Connecting two jumplike unravelings for non-Markovian open quantum systems

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The development and use of Monte Carlo algorithms plays a visible role in the study of non-Markovian quantum dynamics due to the provided insight and powerful numerical methods for solving the system dynamics. In the Markovian case, the connections between the various types of methods are fairly well-understood while for non-Markovian case there has so far been only a few studies. We focus here on two jumplike unravelings of non-Markovian dynamics, the non-Markovian quantum jump (NMQJ) method and the property state method by Gambetta, Askerud, and Wiseman (GAW). The results for simple quantum optical systems illustrate the connections between the realizations of the two methods and also highlight how the probability currents between the system and environment, or between the property states of the total system, associate to the decay rates of time-local master equations, and consequently to the jump rates of the NMQJ method.

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I. INTRODUCTION

The theory of open quantum systems deals with the dynamics of the reduced system which is coupled to its environment [1]. This leads often to decoherence and the loss of quantum properties [2–5], though there also exists schemes to exploit system-reservoir interaction for quantum engineering [6–8]. Recently, non-Markovian dynamics, where memory effects play a crucial role, has become under very active research [9–21]. On one hand this is due to the fact that the fundamental understanding of non-Markovianity is still missing and on the other hand non-Markovianity may be useful for various quantum information or quantum engineering tasks [20, 22].

We show here that there is an inherent connection between the reduced system part of the GAW realizations and the NMQJ realizations. Moreover, we also study how the probability currents between the property states are associated to the decay rates of the time-local master equations, and how the jump rates between the GAW and NMQJ methods are connected. We stress that the NMQJ method can be currently used for systems for which time local non-Markovian master equation can be derived whereas GAW method has greater generality. Our results provide new insight for non-Markovian dynamics in terms of the information flow between the system and the reservoir, and hopefully stimulates further studies of connections between Monte Carlo methods for non-Markovian dynamics.

The paper is organized in the following way. In Section II we describe the basic ingredients of the GAW method and in Sec. III of the NMQJ method. By studying simple quantum optical systems, in Sec. IV we show how the methods are connected and finally, Sec. V concludes the paper.

II. UNRAVELING IN THE TOTAL SYSTEM SPACE: GAW METHOD

We focus on two jumplike unravelings and illustrate their connections by studying simple quantum optical systems. The method by Gambetta, Askerud, and Wiseman (GAW) is based on the generating stochastic realizations for the total system state vectors and monitoring the random jumps between the property states of the total system [36]. On the other hand, the recently developed non-Markovian quantum jump (NMQJ) method generates jumplike realizations for the state vectors within the Hilbert space of the reduced system.

We show here that there is an inherent connection between the reduced system part of the GAW realizations and the NMQJ realizations. Moreover, we also study how the probability currents between the property states are associated to the decay rates of the time-local master equations, and how the jump rates between the GAW and NMQJ methods are connected. We stress that the NMQJ method can be currently used for systems for which time local non-Markovian master equation can be derived whereas GAW method has greater generality. Our results provide new insight for non-Markovian dynamics in terms of the information flow between the system and the reservoir, and hopefully stimulates further studies of connections between Monte Carlo methods for non-Markovian dynamics.

The method by Gambetta, Askerud and Wiseman (GAW) is based on generating piecewise deterministic realizations, or jumplike unraveling within the Hilbert space of the total system, describing the discontinuous transitions between the property states of the system. We give here the basic ingredients of the method suitable for undriven quantum optical systems with spectral mode unraveling. We note that GAW method can also be applied to driven systems and with temporal mode unraveling. More details can be found from the Refs. [36, 45, 46].

We focus on the dynamics of simple undriven quantum optical systems, e.g., two-level and V-systems which are coupled to a continuum of electromagnetic field modes.
at zero temperature. The dynamics of the state vector of the system and the environment in \( \mathcal{H}_S \otimes \mathcal{H}_E \), where \( \mathcal{H}_S \) and \( \mathcal{H}_E \) are the Hilbert spaces of the system and the environment respectively, is given by the Schrödinger equation
\[
\frac{d}{dt} \Psi(t) = -i H |\Psi(t)\rangle.
\] (1)

Here we have set \( \hbar = 1 \). The Hamiltonian \( H = H_S + H_E + H_{SE} \) includes the free evolution of the system \( H_S \) and the environment \( H_E \), and the system-environment interaction \( H_{SE} \). The free evolution of the \( n \)-level system is governed by \( H_S = \sum_{k=1}^{N} \omega_k |k\rangle\langle k| \), where \( |k\rangle \) are the energy eigenstates of the system and \( \omega_k \) the corresponding energies. The free evolution of the \( N \)-mode environment is given by \( H_E = \sum_{j=1}^{N} \nu_j a_j^\dagger a_j \), where the operators \( a_j (a_j^\dagger) \) are the annihilation (creation) operators for the \( j \)-th mode of the environment.

For simplicity we focus on system-environment interactions that under the rotating wave approximation (RWA) include only transition from the excited states to the unique ground state without any cascade structure. The general form of such interaction is
\[
H_{SE} = i \sum_{k=1}^{N} \sum_{j=1}^{N} (g_k |1\rangle\langle k|a_j^\dagger - g_k^* |k\rangle\langle 1|a_j),
\] (2)

From now on we will work in the interaction picture \( H \rightarrow H_I(t) = e^{i(H_S + H_E)t} H e^{-i(H_S + H_E)t} \), where the dynamics is given by Eq. (1) with the Hamiltonian
\[
H_I(t) = i \sum_{k=1}^{N} \sum_{j=1}^{N} (g_k |1\rangle\langle k|a_j^\dagger e^{-i\Omega_{j,k}t} - g_k^* |k\rangle\langle 1|a_j e^{i\Omega_{j,k} t}),
\] (3)

where \( \Omega_{j,k} = \nu_j - \omega_k \) and \( \omega_k \) is the energy difference of the ground state (labeled with index 1) and \( j \)-th excited state of the system. Here \( g_k \) is a frequency-dependent coupling constant.

