}{(N+2k-1)!}.$$

Choose $k=[cN]$ where $c>1/\alpha$ is a constant, we get

$$e^{A(t-s)}(1,N) \gtrsim \frac{N^{(2+\alpha)cN}(t-s)^{N+2cN}}{(N+2cN)!}.$$

Substitute this into the solution of $\boldsymbol{e}_1(t)$ we get the desired estimate. $\square$

We remark that generally $\boldsymbol{y}_1$ does not converge to $\boldsymbol{x}_1$. Using Stirling's approximation we have

$$|\boldsymbol{x}_1(t)-\boldsymbol{y}_1(t)| \gtrsim \exp\Big((\alpha c-1)N\ln N+(1+2c)N\Big)\int_0^t (t-s)^{N+2cN} x_{N+1}(s)\mathrm{d}s.$$

Since $\alpha c>1$ we have the exponential term goes to infinity as $N\to\infty$ if no special behavior of x_{N+1} is provided.

4. Extension to nonlinear problems

In this section, we will extend our analysis to the nonlinear infinite ODE system with similar lower Hessenberg structure. For simplicity, we will only give the detailed proof when $\boldsymbol{x}_i$ are scalar. The vectorial case can be established similarly. Now suppose the original ODE system is

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = f_1(x_1,x_2), \tag{4.1a}$$

$$\frac{\mathrm{d}x_2}{\mathrm{d}t} = f_2(x_1,x_2,x_3), \tag{4.1b}$$

$$\cdots$$

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = f_j(x_1,x_2,\cdots,x_j,x_{j+1}),\cdots. \tag{4.1c}$$

We choose a suitable large integer N and make the corresponding truncation. Denote the truncated equation as

$$\frac{\mathrm{d}y_1}{\mathrm{d}t} = f_1(y_1, y_2), \tag{4.2a}$$

$$\frac{\mathrm{d}y_2}{\mathrm{d}t} = f_2(y_1, y_2, y_3), \tag{4.2b}$$

$$\cdots$$

$$\frac{\mathrm{d}y_N}{\mathrm{d}t} = f_N(y_1, y_2, \cdots, y_N, 0), \cdots. \tag{4.2c}$$

To perform the analysis, we make the following assumption on the functions f_j:

(A4) f_j is Lipschitz with respect to all the variables, e.g.,

$$|f_j(\cdots, x_k, \cdots) - f_j(\cdots, y_k, \cdots)| \le A_{jk}|x_k - y_k|. \tag{4.3}$$

Now let us state the convergence theorem for the nonlinear system (4.1b).

Theorem 4.1. *For an infinite nonlinear ODEs* (4.1b)*, if* (A4) *is satisfied and the Lipschitz coefficients* $\{A_{jk}\}$ *satisfy Assumptions* (A1)-(A3)*, and there exists a positive number* d *such that*

$$d \le 1 - \beta_1, \quad d \ge \frac{\alpha_j - 1}{j}, \quad 0 \le j \le q,$$

then the solution of the lowest order variable y_1 *in truncated equation converges to the original lowest order variable* x_1 *as* N *goes to infinity. We have the estimate*

$$|e_1(t)| \le \frac{N^\beta e^{CNt}}{(N!)^d}\|x_{N+1}\|_\infty, \tag{4.4}$$

where C *is a positive constant independent of* N *and* t *and* $\beta = \beta_1$.

Proof. Define $e_j(t) = x_j(t) - y_j(t)$ and it is easy to see that $e_j(0) = 0$. The equation for $e_j(t)$ $(j < N)$ has the form

$$\begin{aligned}
\frac{\mathrm{d}e_j}{\mathrm{d}t} =& f_j(x_1, x_2, \cdots, x_{j+1}) - f_j(y_1, y_2, \cdots, y_{j+1}) \\
=& f_j(x_1, x_2, \cdots, x_{j+1}) - f_j(y_1, x_2, \cdots, x_{j+1}) \\
&+ f_j(y_1, x_2, \cdots, x_{j+1}) - f_j(y_1, y_2, \cdots, x_{j+1}) \\
&+ \cdots + f_j(y_1, y_2, \cdots, x_{j+1}) - f_j(y_1, y_2, \cdots, y_{j+1}) \\
\le& \sum_{k=1}^{j+1} A_{jk}|e_k|,
\end{aligned}$$

where the last inequality is due to the Lipschitz assumption. Also we have

$$\frac{\mathrm{d}e_j}{\mathrm{d}t} \ge -\sum_{k=1}^{j+1} A_{jk}|e_k|.$$

Similarly we have the estimation for e_N

$$\left|\frac{\mathrm{d}e_N}{\mathrm{d}t}\right| \leq \sum_{k=1}^{N} A_{Nk}|e_k| + A_{N,N+1}|x_{N+1}|.$$

Let us define two ODE systems p_j^ϵ and q_j^ϵ as

$$\frac{\mathrm{d}p_j^\epsilon}{\mathrm{d}t} = \sum_{k=1}^{j+1} A_{jk}p_k^\epsilon + \epsilon, \qquad j < N, \tag{4.5a}$$

$$\frac{\mathrm{d}p_N^\epsilon}{\mathrm{d}t} = \sum_{k=1}^{N} A_{Nk}p_k^\epsilon + A_{N,N+1}|x_{N+1}| + \epsilon, \tag{4.5b}$$

$$\frac{\mathrm{d}q_j^\epsilon}{\mathrm{d}t} = -\sum_{k=1}^{j+1} A_{jk}p_k^\epsilon - \epsilon, \quad j < N, \tag{4.5c}$$

$$\frac{\mathrm{d}q_N^\epsilon}{\mathrm{d}t} = -\sum_{k=1}^{N} A_{Nk}p_k^\epsilon - A_{N,N+1}|x_{N+1}| - \epsilon. \tag{4.5d}$$

