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Author(s): Agasti, Souvik

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Numerical Simulation of Free Dissipative Open Quantum System and Establishment of a Formula for π

Souvik Agasti^{1,2,a)}

¹*Nanoscience center, Dept. of Physics, University of Jyväskylä, Finland*

²*Photonics Laboratory, Physics Unit, Tampere University, Finland*

^{a)}Corresponding author: souvik.s.agasti@jyu.fi

Abstract. We transform the system/reservoir coupling model into a one-dimensional semi-infinite discrete chain with nearest neighbor interaction through a unitary transformation, and, simulate the dynamics of free dissipative open quantum system. We investigate the consequences of such modeling, which is observed as finite size effect causing the recurrence of particle from the end of the chain. Afterwards, we determine a formula for π in terms of the matrix operational form, which indicates a robustness of the connection between quantum physics and basic mathematics.

Introduction

An open quantum system (OQS), described to be a separate entity from its surrounding environment while being coupled with it, has shown importance due to its applicability in the foundation of quantum mechanics, statistical mechanics and atomic, molecular, optical and bio-physics. The theory of OQS has remained useful to describe experimental activities in the field of decoherence measurement and quantum computation, which has applications in quantum networks [1, 2] in mesoscopic systems, which includes photonic crystals [3], ion traps [4, 5] and superconducting circuits [6]. The coupling of system mode to the environment has been used in the sensing and measurement related applications, in a broad range from electromagnetic fields [7] to gravitational waves [8].

The dissipative dynamics of OQS due to the system/bath (S/B) coupling, has been studied with the help of quantum master equation and Heisenberg-Langevin equation [9]. Both the equations are extensions of their classical counterpart, in the quantum regime. Despite of their simplicity, these techniques exhibit limitations while extracting out exact solution when OQS suffers non-Markovianity in the dynamical behavior or non-linearity in the Hamiltonian. For example, the non-Markovian dynamical phenomena has been observed in a type of quantum phase transition between dynamically localized and delocalized states of two level system (TLS) for zero temperature sub-Ohmic and Ohmic baths [10, 11, 12, 13], where one cannot treat effective interaction between oscillator and TLS in a perturbative manner. On another side, the non-linear Hamiltonian appears in case of Kerr nonlinear system [14] or cavity coupled TLS systems [15], where the theory of OQS has been implemented after linearizing the Hamiltonian over nonlinear steady state field amplitude. Therefore, the interesting effects are often missed out, and the limitation of analytics provokes us explicitly to do numerical simulation. The numerical method requires transformation of the degrees of freedom of the environmental modes to a many body system with nearest neighbor interactions.

The idea of such mapping was first introduced in Ref. [13] where a recursive numerical technique was performed on discretised environment, and truncated to form a many body chain. Furthermore, using the properties of orthogonal polynomials, an exact unitary transformation has been presented that maps the Hamiltonian of a linearly coupled system to a continuum of bosonic or fermionic modes, to a Hamiltonian that describes a one-dimensional chain with only nearest-neighbor interactions [16]. Considering applicability, the time-adaptive density matrix renormalisation group (t-DMRG) [17] has been considered recently as one of the most useful tools in optical, atomic and condensed matter physics for the numerical simulation of one-dimensional systems with short-range interactions.

In this paper we present how the S/B coupling model is mapped to a semi infinite chain with nearest neighbor interactions. We construct the Hamiltonian matrix for a single particle located in the entire chain, and use that to simulate the free dissipative OQS. We also discuss the recurrence of particle which comes from the finite size effect

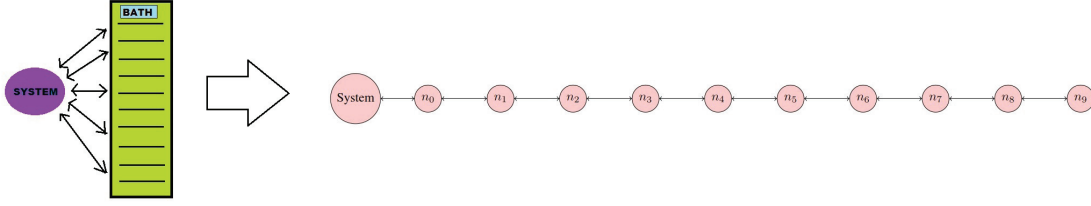


FIGURE 1. Transformation of Hamiltonian from system/bath coupling model to semi infinite chain model.

of the chain. Afterwards, we show that the famous quantity π can be computed from the dissipation dynamics of the OQS, in terms of matrix operational form.