The total system state vector \( |\Psi(t)\rangle \) evolves according to the Eq. (1) with the Hamiltonian (3). Let us define a projective operator valued measure (POVM) as
\[
\pi_{m,N} = I_S \otimes \sum_{j=1}^{N} |n_{j}\rangle\langle n_{j}| = I_S \otimes |m_N\rangle\langle m_N|,
\] (4)

where \( m_N \) is a shorthand notation for arbitrary photon number configuration of the \( N \) environmental modes. In the systems we study we can have at most one excitation in the environment. However, GAW method in general is not limited only to one excitation [36]. We can now define property states of the total system which are conditioned on some particular photon number configuration of the environment. These are
\[
|\Psi_{m,N}\rangle = \pi_{m,N} |\Psi(t)\rangle / \sqrt{N_{m,N}} = \frac{1}{\sqrt{N_{m,N}}} |\phi_{m,N}(t)\rangle_S \otimes |m_N\rangle_E,
\] (5)

where \( N_{m,N} \) is a normalization factor. We denote the un-normalized property states with \( |\tilde{\Psi}_{m,N}\rangle \). From now on we drop the subscript \( N \) for notational convenience and the simple index \( m \) refers to a particular configuration of \( N \) environmental modes.

The GAW method is a piecewise deterministic process (PDP) where the jumps take place between the different property states \( |\Psi_m(t)\rangle \) [36, 37]. Let us define \( P(m,t) \) as the probability for the total system to be in the state \( |\Psi_m(t)\rangle \) at time \( t \) and write the following equation of motion for \( P(m,t) \):
\[
\frac{d}{dt} P(m,t) = \sum_k J_{m,k}(t),
\] (6)

where \( J_{m,k}(t) \) is the probability current from \( |\Psi_k(t)\rangle \) to \( |\Psi_m(t)\rangle \), when \( J_{m,k}(t) > 0 \), and when \( J_{m,k}(t) < 0 \) it is the probability current from \( |\Psi_m(t)\rangle \) to \( |\Psi_k(t)\rangle \), i.e., to the opposite direction. We can define this in the following way
\[
J_{m,k}(t) = T_{m,k}(t) P(k,t) - T_{k,m}(t) P(m,t),
\] (7)

where \( T_{m,k}(t) \) is the transition rate from \( |\Psi_k(t)\rangle \) to \( |\Psi_m(t)\rangle \). From this definition it is clear that \( J_{m,k}(t) = -J_{k,m}(t) \). Given \( J_{m,k}(t) \) and \( P(m,t) \) there are many possible transition rates satisfying Eq. (6). One possibility is to use the following one [36, 37]:

When \( J_{m,k}(t) \geq 0 \),
\[
T_{m,k}(t) = \frac{J_{m,k}(t)}{P(k,t)},
\] (8)

and when \( J_{m,k}(t) < 0 \),
\[
T_{k,m}(t) = 0,
\] (9)

Since we know the total wave function of the system and the environment \( |\Psi(t)\rangle \), the probability of a given property state \( |\Psi_m(t)\rangle \) is \( P(m,t) = \langle \Psi(t)|\pi_m|\Psi(t)\rangle \). Using \( P(m,t) \) and Eq. (1) with the Hamiltonian in Eq. (3) we obtain
\[
J_{m,k}(t) = 2 \text{Im} \{ \langle \Psi(t)|\pi_m H_I(t) \pi_k |\Psi(t)\rangle \}.
\] (10)

The method for generating the realizations of the process begins with solving the total system Schrödinger equation followed by the calculation of the quantities \( J_{m,k}(t) \), \( T_{m,k}(t) \) and \( P(k,t) \). For example, the probability to have a jump between the property states of the total system \( |\Psi_k(t)\rangle \rightarrow |\Psi_m(t)\rangle \), when \( J_{m,k}(t) > 0 \), between \( [t,t+\delta t] \) is \( \delta t T_{m,s}(t) \). Then using random numbers we can decide whether a jump takes place or not. From Eqs. (6) and (7) we see that the term \( \delta t T_{m,k}(t) \) includes the occupation probability of the source state \( k \) in the
ensemble and the rate term from $k$ to $m$ and together they give the transition rate for a single trajectory. After generation of the realizations, the state of the reduced system is
\[
\rho_S(t) = \text{tr}_E\left\{ \sum_m w_m(t)|\Psi_m(t)\rangle\langle \Psi_m(t)| \right\} = \sum_m w_m(t)|\phi_m(t)\rangle\langle \phi_m(t)|,
\]
where $w_m(t) = \frac{\#(m)}{M}$ are the approximations for probabilities $P(m, t)$. $M$ is the size of the statistical ensemble and $(m)$ is the number of ensemble members in state $m$.

### III. UNRAVELING IN THE REDUCED SYSTEM SPACE: NMQJ METHOD

The non-Markovian quantum jump (NMQJ) method is constructed as a piecewise deterministic process in the Hilbert space of the system $H_S$ [11] and the key ingredient is the association of negative decay rates to reverse quantum jumps. The starting point is the time-local non-Markovian master equation, which can be derived, e.g. with time-convolutionless projection operator method (TCL) [1]. General form of such master equation (given here in the interaction picture) is
\[
\frac{d}{dt} \rho_S(t) = -i[H_{LS}(t), \rho_S(t)] + \sum_j \Delta_j(t) \left( C_j \rho_S(t) C_j^\dagger - \frac{1}{2} \{ \rho_S(t), C_j^\dagger C_j \} \right),
\]
where $H_{LS}(t) = \frac{1}{2} \sum_j S_j(t) C_j^\dagger C_j$ is the Lamb shift Hamiltonian, $S_j(t)$ is the Lamb shift rate, $\Delta_j(t)$ is the decay rate which can take negative values and operator $C_j$ is the Lindblad or jump operator to channel $j$. The density matrix of the system at any point of time is decomposed as
\[
\rho_S(t) = \sum_{i=1}^{M_{eff}} P(|\psi_i(t), t\rangle\langle \psi_i(t)|),
\]
where $M$ is the size of the statistical ensemble of the unraveling, $M_{eff}$ is the dimension of the set of different states needed in the simulation (so-called effective ensemble size), and $P(|\psi_i(t), t\rangle)$ is the probability of finding state $|\psi_i(t)\rangle$ in $\rho_S(t)$. The states in the ensemble evolve according to [1]
\[
\frac{d}{dt}|\psi_i(t)\rangle = -i H_{eff}(t)|\psi_i(t)\rangle
\]
\[
= -i \left( H_{LS}(t) - i \frac{1}{2} \sum_j \Delta_j(t) C_j^\dagger C_j \right)|\psi_i(t)\rangle.
\]