Here ϵ is a positive real number and both ODEs start from the initial value 0. It is easy to show that $p_j^\epsilon = -q_j^\epsilon \geq 0$. Now we claim that $q_j^\epsilon \leq e_j(t) \leq p_j^\epsilon(t)$ for all j, i.e., $|e_j(t)| \leq p_j(t)$. Otherwise, define

$$\tau = \inf_t \left\{ t \geq 0,\ \exists j \text{ such that } e_j(t) \geq p_j^\epsilon(t) \text{ or } e_j(t) \leq q_j^\epsilon(t) \right\}.$$

At time τ, there exists an index m such that $e_m(\tau) = p_m^\epsilon(\tau)$ or $e_m(\tau) = q_m^\epsilon(\tau)$. Without loss of generality, we assume $e_m(\tau) = p_m^\epsilon(\tau)$. Since

$$\frac{\mathrm{d}(e_m(t) - p_m^\epsilon(t))}{\mathrm{d}t} \leq -\epsilon < 0 \quad \text{at } t = 0,$$

we have $\tau > 0$ and there must exist an instant $s_0 < \tau$ such that $\phi(s_0) = e_m(s_0) - p_m^\epsilon(s_0) < 0$. Based on the definition of τ, we have $|e_j(t)| \leq p_j^\epsilon(t)$ for $0 \leq t \leq \tau$ and arbitrary j.

If the index $m < N$, we have

$$\phi'(t) = \frac{\mathrm{d}(e_m(t) - p_m^\epsilon(t))}{\mathrm{d}t} \leq \sum_{k=1}^{m+1} A_{mk}(|e_k(t)| - p_k^\epsilon(t)) - \epsilon < 0, \quad t \leq \tau.$$

Similarly if $m = N$, we also have $\phi'(t) < 0$. Together with $\phi(s_0) < 0$ we should have $\phi(\tau) < 0$, which contradicts with $\phi(\tau) = 0$.

Finally, we take a sequence $\{\epsilon_n\}_{n=1}^{\infty}$, $\epsilon_n \to 0+$, then $p_i^{\epsilon_n} \to p_i$ and $|e_1| \le p_1^{\epsilon_n}$. This naturally leads to $|e_1| \le p_1$, where $\{p_j\}$ is defined as

$$\frac{\mathrm{d}p_j}{\mathrm{d}t} = \sum_{k=1}^{j+1} A_{jk} p_k, \quad j < N, \tag{4.6a}$$

$$\frac{\mathrm{d}p_N}{\mathrm{d}t} = \sum_{k=1}^{N} A_{Nk} p_k + A_{N,N+1} |x_{N+1}|. \tag{4.6b}$$

From Theorem 3.2 and the Assumptions on Lipschitz constants A_{jk}, we get the estimate (4.4). $\square$

Based on the final estimate and the whole proof procedure we can make the following remarks.

(1). The theorem is not limited to the case x_j being a scalar. As long as we have the Lipschitz condition to construct a linear system controlling the original system, the final estimate holds from our main Theorem 3.2. The extension to vectorial case is straightforward from the proof above.

(2). The structure of nonlinear system does not have to be exactly the same as (4.1b) in which the parameter $p = 2$. For example, we may have the ODEs as

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = f_j(x_1, \cdots, x_j, x_{j+1}, x_{j+2}),$$

which means $p = 3$. The result is still valid with reasonable modifications. We can similarly construct a linear system to control the original system and apply our general Theorem 3.2.

5. Numerical results

In this section, we will show some numerical results to confirm our analysis. All ODEs are solved by the classical 4th order Runge-Kutta method with time stepsize 10^{-5}.

5.1. Example 1

We test moment closure method on three different SDEs. The SDEs are

$$\text{Case 1:} \quad \mathrm{d}X_t = X_t(W_t + iV_t)\mathrm{d}t + X_t(\mathrm{d}W_t - i\mathrm{d}V_t), \qquad X_0 = 1. \tag{5.1a}$$

$$\text{Case 2:} \quad \mathrm{d}X_t = X_t W_t \mathrm{d}t + X_t \mathrm{d}W_t, \qquad X_0 = 1. \tag{5.1b}$$

$$\text{Case 3:} \quad \mathrm{d}X_t = X_t(W_t + iV_t)^2\mathrm{d}t + X_t(\mathrm{d}W_t - i\mathrm{d}V_t), \qquad X_0 = 1. \tag{5.1c}$$

These three SDEs can be analytically solved, the closed-form solution and mean value is listed below as benchmark to compare with our numerical result.

$$X_t = \exp\left(\int_0^t (W_s + iV_s)\mathrm{d}s + W_t - iV_t\right), \qquad \mathbb{E}X_t = \exp\left(t^2\right). \tag{5.2a}$$

$$X_t = \exp\left(\int_0^t W_s\mathrm{d}s + W_t - \frac{1}{2}t\right), \qquad \mathbb{E}X_t = \exp\left(\frac{t^3}{6} + \frac{t^2}{2}\right). \tag{5.2b}$$

$$X_t = \exp\left(\int_0^t (W_s + iV_s)^2\mathrm{d}s + W_t - iV_t\right), \qquad \mathbb{E}X_t = \exp\left(\frac{4t^3}{3}\right). \tag{5.2c}$$

For SDEs (5.1a), (5.1b) and (5.1c), we define corresponding auxiliary variables $x_n(t) = \mathbb{E}X_t(W_t + iV_t)^n$, $x_n(t) = \mathbb{E}X_tW_t^n$ and $x_n(t) = \mathbb{E}X_t(W_t + iV_t)^n$. To get a uniform expression, we define $x_i(t) = 0$, $i < 0$ for these SDEs. With these notations, the moment closure equation can be written as

