Ensemble of Lindblad's trajectories for non-Markovian dynamics

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Although Lindblad developed a general Markovian theory for open-system dynamics while maintaining the positivity of the density matrix, a practical non-Markovian analog remains a significant problem. Here, we present an extension of Lindblad's theory through an ensemble of Lindbladian trajectories originating from different times in the system's history. This approach provides an account of the system's memory while preserving the positivity of the density matrix. We apply the theory to the Jaynes-Cummings model to capture non-Markovian dynamics in the weak and strong coupling regimes.

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I. INTRODUCTION

Non-Markovian effects are important in a variety of physical quantum systems including but not limited to exciton transport in photosynthetic light harvesting complexes [1–8], qubits and quantum control [9–12], and quantum optics [13]. Yet despite their prevalence there remain many unanswered questions in the theoretical treatment of such systems [14,15]. The most common starting point for treating non-Markovian dynamics is an exact kernel equation, which is challenging to solve in the most general case [14,15]. Many methods approximate the kernel through perturbative techniques, and while they are effective for small perturbations about the Markovian limit, they can in general limit or destroy the positivity of the density matrix [16]. Other methods have been developed to treat non-Markovian dynamics with built-in positivity in specific systems [17–29], but the development of a general, practical framework for non-Markovian approximations that maintains the positive semidefiniteness of the density matrix remains a significant problem [19]. Recent work has produced an exact, closed form master equation which allows the treatment of non-Markovian dynamics for Gaussian environments [30]. Other related work includes quantum jump methods and trajectory approaches [31–37].

Lindblad developed an elegant, completely general theory for treating Markovian dynamics in an open quantum system while maintaining the positive semidefinite property of the density matrix for all time [38–40]. In this paper we present a general extension of Lindblad's theory to the case of non-Markovian quantum systems. While Lindblad examines the equation of motion for a single trajectory that generalizes the Liouville equation to the Markovian case, we consider an ensemble of Lindbladian trajectories (ELT) which allows for an accurate calculation of dynamics in the strong coupling, non-Markovian regime while maintaining the positivity of the density matrix. The constraint of the system's density matrix to be consistent with the total density matrix (i.e., positive semidefinte) has connections to the N-representability problem in which a p-particle density matrix is constrained to represent an N-particle density matrix with $N > p$ [41–45]. The ELT theory is also related to post-Markovian methods [31,33,37] based on Kraus maps, with further details given below. The Jaynes-Cummings model is used to demonstrate the accuracy of the ELT method as it is exactly solvable and many perturbative methods fail at capturing the exact dynamics in the strong coupling regime [46,47].

II. ENSEMBLE OF LINDBLADIAN TRAJECTORIES METHOD

An ensemble of Lindbladian trajectories is used to calculate the density matrix at a given time t. In Fig. 1 the blue density matrix $D(t)$ at time t is the actual density matrix of the quantum system while the green density matrices are auxiliary variables, each of which represents a trajectory in the ensemble. Each green density matrix $\tilde{D}(t, \tau_i)$ is the endpoint of a Lindblad trajectory originating from an actual (blue) density matrix at time $t - \tau_i$. The ensemble of the green density matrices $\tilde{D}(t, \tau_i)$ originating at different times $t - \tau_i$ defines the actual (blue) density matrix at time t. Formally, this is equivalent to

$$D(t) = \sum_{i=1}^{N} \omega(\tau_i)\tilde{D}(t, \tau_i) \tag{1}$$

$$= \sum_{i=1}^{N} \omega(\tau_i)e^{\mathcal{L}(\tau_i)}D(t - \tau_i), \tag{2}$$

where N is an integer controlling the maximum amount of memory, $\omega(\tau_i)$ are the weights of the trajectories and $e^{\mathcal{L}(\tau_i)}$ are the propagators. Each trajectory is a Kraus map which we can represent by the following Lindbladian trajectory:

$$\frac{dD}{ds} = -i[H, D] + \sum_{j=1}^{N} C_j D C_j^\dagger - \frac{1}{2}\{C_j^\dagger C_j, D\}, \tag{3}$$

where s represents an effective time within the mapping and the Lindblad terms C_j account for the interaction of

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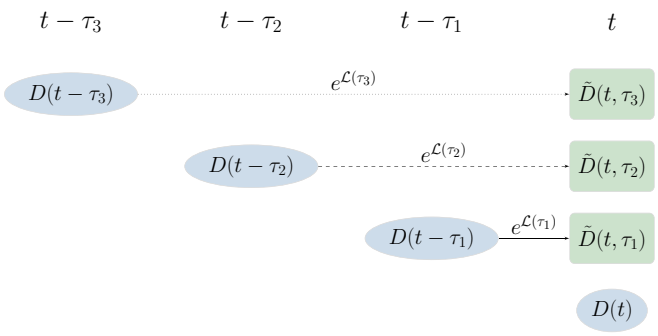