The rate of jumps during positive decay in channel $j$ from state $|\psi_k(t)\rangle$ to state $|\psi_l(t)\rangle$ with jump operator $C_j$ is
\[
R_{kl}^j(t) = \Delta_j(t) |\psi_k(t)\rangle\langle \psi_l(t)| C_j^\dagger C_j |\psi_k(t)\rangle.
\]
The corresponding quantum jump is given by
\[
|\psi_k(t)\rangle \rightarrow |\psi_l(t)\rangle = \frac{C_j |\psi_k(t)\rangle}{\sqrt{\langle \psi_k(t)|C_j^\dagger C_j |\psi_k(t)\rangle}}.
\]
The rate of jumps during negative decay in channel $j$ is
\[
R_{kl}^j(t) = -\frac{P(|\psi_k(t), t\rangle)}{P(|\psi_l(t), t\rangle)} \Delta_j(t) |\psi_k(t)\rangle\langle \psi_l(t)| C_j^\dagger C_j |\psi_k(t)\rangle.
\]

### IV. CONNECTION BETWEEN THE GAW AND NMQJ UNRAVELINGS

To make a connection between the two unravelings, we are interested (i) whether the reduced system part of the total system property state realizations of the GAW method have similarities with the NMQJ realizations, and (ii) if the jumps within the two methods occur with the same rates. As we will show below, the answer for both of these questions is positive.

Comparing the rates, Eqs. (9) and (18), we note that the jump rates for the reverse probability flow and negative decay rates, $J_{m,k} < 0$ and $\Delta_j(t) < 0$ respectively, have similar structure. They both are inversely proportional to the probability to be in the source state of the jump. In the GAW method, the given property state is associated to specific mode to have the excitation (unless the environment is in the vacuum state). In the NMQJ realizations, we know whether the system or the environment has the excitation while in the latter case we do not know which specific mode has the excitation.

In order to reveal the detailed connection between the GAW and NMQJ methods, let us define the following operators
\[
\Pi_0 = I_S \otimes |0_1, 0_2, ..., 0_N\rangle\langle 0_1, 0_2, ..., 0_N| = I_S \otimes |0\rangle\langle 0|,
\]
\[
\Pi_1 = \sum_{k=1}^N I_S \otimes a_k^{\dagger}|0\rangle\langle 0|a_k = \sum_{k=1}^N I_S \otimes |k\rangle\langle 1_k|.
\]

From Eq. (4) we see that $\Pi_0 = \pi_m=0...0$ and $\Pi_1 = \sum_k \pi_k$, where $k = 0\cdots 1_k \cdots 0$ (i.e. $k$ labels all one mode configurations of the environment). We can now ask what is
functions evolve similarly between random jumps in both of the same set of projective rays in $H$. The state space consists of deterministic evolutions of the stochastic wave function of the combined GAW process. We will also see that the wave function is in the same projective ray as the values of the stochastic wave function of the NMQJ method, we can conclude that both methods generate similar realizations in the environment, but not knowing in which mode, there typically occurs probability flow components of the GAW realizations to both directions.

The connection between the GAW and the NMQJ methods is found by re-formulating the GAW method for the following combined property states:

$$|\Psi_0(t)\rangle = \frac{1}{\sqrt{N_0}} \Pi_0 |\Psi(t)\rangle,$$

$$|\Psi_1(t)\rangle = \frac{1}{\sqrt{N_1}} \Pi_1 |\Psi(t)\rangle.$$  \hfill (22)

For this purpose, we must calculate the combined probability current from the system to the environment. This is obtained by considering the total probability current from the $N$-mode vacuum states to all $1_k$-states

$$J_{1,0}(t) = \sum_{k=1}^{N} J_{1_k,0}(t).$$  \hfill (23)

It can be easily shown that the combined probability current satisfies $J_{1,0}(t) = -J_{0,1}(t)$ and

$$\frac{d}{dt} P(1, t) = J_{1,0}(t),$$

$$\frac{d}{dt} P(0, t) = -J_{0,1}(t).$$  \hfill (24)

We have $\sum_{k=1}^{N} \frac{d}{dt} P(1_k, t) = \frac{d}{dt} P(1, t)$ and the r.h.s. of both equations follow from the definition of Eqs. (6) and (23). The transition rates have similar structure as in Eqs. (6) and (23) but we must replace probability with combined probability and probability current with combined probability current.

As we will show below for specific examples, the GAW transition rates defined with combined quantities correspond to the transition rates of the NMQJ method. Here, $|\Psi_1(t)\rangle$ and $|\Psi_0(t)\rangle$, which are defined in the total system Hilbert space $H_S \otimes H_E$, are the possible values of the stochastic wave function of the combined GAW process. If the system part belonging to $H_S$ of the GAW stochastic wave function is in the same projectile ray as the values of the stochastic wave function of the NMQJ method, we can conclude that both methods generate similar realizations for the reduced system. We will also see that the deterministic evolutions of the stochastic wave functions for both processes are identical.

This means that the PDPs of the two methods are the same in the following sense. The state space consists of the same set of projective rays in $H_S$, stochastic wave functions evolve similarly between random jumps in both processes, and random jumps in both processes take place between the same two projective rays in $H_S$ with equal rates. It is sufficient that the states belong to the same projective ray in $H_S$ since we are interested only in the dynamics of the reduced system. Moreover, the states in the same projective ray give equal contribution to the density matrix of the system since the complex phase of the state is not an observable.

