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Tree-Based Implementation of the Small Matrix Path Integral for System-Bath Dynamics

Geshuo Wang[1,*] and Zhenning Cai[1]

[1] *Department of Mathematics, National University of Singapore, Level 4, Block S17, 10 Lower Kent Ridge Road, Singapore 119076.*

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Abstract. The small matrix path integral (SMatPI) method is an efficient numerical approach to simulating the evolution of a quantum system coupled to a harmonic bath. The method relies on a sequence of kernel matrices that defines the non-Markovian dynamics of the quantum system. In the original SMatPI method, these kernels are computed indirectly through the QuAPI method. Instead, we focus on the definition of the kernel matrices and reveal a recurrence relation in these matrices. Using such a relationship, a tree based algorithm (t-SMatPI) is developed, which is shown to be much faster than straightforward computation of the kernel matrices based on their definitions. This algorithm bypasses the step to compute the SMatPI matrices by other path integral methods and provides more understanding of the SMatPI matrices themselves. Meanwhile, it keeps the memory cost and computational cost low. Numerical experiments show that the t-SMatPI algorithm gives exactly the same result as i-QuAPI and SMatPI. In spite of this, our method may indicate some new properties of open quantum systems, and has the potential to be generalized to higher-order numerical schemes.

AMS subject classifications: 81Q80, 82C10

Key words: t-SMatPI, Open quantum system, Catalan number.

1 Introduction

The system-bath dynamics, which successfully models quantum dissipation and quantum decoherence, plays an important role in accurate quantum simulation when the environment plays an non-negligible role. Most simulations of the system-bath dynamics are based on path integrals. Due to the large number of paths, a natural approach is the Monte Carlo methods. For example, the diagrammatic quantum Monte Carlo (dQMC) method applies diagrams to intuitively represent the coupling between the system and

*Corresponding author. *Email addresses:* geshuowang@u.nus.edu (G. Wang), matcz@nus.edu.sg (Z. Cai)

bath [30,37]. For real-time simulations, Monte Carlo based methods suffer from numerical sign problems [5,13]. Different techniques, such as application of bold lines [3,8,31], inclusion-exclusion principle [1,39], combination of thin lines and bold lines [6], are developed to relieve the numerical sign problem or accelerate the computation.

Another idea to simulate the system-bath dynamics is to approximate the dynamics by ignoring the long memory effects so that the system depends only on a finite time in the history. This type of approaches includes the classical iterative quasi-adiabatic propagator path integral (i-QuAPI) [15,27,28], which is efficient when the decay of the memory kernel is fast. However, the i-QuAPI method still has to record the contribution of all the paths within the memory length, leading to prohibitively large memory cost when the time nonlocality is long. Some improvements have been developed in the past decades to reduce the memory cost, among which the blip-summed decomposition [19, 20] reduces the memory cost by ignoring the paths with small contributions, and the differential equation based path integral (DEBPI) studies the continuous form of i-QuAPI and formulates a differential equation system [35]. The small matrix decomposition of the path integral (SMatPI) [21–23,25] successfully overcomes the exponential scaling of the memory cost while preserving the accuracy of i-QuAPI. In this approach, the memory cost scales only linearly with the memory length, leading to a very efficient method for the system-bath dynamics.

The SMatPI method can also be considered as a discrete form of the Nakajima-Zwanzig generalized quantum master equation (GQME) [29, 33, 40, 41], an integro-differential equation with a memory kernel describing the non-Markovian effects. Formally, the SMatPI method is similar to the transfer tensor method (TTM) [2,7,9], which also has a time-convolution form. When the time step Δt tends to zero, the SMatPI and the TTM both converge to the GQME [22], while the special structure of the SMatPI allows it to converge more effectively than the TTM. Both methods allow extension to more complicated models such as spin chain models [24,36].

In this paper, we analyze the structure of the SMatPI matrices and propose a new algorithm for the evaluation of SMatPI matrices directly based on their definitions. It keeps the memory cost and computational cost low. The spin-boson model and the SMatPI method are introduced in Section 2 and Section 3, respectively. In Section 4, we analyze the structure of SMatPI by combining it to Catalan numbers. Some recurrence relations of the SMatPI matrices are discovered in Section 5, which is then turned into a tree-based algorithm in Section 6. Some numerical experiments are carried out in Section 7 showing the accuracy and efficiency of our algorithm. Lastly, in Section 8, we summarize our work and discuss how our method may inspire some new theoretical or numerical findings in our future works.

2 Spin-boson model

In a quantum system, the density matrix $\rho(t)$ satisfies the von Neumann equation