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = x_{n+1}(t) + 2nx_{n-1}(t), \tag{5.3a}$$

$$\frac{\mathrm{d}x_n(t)}{\mathrm{d}t} = x_{n+1}(t) + nx_{n-1}(t) + \frac{1}{2}n(n-1)x_{n-2}(t), \tag{5.3b}$$

$$\frac{\mathrm{d}x_n(t)}{\mathrm{d}t} = x_{n+2}(t) + 2nx_{n-1}(t), \tag{5.3c}$$

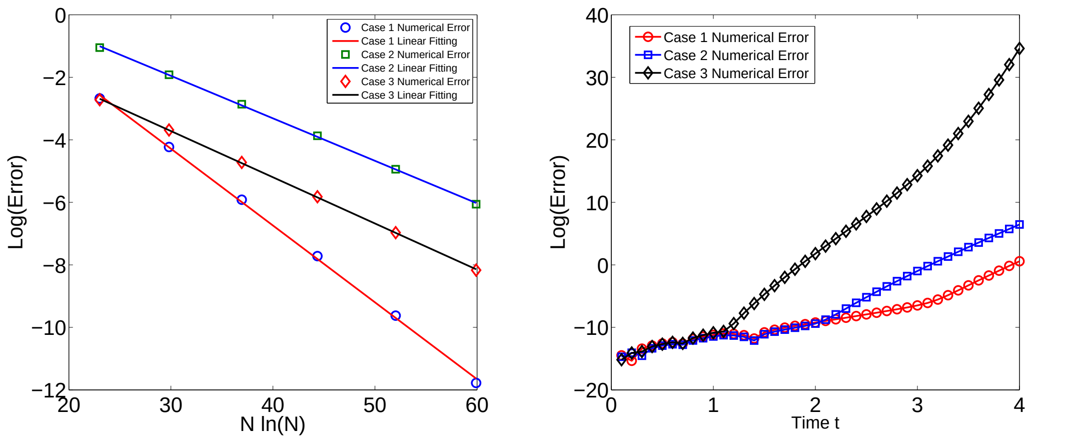
with the same initial conditions $x_i(0) = 0$, $i > 0$ and $x_0(0) = 1$.

These three examples satisfies Theorem 3.2 with different assumptions. For (5.3a), the assumptions hold with $\alpha_0 = 0$, $\alpha_1 = 1$, $\beta_1 = 0$, thus the restriction on d is $0 \le d \le 1$. For (5.3b), the assumptions hold with $\alpha_0 = 0$, $\alpha_1 = 1$, $\alpha_2 = 2$, $\beta_1 = 0$, thus the restriction on d is $\frac{1}{2} \le d \le 1$. For (5.3c), the assumptions hold with $\alpha_0 = 0$, $\alpha_1 = 1$, $\beta_1 = 0$, $\beta_2 = 0$, thus the restriction on d is $0 \le d \le \frac{1}{2}$.

We are interested in two things. One is the convergence rate with respect to the truncation number N when the end time T is fixed. In the discussion of Theorem 3.2, we see the convergence rate with respect to N is $\mathcal{O}(\exp(-N\ln N))$. We can solve these three ODEs (5.3a), (5.3b) and (5.3c) with different truncation number $N = 10, 12, 14, 16, 18, 20$. The numerical error is computed at time $t = 2$, $t = 2$, $t = 1$ for the three examples, respectively. Linear fitting is performed for the logarithm of the numerical errors versus $N\ln N$. The results are shown in Fig. 3(a). It clearly validates our convergence estimates.

The other point of interest is the evolution of numerical error with respect to time t when the truncation number N is fixed. We solve the ODEs to time $t = 4$ and record the numerical error for fixed $N = 25$. The result is shown in Fig. 3(b). We can see that at the beginning, the numerical error is very small. When time increases, the numerical error becomes larger and at last the numerical result is totally incorrect.

We also check the convergence rate for low order moments $x_1(t), \cdots, x_4(t)$ rather than only $x_0(t)$ for Case 1. The analytical solution of x_i can be solved but may be too complicated. We choose a large truncation number $N = 50$ and set the result as a good



(a) Convergence rate (b) Evolution of error

Figure 3: The results of three examples. Left panel: The truncation number N varies in {10,12,14,16,18,20}. The numerical error is computed at time $t=2$, $t=2$ and $t=1$ for three cases separately. Blue $\circ$, green $\square$ and red $\diamond$ represent the logarithm of numerical errors for three cases in Example 1, respectively. Red, blue and green solid lines are the corresponding linear fitting to $N\ln N$. Right panel: The evolution of numerical error with respect to time until $t=4$. Truncation number is fixed at $N=25$ for all three examples.

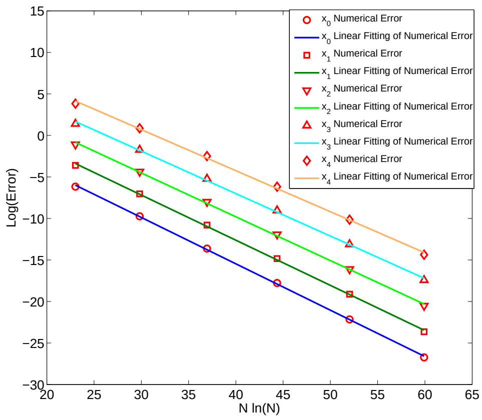


Figure 4: Convergence test of low moments $x_0, x_1, \cdots, x_4$ for Eq. (5.1a) with N varying from 10 to 20. The result supports the convergence rate of type $\exp(-aN\ln N)$.

approximation of analytical solution. We change N from 10 to 20 and compute the numerical error to see the convergence, see Fig. 4. This confirms that the convergence result of lower order terms in our remark is correct.

Remark 5.1. We should remark that the convergence analysis framework may not be suitable for the Case 3 in Example 1. In this case, the maximal admissible exponent $d=1/2$. However, an estimate to $\mathbb{E}X_t(W_t+iV_t)^N$ with Hölder's inequality yields the growth order $\exp((N\ln N-N)/2)$, which exactly cancels the exponential decaying factors obtained from the diagonal matrix D. The perfect performance of the closure approximation shown in Fig. 3 means that the estimate (3.11) may be not sharp and more delicate analysis needs to be developed to handle this situation. This is beyond the scope of this paper, which will be considered in the future.