The summing of the GAW probability currents means that we lose the information to which mode the excitation from the system goes as the system decays. It is intuitive that the sum of the probability currents corresponds to the decay rate since the decay rate describes the total effect of the environment onto the system. However, it is important to note that for a given sign of the decay rate, there typically occurs probability flow components of the GAW realizations to both directions.

In examples below, we will set the frequency dependent couplings to be real-valued and equal to $g_k = \sqrt{d \nu_\text{eff}(\nu_k)}$, where $\nu_\text{eff}(\nu) = \frac{1}{2 \pi} \frac{\gamma_0^2}{\nu - \omega_k^2 + \lambda^2}$ is the spectral density, $d \nu$ is the mode spacing, $\lambda$ is the spectral width, $\omega_k$ is the position of the peak in frequency space, and $\gamma_0$ defines the height of the peak. These parameters are also related to the time scales involved in the dynamics. We have $\tau_S \sim \gamma_0^{-1}$, which is the time scale of the reduced system evolution, and $\tau_c \sim \lambda^{-1}$ is the time scale of the environmental correlation functions. We can also compare our discrete $N$-mode cases to the exact and numerical solutions obtained in the continuum limit $\sum_k |g_k|^2 \to \int d\nu \rho_\text{eff}(\nu)$.

In the following, we make a detailed study for a two-level system (TLA) and a three level atom in a $V$-configuration ($V$-system).

### A. Two-level atom

The Hamiltonian in the interaction picture is now

$$H_I = \frac{i}{\hbar} \sum_{k=1}^{N} g_k (|g\rangle\langle a_k \hat{e}^{i\Omega_k t} - |e\rangle\langle a_k e^{-i\Omega_k t}|),$$  \hfill (25)

where $\Omega_k = \nu_k - \omega_{eg}$. The state of the total system and the initial conditions are

$$|\Psi(t)\rangle = (c_g(t)|g\rangle + c_e(t)|e\rangle)|0\rangle + \sum_{k=1}^{N} c_k(t)|g\rangle|1_k\rangle,$$

$$c_k(0) = 0,$$  \hfill (26)

so that initially the modes of the environment are in a vacuum state. The Schrödinger equation and the interaction picture Hamiltonian lead to the following system of first order differential equations for the amplitudes:

$$\dot{c}_g(t) = 0,$$

$$\dot{c}_e(t) = -\sum_{k=1}^{N} g_k e^{-i\Omega_k t} c_k(t),$$

$$\dot{c}_k(t) = g_k e^{i\Omega_k t} c_e(t).$$  \hfill (27)
Here in the upper equation we use keeping in mind the previously derived results with the combined probability current reduced system part of the corresponding total system which can be easily calculated by using the Hamiltonian which are the two possible states that the stochastic wave function can take, are by using Eq. \[22\]

\[
|\Psi_0(t)\rangle = \frac{c_g(t)|g\rangle + c_c(t)|c\rangle}{\sqrt{|c_g(t)|^2 + |c_c(t)|^2}} |0\rangle,
\]

(29)

\[
|\Psi_1(t)\rangle = \frac{1}{\sqrt{P(1,t)}} \sum_{k=1}^{N} c_k|g\rangle|1_k\rangle
= \frac{1}{\sqrt{P(1,t)}} \sum_{k=1}^{N} c_k|g\rangle|1_k\rangle.
\]

(30)

In the GAW method, the combined property states, which are the two possible states that the stochastic wave function are from Eqs. (20) and (21).

\[
\frac{d}{dt}|\Psi(t)\rangle = \left\{ \begin{array}{ll}
|\Psi(t)\rangle & \text{if } t_1 < t < t_2, \\
0 & \text{otherwise},
\end{array} \right.
\]

\[|\Psi(t)\rangle = \frac{1}{\sqrt{P(1,t)}} \sum_{k=1}^{N} c_k|g\rangle|1_k\rangle.
\]

Here in the upper equation we use \[|\phi_0(t)\rangle\] to denote the reduced system part of the corresponding total system property state. From Eqs. (10) and (23) we get the combined probability current

\[
J_{1,0}(t) = -2\text{Re} \left\{ \frac{\dot{c}_c(t)}{c_c(t)} \right\} |c_c(t)|^2.
\]

(31)

The probabilities \[P(1,t)\] and \[P(0,t)\] satisfy Eq. (24) which can be easily calculated by using the Hamiltonian and the total equation of the system and the environment, or the definitions \[P(1,t), P(0,t)\] and \[J_{1,0}(t)\] [see the text below Eq. (24)]. We can define the transition rates by using Eqs. (8) and (9). When \[J_{1,0}(t) \geq 0\],

\[
T_{1,0}(t) = -2\text{Re} \left\{ \frac{\dot{c}_c(t)}{c_c(t)} \right\} |c_c(t)|^2
\]

\[T_{0,1}(t) = 0,
\]

(32)

and when \[J_{1,0}(t) < 0\],

\[
T_{1,0}(t) = 0,
\]

\[T_{0,1}(t) = 2\text{Re} \left\{ \frac{\dot{c}_c(t)}{c_c(t)} \right\} \frac{|c_c(t)|^2}{1 - |c_c(t)|^2}.
\]

(33)

Finally, the reduced density matrix can be obtained by taking the trace over the environment

\[
\rho_S(t) = \text{tr}_E \{w_0(t)|\Psi_0(t)\rangle\langle\Psi_0(t)| + w_1(t)|\Psi_1(t)\rangle\langle\Psi_1(t)|\}
= w_0(t)|\phi_0(t)\rangle\langle\phi_0(t)| + w_1(t)|g\rangle\langle g|.
\]

Next we will study the TLA with the NMQJ method keeping in mind the previously derived results with the GAW method. The master equation for the TLA unraveled with the NMQJ method is

\[
\frac{d}{dt}\rho_S(t) = -i \left[ \frac{1}{2} S(t) \sigma_+ \sigma_- - \rho_S(t) \right]
+ \Delta(t) \left( \sigma_- \rho_S(t) \sigma_+ - \frac{1}{2} \rho_S(t) \sigma_- \right).
\]