THEORETICAL MODEL

In order to discuss the dissipative dynamics of an OQS, we start with the full Hamiltonian

$$H = H_S + H_B + H_{int} \quad (1)$$

Here, the Hamiltonian of the isolated system is $H_S = \omega_c a^\dagger a$, where ω_c is the frequency, and $a(a^\dagger)$ are the annihilation (creation) operator of the system mode. The Hamiltonian of the bath is represented by a set of bosonic modes $H_B = \sum_{k=-N}^N \omega_k b_k^\dagger b_k$, and, the interaction Hamiltonian between system and environment is $H_{int} = \sum_{k=-N}^N g_k (b_k^\dagger a + a^\dagger b_k)$, where $b_k(b_k^\dagger)$ are the annihilation (creation) operators, and ω_k is the frequency of k^{th} mode of the environmental field. g_k is the coupling strength between the system and k^{th} mode of the bath. The frequency of the bath changes linearly with the change of mode k : $\omega_k \propto k$, and the range is chosen to be symmetric around the system mode (ω_c) due to the fact that, in most of the realistic situation, the system is coupled to the modes of the environment around its own resonating mode (ω_c). Moving to a rotating frame of frequency ω_c , the frequency range of the bath is accepted to be $\omega_k \in [-\epsilon, \epsilon]$.

The dynamics of the bipartite system is determined by a positive function of the mode of the bath, is known as spectral density [13]. In case of a hard cutoff range of the modes of the reservoir, implying wide band limit approximation, i.e. the coupling strength is independent of the mode of the bath ($g_k = c_0$) [18], we obtain the spectral density function as

$$J_k = c_0^2 D \theta(N - k) \theta(N + k) \quad (2)$$

where θ is the Heaviside step function and $D = \frac{\delta k}{\delta \omega_k} = \frac{N}{\epsilon}$ is the density of states (DOS) of the bath.

In case of an empty bath, considering a large cutoff window ($\epsilon \rightarrow \infty$), the dynamics of the system is determined by the Heisenberg equation of motion (HEM): $\dot{a}(t) = -\frac{\gamma}{2} a(t)$ [9], which gives a dissipative nature of the system population ($n_S = \langle a^\dagger a \rangle$) as $n_S(t) = e^{-\gamma t} n_S(0)$, where $\gamma = 2\pi D c_0^2$ is the rate of dissipation of the system. Therefore, if the initial state of the system is a Fock state of only one particle, the occupation probability of the particle decays down exponentially with time as

$$P_S(t) = \exp(-\gamma t) \quad (3)$$

NUMERICAL MODEL

Here, we transform the S/B coupling Hamiltonian to a semi-infinite chain model, using a unitary transformation of the operators of the bath: $d_n = \sum_{k=-N}^N U_n(k) b_k$ [16]. In a case where the spectral density is defined by Eq. (2), normalized shifted Hahn polynomial is a the natural choice as the unitary operator: $U_n^k = \frac{1}{\rho_n} Q_n[(k + N)/2, N]$, where $Q_n(k, N)$ is the Hahn polynomial, and $\rho_n = (-1)^n (N!) \sqrt{\frac{(2n+1)}{(N+n+1)!(N-n)!}}$ is the normalization coefficient. One can check that the