5.2. Example 2

We consider an SDE with two independent Brownian motions W_t and V_t here:

$$\mathrm{d}X_t = X_t W_t \mathrm{d}t + 2X_t V_t \mathrm{d}t + X_t \mathrm{d}W_t + X_t \mathrm{d}V_t), \quad X_0 = 1. \tag{5.4}$$

The analytical solution of X_t and its mean value is

$$X_t = \exp\left(\int_0^t (W_s + 2V_s)\mathrm{d}s + W_t + V_t - t\right), \quad EX_t = \exp\left(\frac{t^3}{3} + t^2\right). \tag{5.5}$$

Take $x_{mn}(t) = EX_t W_t^m V_t^n,\ n \geq 0$ and define

$$x_{-2,0}(t) = x_{0,-2}(t) = x_{-1,-1}(t) = 0,$$

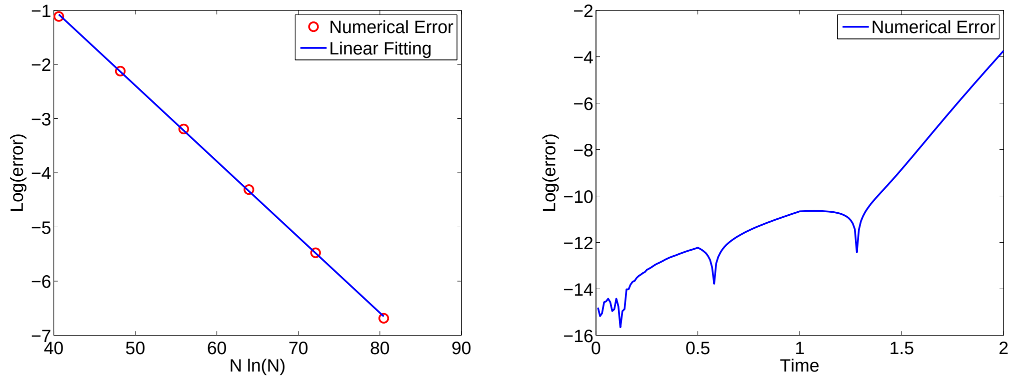
we get the ODEs

$$\begin{aligned}\frac{\mathrm{d}x_{mn}(t)}{\mathrm{d}t} =& x_{m+1,n}(t) + 2x_{m,n+1}(t) + \frac{1}{2}m(m-1)x_{m-2,n}(t) \\ &+ \frac{1}{2}n(n-1)x_{m,n-2}(t) + mx_{m-1,n}(t) + nx_{m,n-1}(t).\end{aligned} \tag{5.6}$$

Such an ODE system corresponds to the case that $\boldsymbol{x}_i$ is no longer a scalar. Define $\boldsymbol{x}_i = (x_{0,i}, x_{1,i-1}, \cdots, x_{i,0})^T$ and we can apply our theorem here. The Assumptions (A1)-(A3) are satisfied with $\alpha_0 = 0,\ \alpha_1 = 1,\ \alpha_2 = 2,\ \beta_1 = 0$ and the restrictions on d is $1/2 \leq d \leq 1$. We want to calculate the mean value in the time interval $[0, 2]$ and compare our numerical result of moment closure method with the analytical result. The truncation of this system is straightforward by setting $\boldsymbol{x}_n = 0,\ n > N$. By varying the truncation number N in $\{15, 17, 19, 21, 23, 25\}$, we testify our theorem. In Fig. 5(a), the logarithm of numerical error at time $t = 2$ with respect to different $N \ln N$ is shown. In Fig. 5(b), the evolution of the logarithm of numerical error is shown with fixed $N = 20$. Both results validate our theoretical estimate and they also suggest the obtained rate of convergence is almost tight.

6. Application to the realistic spin-boson model

In this section, we will apply the established theorems to our motivating spin-boson model, which shows the power of the theoretical results. We will first consider the single-exponential kernel function case, and then the general multi-exponential case.



(a) Convergence rate (b) Evolution of error

Figure 5: Result of Example 2. Left panel: Logarithm of numerical error at time $t = 2$ versus $N \ln N$. N varies in $\{15, 17, 19, 21, 23, 25\}$. Red $\circ$ represents the numerical error and blue solid line is the linear fitting result. Right panel: Logarithm of numerical error with respect to time with fixed truncation number $N = 20$.

6.1. Single-exponential case

In the single-exponential case, we have the kernel function $\alpha(t) = \gamma \exp(-\Omega t)$. The moments ρ_{mn} defined in (2.4) satisfies the system (2.5). Here we only consider the simple truncation closure as

$$\begin{aligned}\frac{\mathrm{d}y_{mn}}{\mathrm{d}t} =& - i[H_s, y_{mn}] - i[f_s, y_{m+1,n} + y_{m,n+1}] \\ &+ i\gamma(n y_{m,n-1} f_s - m f_s y_{m-1,n}) \\ &- (m\Omega + n\Omega^*) y_{mn} \quad \text{for } \ m, n \in \mathbb{N} \text{ and } \ m + n = 0, 1, \cdots, N, \end{aligned} \tag{6.1}$$

where $y_{mn} \in \mathbb{C}^{2\times 2}$ and $y_{mn} := 0$ if $m + n < 0$ or $m + n > N$.