FIG. 1. An ensemble of Lindbladian trajectories whose weighted ensemble produces the density matrix at time t.

the N-electron system with its environment through different dissipative channels [39]. From the properties of Kraus maps the trajectories produce positive semidefinite density matrices whose ensemble is also positive semidefinite [48]. If the Hamiltonian and the Lindbladian matrices are all time dependent, that is dependent on the effective time s, then the Lindblad trajectory can approach an arbitrary Kraus map. The proof follows from writing the Lindblad trajectory as a composition of Kraus maps where all but one of the Kraus maps can be chosen to be the identity operation.

This ansatz is an extension of the Lindbladian theory to the general case of non-Markovian dynamics under the mild assumption that each point in history can be mapped to the present using a Kraus map. Because any positive semidefinite density matrix at time t can be generated by a Kraus map from a historical density matrix at $t-\tau$ [9–12,48], the assumption is equivalent to requiring that each trajectory's density matrix be positive semidefinite. Any positive semidefinite density matrix can be generated from an initial density matrix from a Kraus map. By assuming the positivity of each individual map in the ensemble average, we can select the nonnegative weights in the ensemble average without any additional restriction. Although Kraus maps are employed in other open-system theories such as the post-Markovian methods [31,33,37], ELT does not rely on measurement theory to generalize the Lindblad equation, which leads to a different set of final equations.

III. RELATIONSHIP TO KERNEL METHODS

The general kernel equation is given by

$$\frac{dD}{dt} = \int_0^t \mathcal{K}(t,\tau)D(t,\tau)d\tau, \tag{4}$$

where $D(t,\tau)$ is the reduced density matrix at time $t-\tau$ and $\mathcal{K}(t,\tau)$ is the memory kernel [14,15]. We can convert Eq. (2) into the form of Eq. (4) by taking the summation in Eq. (2) to the continuous limit, differentiating each side of Eq. (2) with respect to t, and invoking the Leibnitz rule:

$$\frac{dD(t)}{dt} = \int_0^t \omega(\tau)e^{\mathcal{L}(\tau)}\frac{dD(t,\tau)}{dt}d\tau, \tag{5}$$

where t is the current time, $t-\tau$ is the initial time for each trajectory, $e^{\mathcal{L}(\tau)}$ are the Kraus maps, and $\omega(\tau)$ are the weights. The key difference between the Eq. (5) and the standard kernel equation in Eq. (4) is that the integral depends on the first derivative of the density matrix with respect to time while the standard method relies on just the density matrix. Equation (5) is the key equation because the time derivative is central to the process of maintaining a positive semidefinite density matrix. It also has the benefit of transforming the integro-differential equation in Eq. (4) into a simplified type 2 Volterra equation [49,50], which has well-developed numerical solutions [51].

IV. JAYNES-CUMMINGS MODEL

To illustrate this theory, we consider the damped Jaynes-Cummings model on resonance with and without detuning. This model consists of a single excitation in a two-level system coupled to a reservoir of harmonic oscillators [14,17,46,47]. The Hamiltonian for the model is

$$\hat{H} = \frac{\omega_0}{2}\hat{\sigma}_z + \int \omega\hat{a}_\omega^\dagger\hat{a}_\omega + \lambda(\hat{\sigma}_+\hat{a}_\omega + \hat{\sigma}_-\hat{a}_\omega^\dagger)d\omega, \tag{6}$$

where ω_0 is the two-level system's transition frequency and λ is inversely proportional to the reservoir correlation time. The $\hat{a}_\omega^\dagger$ and $\hat{a}_\omega$ are the creation and annihilation operators for frequency modes ω, and $\hat{\sigma}_{x,y,z}$ are the Pauli spin operators with $\hat{\sigma}_\pm = (\hat{\sigma}_x \pm \hat{\sigma}_y)/2$ [17]. The spectral density of the bath is

$$J(\omega) = \frac{1}{2\pi}\frac{\gamma_0\lambda^2}{(\omega_0-\Delta-\omega)^2+\lambda^2}, \tag{7}$$

where γ_0 is inversely proportional to the time scale of system changes and Δ is the amount of detuning [14]. Here the decay rates and populations in the excited level from our method are compared to those calculated exactly from the spectral density of the bath [14,17]. We also compare our results with the Markovian solution, the solution to the generalized master equation to second order (GME2), and the time convolutionless solution to second (TCL2) and fourth (TCL4) orders [52,53].