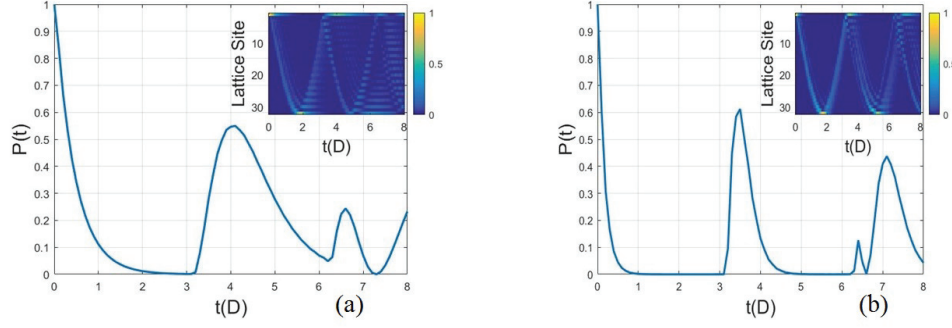


FIGURE 2. Occupation probability in system determined numerically for different rates of dissipation (a) $c_0 = 0.6D^{-1}$ and (b) $c_0 = 1D^{-1}$. Total number of modes of the bath $N = 30$. In the inset the image plot is given for the population on the sites which shows how the particle reflects back from the boundary.

new modes of the bath satisfy bosonic commutation relation $[d_n, d_m^\dagger] = \delta_{mn}$. Essentially, the transformed Hamiltonian becomes

$$\tilde{H} = \eta' (a^\dagger d_0 + a d_0^\dagger) + \sum_{n=0}^{N-1} \eta_n (d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n) \quad (4)$$

The diagrammatic representation of this transformation is shown in Fig. 1. Using the recurrence relation of Hahn polynomial [16, 19], the coefficients are determined as $\eta' = c_0 \sqrt{2N}$ and $\eta_n = \frac{(n+1)}{D} \sqrt{\frac{(N-n)(N+n+2)}{(2n+1)(2n+3)}}$. The mapping is useful for the simulation of the time dynamics of OQS using DMRG method. Recently, similar mapping was introduced in Ref. [16] aiming to be applied on spin-boson models [20] and biomolecular systems [21]. However, instead of using DMRG, we use the Hamiltonian for a system where one particle of boson is located in entire chain.

FREE DISSIPATIVE SYSTEM

In a situation where only one particle located in the entire system and environment, which is initially localized in system, leaving the bath completely empty, the state of the corresponding 1-D chain is represented by $|S\rangle = [1\ 0\ 0\ 0\ \dots]^T$. Essentially, the corresponding matrix representation of the chain Hamiltonian gives

$$\tilde{H} = \begin{bmatrix} 0 & \eta' & & & 0 \\ \eta' & 0 & \eta_0 & & \\ & \eta_0 & 0 & \eta_1 & \\ & & \eta_1 & \ddots & \\ & & & \ddots & \eta_{N-1} \\ 0 & & & & \eta_{N-1} & 0 \end{bmatrix} \quad (5)$$

After time t , the occupation probability of the particle in the system is determined from the time evolved state $|S_t\rangle = e^{-i\tilde{H}t}|S\rangle$ as $P_S(t) = |\langle S|S_t\rangle|^2$. We determine the time evolved state numerically, and plot the dissipative nature of the system population in Fig. 2, where we observe that the system population increases again after a certain time, which comes from the fact that the particle reflects back from the end of the chain, which is visible from the population plot of the entire chain shown in the inset of Fig. 2. The recurrence of the particle is dependent on the DOS, which is explained explicitly in appendix.

Comparing to the Eq. (3), we estimate the rate of dissipation from the numerically determined population dynamics of the system as

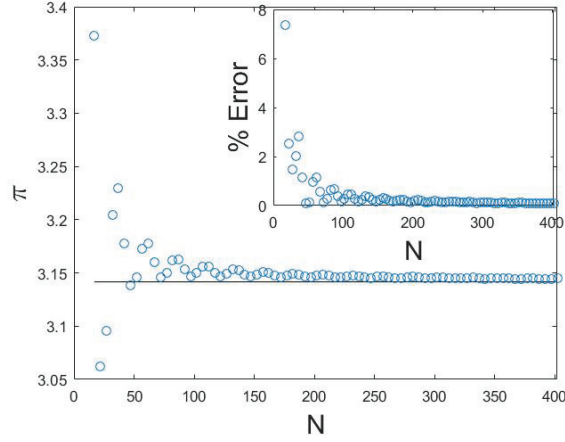


FIGURE 3. Plot of the value of π determined numerically, for increasing size of matrix. The black line corresponds to the actual value. In the inset, % error is calculated for increasing size of matrix.