To apply Theorem 3.2, we need to rearrange the variables ρ_{mn} and y_{mn} to form a single vector. The rule to transform each matrix ρ_{mn} into the vector $\boldsymbol{\rho}_{mn}$ is defined as

$$\rho_{mn} = \begin{pmatrix} \rho_{mn}^{(11)} & \rho_{mn}^{(12)} \\ \rho_{mn}^{(21)} & \rho_{mn}^{(22)} \end{pmatrix} \mapsto \boldsymbol{\rho}_{mn} = (\rho_{mn}^{(11)}, \rho_{mn}^{(12)}, \rho_{mn}^{(21)}, \rho_{mn}^{(22)}). \tag{6.2}$$

Define $\boldsymbol{x} = (\boldsymbol{x}_0, \boldsymbol{x}_1, \cdots, \boldsymbol{x}_r, \cdots)$ where $\boldsymbol{x}_r = (\boldsymbol{\rho}_{0r}, \boldsymbol{\rho}_{1,r-1}, \cdots, \boldsymbol{\rho}_{r0}) \in \mathbb{C}^{4(r+1)}$. We have the ODE system for $\boldsymbol{x}$ as

$$\frac{\mathrm{d}\boldsymbol{x}_r}{\mathrm{d}t} = L_{r,r-1}\boldsymbol{x}_{r-1} + L_{r,r}\boldsymbol{x}_r + U_{r,r+1}\boldsymbol{x}_{r+1}, \qquad r \in \mathbb{N}, \tag{6.3}$$

where $L_{r,r-1} \in \mathbb{C}^{4(r+1)\times 4r}$, $L_{r,r} \in \mathbb{C}^{4(r+1)\times 4(r+1)}$ and $U_{r,r+1} \in \mathbb{C}^{4(r+1)\times 4(r+2)}$ are matrices with 4-by-4 subblocks

$$(L_{r,r-1})_{jk} = \begin{cases} -i\gamma j \Gamma_{(f_s\cdot)}, & j = k+1, \\ i\gamma(r-j)\Gamma_{(\cdot f_s)}, & j = k, \\ 0, & \text{otherwise}, \end{cases} \tag{6.4}$$

for $j=0,\cdots,r$ and $k=0,\cdots,r-1$,

$$(L_{rr})_{jk}=\begin{cases}-(j\Omega+(r-j)\Omega^*)\mathrm{I}-i\Gamma_{[H_s,\cdot]}, & j=k,\\ 0, & \text{otherwise},\end{cases} \tag{6.5}$$

for $j=0,\cdots,r$ and $k=0,\cdots,r$,

$$(U_{r,r+1})_{jk}=\begin{cases}-i\Gamma_{[f_s,\cdot]}, & k=j \text{ or } k=j+1,\\ 0 & \text{otherwise},\end{cases} \tag{6.6}$$

for $j=0,\cdots,r$ and $k=0,\cdots,r+1$. Here the symbols $\Gamma_{(f_s\cdot)}$, $\Gamma_{(\cdot f_s)}$, $\Gamma_{[f_s,\cdot]}$ and $\Gamma_{[H_s,\cdot]}$ are constant matrices derived by transforming the matrix product and Poisson bracket into matrix-vector product operations, which can be explicitly written as

$$\Gamma_{(f_s\cdot)}=\frac{1}{2}\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix},\qquad \Gamma_{(\cdot f_s)}=\frac{1}{2}\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&-1\end{bmatrix},$$

$$\Gamma_{[H_s,\cdot]}=\frac{1}{2}\begin{bmatrix}0&1&-1&0\\1&0&0&-1\\-1&0&0&1\\0&-1&1&0\end{bmatrix},\qquad \Gamma_{[f_s,\cdot]}=\begin{bmatrix}0&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&0\end{bmatrix}.$$

It remains to show that this system actually satisfies the conditions of Theorem 3.2. The Eqs. (6.4) and (6.5) show that we have $L_{r,r-1}\lesssim r$ and $L_{r,r}\lesssim r$ so the assumption **(A1)** is satisfied with $q=1$, $\alpha_0=1$ and $\alpha_1=1$. The Eq. (6.6) shows that we have $U_{r,r+1}\lesssim 1$ so **(A2)** is satisfied with $p=1$ and $\beta_1=0$. The number of non-zeros in each row of the matrix is obviously independent of N, so **(A3)** is satisfied as well. Finally we have the constraint $0\le d\le 1$ from Theorem 3.2, and the theorem holds with $d=1$, which results in the error estimate

$$\|\rho_{mn}(t)-y_{mn}(t)\|_\infty\lesssim\frac{Ne^{CNt}}{(N+1)!}\|\boldsymbol{x}_{N+1}\|_\infty \tag{6.7}$$

for m,n independent of N. The estimate of $\|\boldsymbol{x}_{N+1}\|_\infty$ in the Appendix B ensures the exponential convergence of the closure approximation.

6.2. Multi-exponential case

When the kernel function $\alpha(t)$ has the multi-exponential form

$$\alpha(t)=\sum_{l=1}^{L}\gamma_l\exp(-\Omega_l t),$$

where γ_l are real and Ω_l are complex with positive real parts, we can also show the exponential convergence of the closure approximations. To do this, let us derive the closure system at first.

Define I the multi-indices

$$I = (m_1, m_2, \cdots, m_L, n_1, n_2, \cdots, n_L), \quad m_l, n_l \in \mathbb{N},$$

and $\rho_I(t)$ as

$$\rho_I(t) = \mathbb{E}\Big(\rho_s(t) \prod_{l=1}^{L} g_l^{m_l}(t) h_l^{n_l}(t)\Big), \tag{6.8}$$

where g_l, h_l for $l = 1, 2, \cdots, L$ are scalar functions defined as

$$g_l(t) = \int_0^t \gamma_l e^{-\Omega_l(t-s)} (\mathrm{d}W_1(s) - i\mathrm{d}W_4(s) - i\mathrm{d}W_2(s) + \mathrm{d}W_3(s)), \tag{6.9a}$$

$$h_l(t) = \int_0^t \gamma_l e^{-\Omega_l^*(t-s)} (\mathrm{d}W_1(s) - i\mathrm{d}W_4(s) + i\mathrm{d}W_2(s) - \mathrm{d}W_3(s)). \tag{6.9b}$$

Similar as in the single-exponential case, g_l and h_l satisfy the SDEs

$$\mathrm{d}g_l = -\Omega_l g_l \mathrm{d}t + \frac{\gamma_l}{2}(\mathrm{d}W_1(s) - i\mathrm{d}W_4(s) - i\mathrm{d}W_2(s) + \mathrm{d}W_3(s)), \tag{6.10a}$$

$$\mathrm{d}h_l = -\Omega_l^* h_l \mathrm{d}t + \frac{\gamma_l}{2}(\mathrm{d}W_1(s) - i\mathrm{d}W_4(s) + i\mathrm{d}W_2(s) - \mathrm{d}W_3(s)). \tag{6.10b}$$