(34)

where the decay rate \[\Delta(t)\] and Lamb shift rate \[S(t)\] are \[1\]

\[
\Delta(t) = -2\text{Re} \left\{ \frac{\dot{c}_c(t)}{c_c(t)} \right\} c_c(t),
\]

\[S(t) = -2\text{Im} \left\{ \frac{\dot{c}_c(t)}{c_c(t)} \right\} c_c(t).
\]

(35)

and the non-hermitian Hamiltonian giving the deterministic evolution of the stochastic wave function is \[1\]

\[
H_{\text{eff}}(t) = \frac{1}{2} \left[ S(t) - i \Delta(t) \right] \sigma_+ \sigma_- - \rho_S(t).
\]

(36)

All the amplitudes \[c(t)\] in Eq. (26) are solutions of the Schrödinger equation for the system and the environment with the Hamiltonian from Eq. (25). These amplitudes have the following connection to the normalized state vectors of the effective ensemble of the NMQJ method

\[
|\psi_0(t)\rangle = \frac{c_g(t)|g\rangle + c_c(t)|c\rangle}{\sqrt{|c_g(t)|^2 + |c_c(t)|^2}},
\]

\[
|\psi_1(t)\rangle = |g\rangle,
b_g(0) = c_g(0), b_c(0) = c_c(0).
\]

(37)

Comparing these with the property state \[|\Psi_0(t)\rangle\] of the GAW method in Eq. (29), we can see that

\[
\text{tr}_E \{ |\Psi_0(t)\rangle\langle\Psi_0(t)| \} = |\phi_0(t)\rangle\langle\phi_0(t)| = |\psi_0(t)\rangle\langle\psi_0(t)|,
\]

\[
\text{tr}_E \{ |\Psi_1(t)\rangle\langle\Psi_1(t)| \} = |g\rangle\langle g| = |\psi_1(t)\rangle\langle\psi_1(t)|.
\]

(38)

This shows that the reduced system part of the GAW realizations and the NMQJ realizations are identical. We are left with showing in detail that also the transition rates are the same.

The reduced density matrix in NMQJ is

\[
\rho_S(t) = P(|\psi_0(t)\rangle, t)|\phi_0(t)\rangle\langle\phi_0(t)| + P(|\psi_1(t)\rangle, t)|\psi_1(t)\rangle\langle\psi_1(t)|.
\]

(39)

When \[\Delta(t) \geq 0\] we have transitions from \[|\psi_0(t)\rangle\rightarrow |\psi_1(t)\rangle\] and from Eq. (15) we obtain

\[
R_{1,0}(t) = \Delta(t) \frac{|c_c(t)|^2}{|c_g(t)|^2 + |c_c(t)|^2}.
\]

(40)

This is identical to \[T_{1,0}(t)\] when \[J_{1,0}(t) \geq 0\], see Eqs. (32) and (35).

When \[\Delta(t) < 0\] we have transitions from \[|\psi_1(t)\rangle\rightarrow |\psi_0(t)\rangle\] and

\[
R_{0,1}(t) = -P(|\psi_0(t)\rangle, t) \Delta(t) \frac{|c_c(t)|^2}{|c_g(t)|^2 + |c_c(t)|^2}.
\]

(41)

Since \[\rho_S(t)\] must be a positive operator we know that the decay rate \[\Delta(t)\] and therefore also \[J_{1,0}(t)\], must initially be positive. Let us call \[t_1\] the time when \[\Delta(t)\] turns negative for the first time. Now \[\rho_S(t)\], when \[t < t_1\], generated by GAW and NMQJ must be the same, since from Eq. (38) we see that the states in
the decomposition of $\rho_S(t)$ belong to the same projective ray and $R_{1,0}(t) = \mathcal{T}_{1,0}(t)$ for $t < t_1$. Therefore we have $P(0, t) = |c_0(t)|^2 + |c_1(t)|^2 = P(\psi_0(t), t)$ and $P(1, t) = P(\psi_1(t), t)$. Now we can rewrite $R_{0,1}(t)$ as

$$R_{0,1}(t) = -\frac{P(0, t)}{P(1, t)} \frac{\Delta(t)|c_1(t)|^2}{\Delta(t)|c_0(t)|^2} = -\frac{\Delta(t)|c_1(t)|^2}{\Delta(t)|c_0(t)|^2},$$

(42)

which is the same as $\mathcal{T}_{0,1}(t)$, when $J_{1,0}(t) < 0$, see Eqs. [33] and [35]. It is also clear now that at $t = t_1$ both $J_{1,0}(t)$ and $\Delta(t)$ turn negative.

Thus we have shown that we can derive the NMQJ results from the GAW method for this system. This means (i) that we can obtain the decay rate in the master equation (34) from the probability currents between the total system property states of the GAW method, and (ii) that the random state vector in $\mathcal{H}_S$ in both methods obtains its possible values from the same set of states, namely $\{g\}$ and $\{\psi_0\}$ (we neglect the global phase since it plays no role here).

In the first example we have chosen the parameters as $|\Psi(t)\rangle = |e\rangle|0\rangle$, time scale $[t] = 1/\gamma$, $\delta = 3\lambda$ and $\gamma_0 = 0.8\lambda$. We use 180 environmental modes and a statistical ensemble with $10^4$ members. With the parameters mentioned above, the decay rate in the master equation (34) is time dependent but always positive, thus corresponding to the time-dependent Markovian case. This also means that there are no reverse jumps in the NMQJ method in this parameter regime. However, as Fig. 1 shows, there are negative probability currents in the GAW method for specific modes or individual property states, while the total probability current between the system and the environment, $J_{1,0}(t)$, remains positive indicating net current from the system to the environment. This means that while there are individual transitions from one photon to zero photon states in GAW, the number of transitions from zero photon states to one photon states is larger keeping the total probability current positive, which then matches the probability current obtained from NMQJ.

In the second example we have chosen the parameters as in the first example except for $\gamma_0 = 4\lambda$ and $\delta = -4\lambda$. The system is now in the non-Markovian regime displaying also negative values for the decay rate. Figure 2 shows the individual probability currents for this case. The results show that the region $\nu_k - \omega_c \approx 0$ (or $\nu_k \approx \omega_c$) gives the dominant contribution to the total probability current and it has also dominant negative contribution. As a consequence, the total current has negative periods, which is reflected in the negative regions for the decay rate, and thus the system is driven to the non-Markovian regime.