In the weak coupling case without detuning the correlation time of the reservoir is set to one-fifth of the system's timescale, and in the strong coupling case without detuning the correlation time of the reservoir is set to five times the system's timescale. In all calculations we set the Markovian decay rate γ_0 to 1.091. The trajectory of each density matrix in the ELT method was computed with the computer algebra system Maple [54].

The excited-level population of the Jaynes-Cummings model has the following closed-form solution in the Markovian limit:

$$D_{11}(t) = D_{11}(0)e^{-\gamma_0 t}. \tag{8}$$

In the ELT method we consider an ensemble of such Lindbladian trajectories, one trajectory from each historical point in time,

$$D_{11}(t) = \sum_i \omega(\tau_i)\tilde{D}_{11}(t,\tau_i), \tag{9}$$

where $\tilde{D}_{11}(t,\tau_i) = D_{11}(t-\tau_i)e^{-\gamma(\tau_i)(t-\tau_i)}$. To match the dynamics from the ELT method with the dynamics from the full quantum system including both system and bath, we optimized both the weights $\omega(\tau_i)$ and the decay parameters $\gamma(\tau_i)$ simultaneously with a least squares fit to the

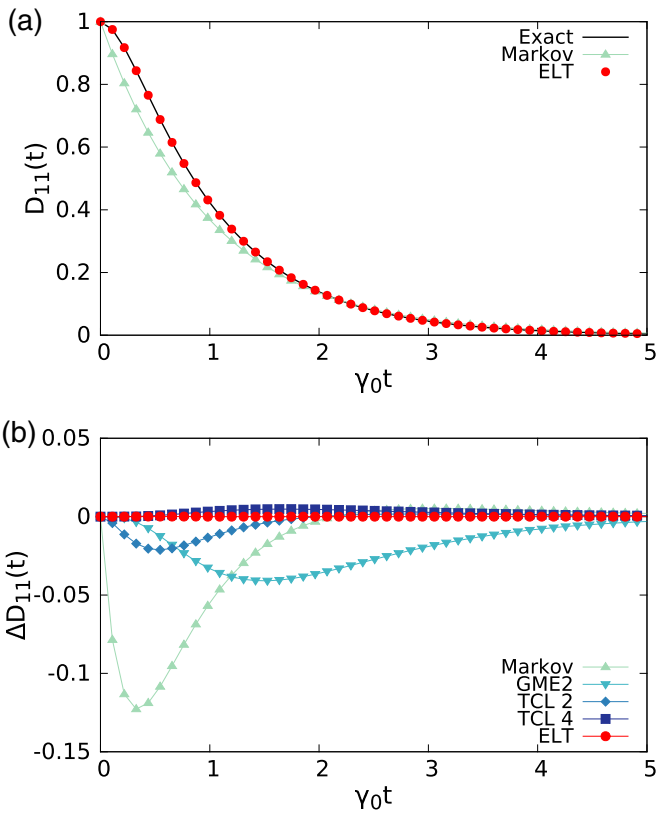

FIG. 2. The exact (black line), Markovian (green triangles), GME2 (green-blue inverted triangles), TCL2 and TCL4 (teal diamonds and blue squares respectively), and ELT (red circles) (a) populations of the excited level and (b) errors relative to the exact solution are shown for the weak coupling limit ($\lambda = 5\gamma_0$, $\gamma_0 = 1.091$, $\Delta = 0$) in the Jaynes-Cummings model. The ELT method shows closest agreement to the exact solution.

exact solution by a sequential programming algorithm in Maple [55].

Figure 2(a) shows the excited-level populations of the Markovian, ELT, and exact solutions while Fig. 2(b) shows the errors in the excited-level population from all methods relative to the exact solution. The excited-level population of the Markovian solution decays too quickly at short times and too slowly at longer times. While the perturbative methods, GME2, TCL2, and TCL4, improve upon this behavior, only the ELT method agrees with the exact solution to the precision of the numerical solution.

In the strong coupling limit the excited-level population of each method is shown in Fig. 3. The Markovian, TCL2, and TCL4 methods give physical results and the correct long-time behavior; they capture only the decay of the population and not its recovery. The GME2 solution exhibits unphysical behavior in the form of large negative probabilities for finding the model in its excited level. The ELT method correctly predicts the recovery, matching the exact solution to the precision of the numerical methods. Physically, the recovery arises from the energy previously transferred to the surroundings driving the system back into the excited state, which is often referred to as a back-flow of energy or information.