For national ease, we also define

$$\rho_{I,m_l-} := \Big(\rho_s(t) \prod_{k=1}^{L} (g_k^{m_k}(t) h_k^{n_k}(t))/g_l(t)\Big), \quad \rho_{I,m_l+} := \Big(\rho_s(t) \prod_{k=1}^{L} (g_k^{m_k}(t) h_k^{n_k}(t)) \cdot g_l(t)\Big),$$

$$\rho_{I,n_l-} := \Big(\rho_s(t) \prod_{k=1}^{L} (g_k^{m_k}(t) h_k^{n_k}(t))/h_l(t)\Big), \quad \rho_{I,n_l+} := \Big(\rho_s(t) \prod_{k=1}^{L} (g_k^{m_k}(t) h_k^{n_k}(t)) \cdot h_l(t)\Big).$$

Here we naturally assume ρ_{I,m_l-} and ρ_{I,n_l-} only defined for $m_l, n_l \geq 1$. It is not difficult to show that the moments ρ_I satisfy the following infinite system

$$\begin{aligned}\frac{\mathrm{d}\rho_I}{\mathrm{d}t} = &-i[H_s, \rho_I] - \sum_{l=1}^{L} i[f_s, \rho_{I,m_l+} + \rho_{I,n_l+}] \\ &+ \sum_{l=1}^{L} i\gamma_l (n_l \rho_{I,n_l-} f_s - m_l f_s \rho_{I,m_l-}) - \sum_{l=1}^{L} (m_l \Omega_l + n_l \Omega_l^*) \rho_I.\end{aligned} \tag{6.11}$$

Especially, $\rho_I(t)$ for $I = (0, \cdots, 0, 0, \cdots, 0)$ is the desired solution.

Define the order of the multi-index I as

$$|I| = \sum_{l=1}^{L} (m_l + n_l).$$

The straightforward closure by truncating the terms with $|I| \leq N$ can be made as in the single-exponential case. To analyze the convergence, define $\boldsymbol{x} = (\boldsymbol{x}_0, \boldsymbol{x}_1, \cdots, \boldsymbol{x}_r, \cdots)$, where $\boldsymbol{x}_r = (\boldsymbol{\rho}_{I_{r0}}, \boldsymbol{\rho}_{I_{r1}}, \cdots, \boldsymbol{\rho}_{I_{r,K_r}})$ for all the multi-indices $|I_{rk}| = r$ and $I_{r,k} < I_{r,k+1}$. Here $\boldsymbol{\rho}$ is the 4-vector formed by rearranging the entries of matrix ρ as in the single-exponential case, K_r is the combinatorial number of partitioning r into $2L$ natural numbers, and '$<$' is the natural partial ordering for multi-indices. From (6.11) one can deduce the system of ODEs satisfied by $\boldsymbol{x}$

$$\frac{\mathrm{d}\boldsymbol{x}_r}{\mathrm{d}t} = L_{r,r-1}\boldsymbol{x}_{r-1} + L_{r,r}\boldsymbol{x}_r + U_{r,r+1}\boldsymbol{x}_{r+1}, \quad r \geq 0. \tag{6.12}$$

Finding the exact form of $L_{r,r-1}$, $L_{r,r}$ and $U_{r,r+1}$ is cumbersome and unnecessary. It is not difficult to find that $L_{r,r-1}$ is only related to

$$\sum_{l=1}^{L} i\gamma_l(n_l\rho_{I,n_l-}f_s - m_l f_s \rho_{I,m_l-}),$$

thus we have $L_{r,r-1} \lesssim r$. Similarly, $L_{r,r}$ is only related to

$$i[H_s, \rho_I] - \rho_I \sum_{l=1}^{L}(m_l\Omega_l + n_l\Omega_l^*),$$

and we also have $L_{r,r} \lesssim r$. $U_{r,r+1}$ is only related to

$$\sum_{l=1}^{L} i[f_s, \rho_{I,n_l+} + \rho_{I,m_l+}]$$

and thus

$$U_{r,r+1} \lesssim 1.$$

Thus we find that the Assumptions **(A1)-(A3)** in Theorem 3.2 hold as well. With the same argument as in the single-exponential case, we can choose $d = 1$ and get similar error estimate like (6.7).

Now we numerically test the convergence rate of the closure approximation method for the spin-boson model when $L = 1, 2$. For the single-exponential case we choose $\gamma = 400, \Omega = 20$. For the double-exponential case we choose $\gamma_1 = 400, \gamma_2 = -100, \Omega_1 = 20, \Omega_2 = 10$. The truncated ODE system is solved with an explicit 3rd-order Runge-Kutta method with step size 10^{-4}. The computation is carried on from $t = 0$ to $t = 100$. As the exact solution to the system is unknown, the solution of the system truncated with a sufficiently large cutoff N_{ref} is chosen to be the reference solution for comparison. We take $N_{\text{ref}} = 18$ for the single-exponential case and $N_{\text{ref}} = 15$ for the double-exponential case, which is already accurate enough. The error for the $\rho_s(t)$ agains the cutoff number N is plotted in Fig. 6. The linear relation between the $\ln$(error) and $N \ln N$ clearly indicates the exponential convergence of the closure approximations.

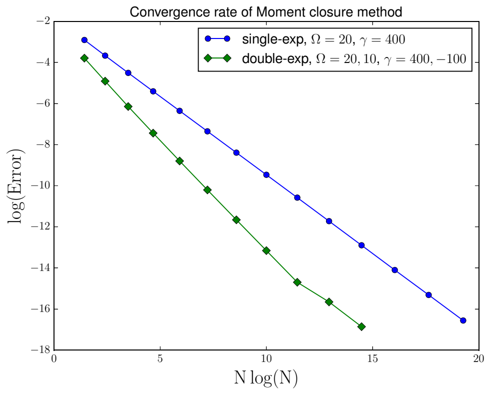


Figure 6: Convergence rate of the closure approximation for spin-boson model. The blue • and green ♦ represent the logarithm of numerical errors against $N \ln N$ for single and double-exponential cases, respectively. The linear relation between the $\ln$(error) and $N \ln N$ clearly indicates the exponential convergence of the closure approximations.