In Fig. 3 we have plotted the decay rate which is calculated from the probability current components. We compare it to the exact decay rate calculated in the continuum limit and see that the agreement of the curves is good. In the same figure we have also plotted the exact solution for the density matrix and compare it to the simulated ones, and we can see that the agreement of the curves is excellent.

FIG. 1. Probability currents $J_{1,0}(t)$ for TLA in the Markovian case. Initial state is $|e\rangle|0\rangle$, $[t] = 1/\lambda$, $\delta = 3\lambda$, $\gamma_0 = 0.8\lambda$ and we use 180 environmental modes. When $t \approx 1$ we see that there occurs negative probability currents.

FIG. 2. Probability currents $J_{1,0}(t)$ for TLA. The parameters are as in Fig. 1 except that $\gamma_0 = 4\lambda$ and $\delta = -4\lambda$. We can identify the modes for which $\nu_k \approx \omega_c$ responsible for the non-Markovian effects. See the text for details.

### B. V-system

The Hamiltonian for the V-system in the interaction picture is

$$H_I = i \sum_{k=1}^N g_k (|c\rangle \langle a| a_k e^{i\Omega_k \cdot a} + |c\rangle \langle b| a_k e^{i\Omega_k \cdot a} + \text{h.c}),$$

(43)
where \( \Omega_{k,i} = \nu_k - \omega_i, \) \( i = a, b, \) and we have denoted with \(|a\rangle\) and \(|b\rangle\) the two upper states and with \(|c\rangle\) the ground state. Differential equations for the amplitudes obtained from Schrödinger equation are

\[
\begin{align*}
\dot{c}_c(t) &= 0, \\
\dot{c}_a(t) &= -\sum_{k=1}^N g_k e^{-i\Omega_{k,a} t} c_k(t), \\
\dot{c}_b(t) &= -\sum_{k=1}^N g_k e^{-i\Omega_{k,b} t} c_k(t), \\
\dot{c}_k(t) &= g_k (c_a(t) e^{i\Omega_{k,a} t} + c_b(t) e^{i\Omega_{k,b} t}).
\end{align*}
\] (44)

As we have seen in Sec. IV.A, the sum of the probability currents over all modes is related to the decay rate. By using the same procedure as in Sec. IV.A, it is possible to derive the following equations for the probabilities

\[
\begin{align*}
\frac{d}{dt} P(0,t) &= -\mathcal{J}_{1,0}(t), \\
\frac{d}{dt} P(1,t) &= \mathcal{J}_{1,0}(t).
\end{align*}
\] (45)

The reduced system dynamics corresponding to these equations is given by a non-secular master equation which is not in general compatible with the form given in Eq. (12) used as a starting point for the NMQJ.

To find the connection between GAW and NMQJ in this system, we approximate the exact non-secular dynamics by de-coupling the evolution of the coherences and populations [28]. Eventually this means that the emission of the photon can be associated to one of the two decay channels and we write the Hamiltonian as

\[
H_I = i \sum_{k=1}^N g_k (|c\rangle\langle a| a_k e^{i\Omega_{k,a} t} + |c\rangle\langle b| b_k e^{i\Omega_{k,b} t} + \text{h.c.}),
\] (46)

and these equations are a good approximation for Eq. (44) in certain parameter regions.

We assume that initially the environmental modes are empty. Then we can give the total state of the system and the environment as

\[
|\Psi(t)\rangle = c_c(t)|c\rangle|0\rangle_a|0\rangle_b + c_a(t)|0\rangle_a|0\rangle_b + c_b(t)|0\rangle_a|0\rangle_b + \sum_{k=1}^N c_k^*(t)|1\rangle_a|0\rangle_b + \sum_{k=1}^N c_k^*(t)|0\rangle_a|1\rangle_b.
\] (48)

From now on we drop the subscripts referring to different Hilbert spaces. We want to know the probabilities to find a photon in the environment and we want to identify which of the excited states has decayed. Therefore it is natural to use the following operators

\[
\begin{align*}
\Pi_0 &= I_S \otimes |0\rangle \langle 0| \otimes |0\rangle \langle 0|, \\
\Pi_{1,a} &= \sum_{k=1}^N I_S \otimes |1\rangle_a \langle 1|_k \otimes |0\rangle \langle 0|, \\
\Pi_{1,b} &= \sum_{k=1}^N I_S \otimes |0\rangle \langle 0| \otimes |1\rangle_a \langle 1|_k.
\end{align*}
\] (49)

The probability to have one photon in the environment which has been created when the excited state \( i \) decayed, is \( P^i(1,t) \), where \( i = a, b, \) and the probability to have zero photons in the environment is \( P(0,t) \). Following a similar procedure as for the earlier presented TLA case, we can calculate them as

\[
\begin{align*}
P^i(1,t) &= \langle \Psi(t)|\Pi_{1,i}|\Psi(t)\rangle = \sum_{k=1}^N |c_k^*(t)|^2, \\
P(0,t) &= \langle \Psi(t)|\Pi_0|\Psi(t)\rangle = |c_c(t)|^2 + |c_a(t)|^2 + |c_b(t)|^2.
\end{align*}
\] (50)
Subsequently, the combined property states are
\[
|\Psi_0(t)\rangle = \frac{c_a(t)|c|0\rangle|0\rangle + c_a(t)|a\rangle|0\rangle + c_b(t)|b\rangle|0\rangle}{\sqrt{P(0,t)}},
\]
(51)
\[
|\Psi_{1,a}(t)\rangle = \frac{\sum_{k=1}^N c^*_k(t)|c\rangle|1_k\rangle|0\rangle}{\sqrt{P^n(1,t)}},
\]
\[
|\Psi_{1,b}(t)\rangle = \frac{\sum_{k=1}^N c^*_k(t)|c\rangle|1_k\rangle|0\rangle}{\sqrt{P^n(1,t)}}.
\]