$$\gamma = -\frac{\delta \ln(P_S(t))}{\delta t} \Big|_{t < \text{recurrence time}} \quad (6)$$

In the next step, we fix $D = 1$, $c_0 = 1$ and $t = 1$ (which satisfies the condition $t < \text{recurrence time}$), in order to get the simplest formula of π in terms of the matrix operational form. It is to be noted that Eq. (3) is obtained by considering a large cutoff frequency which is ideally infinite. Therefore, the accuracy of the value of π determined by this new formula, is anticipated when we increase the size of the matrix. It is also true that π is an irrational number, which demands the ideal size of the matrix to be infinite. Fig. 3 presents a comparison between actual and numerically determined value of π , which shows how the numerically determined value gets closer to actual one when we increase the size of matrix.

Remark: Note that the unitary transformation of S/B coupling Hamiltonian is done using Hahn polynomial which is given by $Q_n(k; N) = {}_3F_2(-n, -k, n+1; 1, -N+1; 1)$, where ${}_3F_2$ is generalized hyper-geometric function which is constructed by Gamma function [19]. Therefore, the value of π has not been used anywhere in the process of transformation of Hamiltonian to 1-D chain. On the other side, in the analytically determined dynamics of open quantum system, the quantity π appears in the rate of dissipation from the Fourier transformation of delta function.

CONCLUSION

We present a model that represents the transformation of Hamiltonian of an OQS coupled linearly to a discrete set of modes of bosonic reservoir, to a Hamiltonian of a one-dimensional chain having nearest-neighbour interactions. Using the model, we study free dissipation of a particle, located initially in the system, to a zero temperature empty bath. We observe that the finite length of the chain causes recurrence of particle from the end. The mapping seems promising to investigate the dynamics of OQS through the numerical simulation of many body systems. We also determine a formula for π in terms of matrix operations through this method. As anticipated from the fact that π is an irrational number, the accuracy increases as the size of the matrix increases. Such kind of formulation indicates the robustness of the establishment of quantum physics and its connection to the fundamental mathematics.

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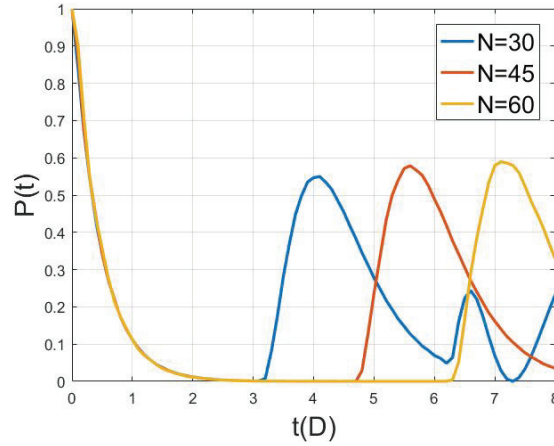


FIGURE 4. Plot of time evolution of a free dissipative system for the variation of DOS ($1D$, $3/2D$ and $2D$), which is obtained by fixing the cutoff frequency ($30D^{-1}$) and changing number of lattice sites. $\gamma = 2.2619D^{-1}$ (the actual value of π has been used here).

Appendix

The recurrence time of the particle is dependent on the group velocity in the lattice. The group velocity is defined by $v_g = \frac{\delta\omega_k}{\delta k_N}$, where k_N is the wavenumber determined by the number of lattice sites ($k_N \propto N$), and ω_k is the frequency. The higher group velocity causes the phonon traveling faster in lattice. However, the group velocity is inversely proportional to the density of states ($v_g \propto D^{-1}$), and therefore, the recurrence time increases linearly when the DOS increases. In the Fig. 4, we increased the DOS by increasing the number of sites keeping the cutoff frequency fixed. The increment of DOS forces to take more number of lattice into account, and therefore, which causes an increment in the recurrence time.

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