7. Conclusions

In this paper, we have explored the validity and convergence rate of one type of moment closure method. The method is straightforward and easy to implement. The convergence rate is proven to be exponential which is much faster than most classical methods. Such a fast convergence ensures that a moderate truncation number N will give an acceptable result. The numerical results also show moment closure method is fast and accurate compared with Monte Carlo simulations and WCE.

The way we get the closure system depends on the special structure of the model. When a dynamical system is given, how to choose the appropriate moment closure variables is beyond our discussions. But our framework is not limited to systems described by SDEs. Our assumptions are put on the infinite ODEs rather than the original SDEs. In this sense, as long as we have a infinite ODEs and the assumptions are satisfied, no matter where it comes from, we will get a convergence result.

Future work may include the construction of efficient moment closure methods and analysis of the moment closure for more general SDEs. Both topics are challenging and interesting in real applications.

Appendix A

Proof of (3.6a). From (1.1) we can obtain by Ito's formula

$$d|X_t|^2 = (2\mathrm{Re}(\mu) + 2 + 2W_t)|X_t|^2 dt + 2|X_t^2|dW_t.$$

Define $Y_t = |X_t|^2$, we get

$$Y_t = e^{\int_0^t (2\mathrm{Re}(\mu)+2+2W_s)ds} Y_0 + 2\int_0^t e^{\int_s^t (2\mathrm{Re}(\mu)+2+2W_\tau)d\tau} Y_s dW_s.$$

This gives

$$\mathbb{E}Y_t = \mathbb{E}\Big(e^{\int_0^t (2\mathrm{Re}(\mu)+2+2W_s)ds} Y_0\Big) = e^{(2\mathrm{Re}(\mu)+2)t+\frac{2}{3}t^3}\mathbb{E}Y_0.$$

Here we naturally assume Y_0 is independent of W_t. $\square$

Appendix B

In this part, we will show that

$$\frac{1}{N!}\|\rho_I\|_\infty = \frac{1}{N!}\Big\|\mathbb{E}\Big(\rho_s(t)\prod_{l=1}^L g_l^{m_l}(t)h_l^{n_l}(t)\Big)\Big\|_\infty \lesssim \exp\Big(-\frac{N}{2}\ln N + B_0 N\Big)K(t) \quad \text{(B.1)}$$

for $|I| = N$ in the multi-exponential case, where $B_0 = (\ln(4L)+1)/2 + \max_l \sigma_l$ and $K(t)$ is independent of N. This covers the single-exponential as a special case.

To do this, we first note that

$$\Big|\mathbb{E}\Big(\rho_s(t)\prod_{l=1}^L g_l^{m_l}(t)h_l^{n_l}(t)\Big)\Big| \le \big(\mathbb{E}|\rho_s|^2\big)^{\frac{1}{2}}\prod_{l=1}^L \big(\mathbb{E}|g_l|^{4m_lL}|\big)^{\frac{1}{4L}}\big(\mathbb{E}|h_l|^{4n_lL}\big)^{\frac{1}{4L}}. \quad \text{(B.2)}$$

Here g_l and h_l are both complex Gaussian random variables with mean 0. Denote $g_l(t) = a_l(t) + ib_l(t)$, where $a_l = \mathrm{Re}(g_l)$, $b_l = \mathrm{Im}(g_l)$ are the corresponding real and imaginary parts of g_l. We have

$$\mathbb{E}(a_l(t)b_l(t)) = 0, \qquad \mathbb{E}a_l^2 = \mathbb{E}b_l^2$$

from the fact $\mathbb{E}g_l^2 = 0$. Furthermore, we have

$$\mathbb{E}a_l^2(t) = \mathbb{E}b_l^2(t) = \frac{\gamma_l^2}{R_l}(1-e^{-2R_lt}) =: \sigma_l^2(t),$$

from $\mathbb{E}|g_l|^2 = \mathbb{E}(a_l^2+b_l^2)$, where $R_l = \mathrm{Re}(\Omega_l) > 0$. Direct calculation gives

$$\mathbb{E}|g_l|^n = \mathbb{E}(|g_l|^2)^{\frac{n}{2}} = \mathbb{E}(a_l^2+b_l^2)^{\frac{n}{2}} = \sqrt{\frac{\pi}{2}}\sigma_l^n(t)\mathbb{E}|X|^{n+1}, \quad n \in \mathbb{N}, \quad \text{(B.3)}$$

where $X \sim N(0,1)$ the standard normal distribution. Eq. (B.3) shows that for the indices $|I| = N$

$$\begin{aligned}
&\prod_{l=1}^L \big(\mathbb{E}|g_l|^{4m_lL}|\big)^{\frac{1}{4L}}\big(\mathbb{E}|h_l|^{4n_lL}\big)^{\frac{1}{4L}}\\
\le&\Big(\prod_{l=1}^L \sigma_l^{m_l+n_l}\Big)\prod_{l=1}^L\Big((4m_lL)!!(4n_lL)!!\Big)^{\frac{1}{4L}}\\
\le&\Big(\max_{l=1,\cdots,L}\sigma_l\Big)^N 2^{\frac{N}{2}}\prod_{l=1}^L\Big((2m_lL)!(2n_lL)!\Big)^{\frac{1}{4L}}, \qquad \text{(B.4)}
\end{aligned}$$

where $\sigma_l := \gamma_l/\sqrt{R_l}$. Utilizing the Stirling's formula we get

$$\begin{aligned}
&\prod_{l=1}^{L}\Big((2m_lL)!(2n_lL)!\Big)^{\frac{1}{4L}}\\
\sim&\Big(\exp\Big(\sum_{l=1}^{L}2m_lL\ln(2m_lL)+2n_lL\ln(2n_lL)-2m_lL-2n_lL\Big)\Big)^{\frac{1}{4L}}\\
\leq&\exp\Big(\frac{N}{2}\ln(2NL)-\frac{N}{2}\Big).
\end{aligned}\tag{B.5}$$