The differential equations for probabilities \(P(0,t)\) and \(P^n(1,t)\) can be calculated with the help of Eqs. (23), (47) and (48). We obtain
\[
\frac{d}{dt}P(0,t) = -J_1^{a,b} - J_{1,0}(t),
\]
\[
\frac{d}{dt}P^n(1,t) = J_1^{a,b},
\]
\[
\frac{d}{dt}P^b(1,t) = J_1^{b,0}(t),
\]
(52)
where the combined probability currents \(J_1^{a,b}\) and \(J_1^{b,0}\) tell how much probability is flowing from the system to the environment in each channel separately. The combined probability currents are now
\[
J_1^{a,b}(t) = -2\Re \left\{ \frac{\dot{c}_i(t)}{c_i(t)} \right\} |c_i(t)|^2,
\]
(53)
where \(i = a, b\). We can define transition rates as in Eqs. (3) and (4) separately for each decay path since we can partition the combined probability current into two independent parts. They are, when \(J_1^{a,b}(t) \geq 0\),
\[
T_1^{a,b}(t) = \frac{J_1^{a,b}(t)}{P(0,t)} = -2\Re \left\{ \frac{\dot{c}_i(t)}{c_i(t)} \right\} \frac{|c_i(t)|^2}{P(0,t)},
\]
\[
T_0^{a,b}(t) = 0,
\]
(54)
and when \(J_1^{a,b}(t) < 0\),
\[
T_1^{a,b}(t) = 0,
\]
\[
T_0^{a,b}(t) = -J_1^{a,b}(t) = 2\Re \left\{ \frac{\dot{c}_i(t)}{c_i(t)} \right\} \frac{|c_i(t)|^2}{P(1,t)},
\]
(55)
where \(i = a, b\).

The reduced density matrix generated by the GAW method is now
\[
\rho_S(t) = \text{tr}_E \{ w_0(t)|\Psi_0(t)\rangle\langle\Psi_0(t)| + w_{1,a}(t)|\Psi_{1,a}(t)\rangle\langle\Psi_{1,a}(t)|
+ w_{1,b}(t)|\Psi_{1,b}(t)\rangle\langle\Psi_{1,b}(t)| \}.
\]
(56)

Next we will study the NMQJ method for this system. The master equation describing the reduced system dynamics under secular approximation is
\[
\frac{d}{dt}\rho_S(t) = -i\frac{1}{2}S_a(t)|a\rangle\langle a|\rho_S(t) - i\frac{1}{2}S_b(t)|b\rangle\langle b|\rho_S(t]
+ \Delta_a(t)\{ |c\rangle\langle b|\rho_S(t)|a\rangle\langle c| - \frac{1}{2}\rho_S(t)|a\rangle\langle a| \}
+ \Delta_b(t)\{ |c\rangle\langle b|\rho_S(t)|b\rangle\langle c| - \frac{1}{2}\rho_S(t)|b\rangle\langle b| \}.
\]
(57)
The total state of the system and the environment has been given in Eq. (48), and by tracing out the environmental degrees of freedom and taking the time derivative of the expression \(|\Psi(t)\rangle\langle\Psi(t)|\) we can identify the Lamb shifts and the decay rates to be
\[
\Delta_i(t) = -2\Re \left\{ \frac{\dot{c}_i(t)}{c_i(t)} \right\},
\]
\[
S_i(t) = -2\Im \left\{ \frac{\dot{c}_i(t)}{c_i(t)} \right\},
\]
(58)
where \(i = a, b\). The non-Hermitian Hamiltonian for NMQJ in this system is
\[
H_{\text{eff}}(t) = \sum_i \frac{1}{2} (S_i(t) - i\Delta_i(t))|i\rangle\langle i|,
\]
(59)
where again \(i = a, b\). We can give the deterministically evolving state of the NMQJ process and the initial condition as
\[
|\psi_0(t)\rangle = d_a(t)|c\rangle + d_a(t)|a\rangle + d_b(t)|b\rangle,
\]
\[
d_j(0) = c_j(0),
\]
(60)
where \(j = c, a, b\) and \(c_j(t)\) are probability amplitudes from Eq. (48). By solving the time evolution given by the Hamiltonian of Eq. (59), we see that \(c_a(t) = d_a(t)\), \(c_b(t) = d_a(t)\), and \(c_a(t) = d_b(t)\). In NMQJ, the realizations of the process are normalized and therefore we can write
\[
|\psi_0(t)\rangle = \frac{c_a(t)|c\rangle + c_a(t)|a\rangle + c_b(t)|b\rangle}{\sqrt{|c_a(t)|^2 + |c_b(t)|^2 + |c_a(t)|^2}},
\]
\[
|\psi_1(t)\rangle = |c\rangle
\]
(61)
The reduced density matrix of the NMQJ process is then
\[
\rho_S(t) = P(|\psi_0(t)\rangle, t)|\psi_0(t)\rangle\langle\psi_0(t)| + P(|\psi_1(t)\rangle, t)|\psi_1(t)\rangle\langle\psi_1(t)|.
\]
(62)
As in Eqs. (15) and (18), and using Eqs. (50), we can write the transition rates, where \(\Delta_i(t) \geq 0\),
\[
R^{i}_{10}(t) = \frac{|c_i(t)|^2}{P(0,t)}
\]
\[
R^{i}_{01}(t) = 0,
\]
(63)
and when $\Delta_i(t) < 0$,

$$R_{10}^i(t) = 0,$$

$$R_{01}^i(t) = -\frac{P(\psi_0(t), t)}{P(\psi_1(t), t)} \Delta_i(t) \frac{|\psi_i(t)|}{P(0, t)}, \quad (64)$$

where $i = a, b$. By using Eqs. (51) and (61), we obtain the connection between the GAW and NMQJ state vectors

$$\text{tr}_E[|\Psi_0(t)\rangle\langle\Psi_0(t)|] = |\psi_0(t)|^2,$$

$$\text{tr}_E[|\Psi_{1,i}(t)\rangle\langle\Psi_{1,i}(t)|] = |\psi_1(t)|^2,$$

where $i = a, b$.