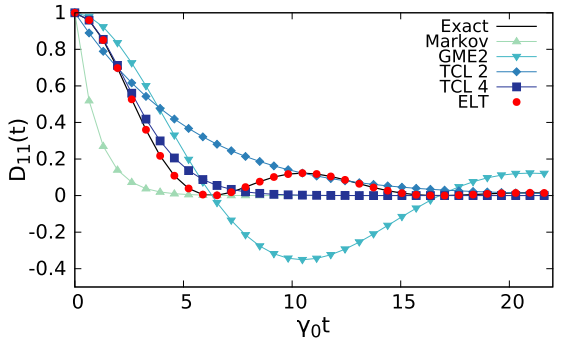

FIG. 3. The population of the Jaynes-Cummings excited level in the strong coupling limit ($\lambda = 0.2\gamma_0$, $\gamma_0 = 1.091$, $\Delta = 0$) is shown as a function of time for the exact (black line), Markovian (green triangles), GME2 (green-blue inverted triangles), TCL2 and TCL4 (teal diamonds and blue squares respectively), and ELT (red circles) solutions. The ELT method agrees with the exact solution for all times.

Finally, we consider the Jaynes-Cummings model with detuning, comparing the Markovian, TCL4, and ELT solutions in Fig. 4, where $\lambda = 0.3\gamma_0$ and $\Delta = 2.4\gamma_0$. In this case the ensemble of such Lindbladian trajectories is augmented with trajectories of the hole density matrix:

$$D_{11}(t) = \sum_i [\omega(\tau_i)\tilde{D}_{11}(t,\tau_i) + \tilde{\omega}(\tau_i)\{1 - \tilde{Q}_{11}(t,\tau_i)\}] \quad (10)$$

where $\tilde{Q}_{11}(t,\tau_i) = Q_{11}(t-\tau_i)e^{-\gamma(\tau_i)(t-\tau_i)}$ in which $Q_{11}(t) = 1 - D_{11}(t)$. Physically, consideration of the hole density matrix is equivalent to including an additional Lindbladian channel corresponding to the decay of a hole from the upper level (or excitation of a particle from the lower level). It is seen that although the detuning case is inherently non-Lindbladian by nature [14], due to the ensemble nature of the ELT method, the exact dynamics are still captured.

V. CONCLUSIONS

The most general form of treating non-Markovian dynamics in open quantum systems is with the kernel equation (4). However, practical use of the kernel equation is computationally challenging in its general form. Approximations to the kernel, especially those that rely

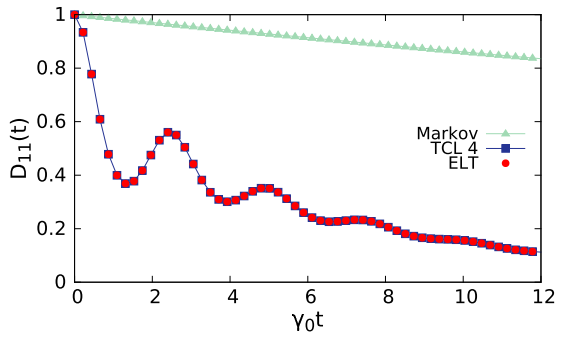

FIG. 4. The population of the excited level of the Jaynes-Cummings model in the strong coupling, detuning limit ($\lambda = 0.3\gamma_0$, $\gamma_0 = 1.091$, $\Delta = 2.4\gamma_0$) is shown as a function of time for the Markovian (green triangles), TCL4 (blue squares), and ELT (red circles) solutions. The ELT agrees with the TCL4 solution.

upon perturbative arguments, tend to sacrifice the positive semidefiniteness of the density matrix. Here, we have presented a general theory that considers an ensemble of Lindbladian trajectories originating from different times in the system's history. In this manner the approach provides a complete account of the system's memory in a framework that preserves the positivity of the system's density matrix for all time. The Lindbladian trajectories capture the full range of potential dynamics because of the one-to-one mapping between Lindbladian trajectories and Kraus maps. Application of ELT to the Jaynes-Cummings model demonstrates its ability to capture non-Markovian dynamics in both the weak and strong coupling regimes. As with Lindblad's theory, the present generalization requires physical insight from theory and/or experiments to select the appropriate system-bath parameters. Future work will further explore the application of these results to the more accurate description of non-Markovian quantum systems.

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