To estimate $\mathbb{E}|\rho_s|^2$, we first rewrite (2.1) in a vectorial form as in (6.3):

$$\begin{aligned}
\mathrm{d}\boldsymbol{x}=&\big(-i\Gamma_{[H_s,\cdot]}\boldsymbol{x}-i\bar{g}(t)\Gamma_{[f_s,\cdot]}\boldsymbol{x}\big)\,\mathrm{d}t\\
&-\frac{i}{2}\Gamma_{[f_s,\cdot]}\boldsymbol{x}(\mathrm{d}W_1+i\mathrm{d}W_4)+\frac{1}{2}\Gamma_{\{f_s,\cdot\}}\boldsymbol{x}(\mathrm{d}W_2-i\mathrm{d}W_3),
\end{aligned}\tag{B.6}$$

where $\boldsymbol{x}=(\rho_s^{(11)},\rho_s^{(12)},\rho_s^{(21)},\rho_s^{(22)})$, $\Gamma_{\{f_s,\cdot\}}$ is defined as

$$\Gamma_{\{f_s,\cdot\}}=\begin{bmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&-1\end{bmatrix}.$$

We have the following identity by Ito's formula

$$\begin{aligned}
\mathrm{d}|\boldsymbol{x}|^2=&\mathrm{d}\boldsymbol{x}\cdot\boldsymbol{x}^*+\boldsymbol{x}\cdot\mathrm{d}\boldsymbol{x}^*+\mathrm{d}\boldsymbol{x}\cdot\mathrm{d}\boldsymbol{x}^*\\
=&2\mathrm{Re}\left(-i\boldsymbol{x}^*\Gamma_{[H_s,\cdot]}\boldsymbol{x}-i\bar{g}(t)\boldsymbol{x}^*\Gamma_{[f_s,\cdot]}\boldsymbol{x}\right)\mathrm{d}t\\
&-\frac{i}{2}\boldsymbol{x}^*\Gamma_{[f_s,\cdot]}\boldsymbol{x}(\mathrm{d}W_1+i\mathrm{d}W_4)+\frac{1}{2}\boldsymbol{x}^*\Gamma_{\{f_s,\cdot\}}\boldsymbol{x}(\mathrm{d}W_2-i\mathrm{d}W_3)\\
&+\frac{i}{2}\boldsymbol{x}\Gamma_{[f_s,\cdot]}\boldsymbol{x}^*(\mathrm{d}W_1-i\mathrm{d}W_4)+\frac{1}{2}\boldsymbol{x}\Gamma_{\{f_s,\cdot\}}\boldsymbol{x}^*(\mathrm{d}W_2+i\mathrm{d}W_3)\\
&+\frac{1}{2}\boldsymbol{x}^*\Gamma^2_{[f_s,\cdot]}\boldsymbol{x}\mathrm{d}t+\frac{1}{2}\boldsymbol{x}^*\Gamma^2_{\{f_s,\cdot\}}\boldsymbol{x}\mathrm{d}t.
\end{aligned}\tag{B.7}$$

Simple calculations yield the estimates

$$\begin{aligned}
&|\boldsymbol{x}^*\Gamma_{[H_s,\cdot]}\boldsymbol{x}|\leq 2|\boldsymbol{x}|^2,\quad &&|\boldsymbol{x}^*\Gamma_{[f_s,\cdot]}\boldsymbol{x}|\leq|\boldsymbol{x}|^2,\quad |\boldsymbol{x}^*\Gamma_{\{f_s,\cdot\}}\boldsymbol{x}|\leq|\boldsymbol{x}|^2,\\
&|\boldsymbol{x}^*\Gamma^2_{[f_s,\cdot]}\boldsymbol{x}|\leq|\boldsymbol{x}|^2, &&|\boldsymbol{x}^*\Gamma^2_{\{f_s,\cdot\}}\boldsymbol{x}|\leq|\boldsymbol{x}|^2.
\end{aligned}$$

Substitute them into (B.7), employ the Ito isometry and Gronwall's inequality, we get the estimate

$$\mathbb{E}|\boldsymbol{x}(t)|^2\leq\mathbb{E}\left(\exp\left(\int_0^t A(s)ds\right)\right)\mathbb{E}|\boldsymbol{x}(0)|^2,\tag{B.8}$$

where $A(t):=5+2|\bar{g}(t)|$, and we have already taken the natural assumption that the Wiener processes are independent of initial condition $\boldsymbol{x}(0)$.

To estimate of the exponential moment in (B.8), we first note that it is enough to consider $|g_l(s)|$ instead of $A(s)$. We can get the following estimate

$$\begin{aligned}
&\mathbb{E}\left(\exp\left(\int_0^t |g_l(s)|ds\right)\right) = \mathbb{E}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\int_0^t |g_l(s)|ds\right)^n \\
\leq&\mathbb{E}\sum_{n=0}^{\infty}\frac{t^{n-1}}{n!}\int_0^t |g_l(s)|^n ds \lesssim \sum_{n=0}^{\infty}\frac{(\sigma_l t)^n}{n!}\mathbb{E}|X|^{n+1} \\
=&\mathbb{E}\Big(|X|\exp(\sigma_l t|X|)\Big) \leq \sqrt{\frac{2}{\pi}} + \exp\left(\frac{\sigma_l^2 t^2}{2}\right)\cdot 2\sigma_l t,
\end{aligned}$$

where we utilized (B.3), $\sigma_l := \gamma_l/\sqrt{R_l}$ and $X \sim N(0,1)$.

Combing the above estimate with (B.2)-(B.5) and (B.8) gives the desired estimate about $\|\rho_I\|_\infty$ for $|I| = N$.

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