This means that the system Hilbert space part of the possible realizations of the combined GAW process and the NMQJ process with the same index belong to the the same projective ray in $\mathcal{H}_S$. We also see that there is redundancy in $\text{tr}_E[|\Psi_{1,i}(t)\rangle\langle\Psi_{1,i}(t)|]$ since both states when $i = a, b$ belong to the same projective ray in $\mathcal{H}_S$. It means that we can combine $w_{1,b}(t) + w_{1,a}(t) = w_1(t)$ in Eq. (65) and that both transition rates $T^a$ and $T^b$ induce jumps between the same two projective rays but the rates of the jumps are generally different.

We assume that from some initial time $t_0$ to $t_1$ the rates $\Delta_a(t)$ and $\Delta_b(t)$ are positive. Then from Eqs. (54), (58) and (63) we see that $R_{10}^a(t) = T_{01}^a(t)$ and $R_{01}^a(t) = T_{10}^a(t)$. This implies that the density matrices generated by GAW and NMQJ are the same at least to $t_1$ when at least one of the decay rates or collective probability currents turns negative. Since NMQJ and GAW both have normalized realizations we can deduce that $w_0(t) = P(0, t) = P(|\psi_0(t)|, t)$ and $w_1(t) = P(1, t) = P(|\psi_1(t)|, t)$ when $t \in [t_0, t_1]$.

Now when negative currents ($J_{10}^i(t) < 0$) or decay rates ($\Delta_i(t) < 0$) emerge when $t > t_1$, the transition rates are $T_{01}^a(t) = R_{01}^a(t)$ and $T_{10}^a(t) = R_{10}^a(t)$ since we have $P(0, t) = P(|\psi_0(t)|, t)$ and $P(1, t) = P(|\psi_1(t)|, t)$ (the calculation is the same as we did in Eq. (42)). Thus we have shown that the GAW process for the combined property state is an equivalent process to NMQJ in $\mathcal{H}_S$ in the sense we defined in the beginning of Sec. IV.

Next we study a numerical example where the initial state is written in non-secular case as $|\Psi(t)| = \frac{1}{\sqrt{3}}(|a\rangle_S|0\rangle_E + |b\rangle_S|0\rangle_E)$ and under secular approximation, where each channel has independent environment, as $|\Psi(t)| = \frac{1}{\sqrt{2}}(|a\rangle_S|0\rangle_{E_a}|0\rangle_{E_b} + |b\rangle_S|0\rangle_{E_a}|0\rangle_{E_b})$. We are written here the different Hilbert spaces explicitly for clarity but from now on we omit this for compactness of notation. Other parameters are defined as $|t| = 1/\lambda$, $\gamma_0 = 4\lambda$, $\delta_a = 3\lambda$, $\delta_b = -3\lambda$ and we have used 240 environmental modes.

We start with the non-secular case. Figure 4 shows the corresponding probability currents between the property states of the GAW method. The interference of probability currents is visible. In the secular case Fig. 5 shows probability currents under the secular approximation which decouples the two excited states. Probability currents can not interfere because each excited state interacts with its separate environment. The comparison between the density matrices for the two cases are shown in Fig. 6. In the same figure we can also see that under secular approximation the reduced dynamics are governed by master equation (57). We can clearly see the effect of the interference of the probability currents to the reduced system dynamics in the non-secular case.

In Fig. 7 we show the effect of the secular approximation to the combined probability current from the system to the environment, i.e. the difference of $J_{1,0}^a(t)$ and $J_{1,0}^b(t)$ + $J_{1,0}^b(t)$. There are fast oscillations in $J_{1,0}(t)$ and it can even be negative when $J_{1,0}^b(t) + J_{1,0}^b(t)$ is positive. In Fig. 7 we compare the secular approximation decay rate calculated from GAW to the TCL2 [1] decay rate and we see that the match is very good.

![FIG. 4](image-url) Probability currents in the non-secular case. The initial state is $\frac{1}{\sqrt{2}}(|a\rangle|0\rangle + |b\rangle|0\rangle)$, $|t| = 1/\lambda$, $\gamma_0 = 4\lambda$, $\delta_a = 3\lambda$, $\delta_b = -3\lambda$, and we have used 240 environmental modes.

![FIG. 5](image-url) Probability currents in the secular case. The parameters are as in Fig. 4 but the initial state is $\frac{1}{\sqrt{2}}(|a\rangle|0\rangle|0\rangle + |b\rangle|0\rangle|0\rangle)$.
FIG. 6. Density matrix elements for the V-system. The parameters are as in Figs. 4 and 5. For the chosen parameter values $\rho_{aa}(t) = \rho_{bb}(t)$.

FIG. 7. Top: Sum of probability currents from the system to the environment. Solid red line is the non-secular case where we can not distinguish different decay channels. Blue circles are the secular case where we have two different decay channels. Bottom: Decay rates calculated from GAW method for the secular case (solid blue line) and decay rate of TCL2 master equation (red circles). Parameters are as in Figs. 4 and 5.

V. CONCLUSIONS

We have studied the non-Markovian dynamics of simple quantum optical systems by means of two jump-like unravelings. The GAW method uses piecewise deterministic realizations within the Hilbert space of the total system while the NMQJ method exploits piecewise deterministic realizations within the Hilbert space of the reduced system. Our analysis shows that there exists a connection between the two methods. In particular, we have demonstrated that the reduced system part of the property states of the GAW are identical for the NMQJ state vectors in the considered cases. Moreover, the summation over the probability currents appearing in the GAW formalism are directly connected to the decay rates of the time-local master equations and hence to the rates of jumps in the NMQJ method. While there exists quite a large variety of Monte Carlo methods for non-Markovian systems [11–13, 27–37], both jump and diffusion type, generally the connections between the methods have not yet been extensively investigated apart of a few studies [35, 44]. We expect that the results presented here stimulate further research in this area leading to improved insight to the often complex quantum dynamics of non-Markovian systems. Moreover, analyzing the probability currents in similar manner as treated here, may lead to further understanding of the information flow between the system and the environment, a topic which is currently vividly discussed in the context of open quantum systems.

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