Embedding dissipation and decoherence in unitary evolution schemes

A. R. P. Rau* and R. A. Wendell
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001

Dissipation and decoherence, and the evolution from pure to mixed states in quantum physics are handled through master equations for the density matrix. By embedding elements of this matrix in a higher-dimensional Liouville-Bloch equation, the methods of unitary integration are adapted to solve for the density matrix as a function of time. Results are illustrated for a damped, driven two-level system, the work involved being nearly all analytical.

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The study of open quantum systems is of widespread interest across different areas of physics particularly in the irreversible processes of dissipation and decoherence afforded by coupling to an external reservoir or environment. Quantum optics is replete with such studies for optical bistability, resonance fluorescence, and the general evolution from pure to mixed states, often considered through damped, driven two-level atoms [1]. Coupled quantum wells in a wider context and the study of quantum Brownian motion, dissipation and fluctuations have also received much attention [2]. Application of such considerations to "quantum non-demolition" in the emerging field of laser-interferometric gravitational wave detection, and of quantum noise and decoherence in the field of quantum computation, add to the importance of this subject. Finally, this evolution from pure to mixed states is at the heart of the problem of measurement in quantum theory [3].

On the other hand, unitary integration schemes for the evolution operator of time-dependent Hamiltonians, when available, are powerful because they preserve invariants and are stable, also in numerical application. In this Letter, we present a general procedure and illustrate with an example how to preserve most of these advantages even while working with systems exhibiting dissipation and decoherence. There are two key steps. First, the n-dimensional Liouville-von Neumann-Lindblad (LvNL) equation containing dissipation and decoherence is embedded in a (n^2-1)-dimensional Liouville-Bloch form with a non-Hermitian Hamiltonian. Second, this Liouville-Bloch equation is handled by a "unitary integration" procedure that has been described in recent years [4, 5, 6] wherein the evolution operator is written as a product of exponentials, each exponent involving an element of a closed Lie algebra of operators together with a multiplicative classical function of time. With all the non-commutativity handled analytically, the entire problem is reduced to solving coupled, first-order differential equations for this set of *classical* functions. In many cases, this set reduces to a single non-trivial Riccati (first order, quadratically nonlinear) equation for one of the classical functions, all the rest then obtained through trivial quadratures [6]. All of the above features remain valid even when the Hamiltonian is non-Hermitian and the evolution non-unitary.

Two other papers share our aims in setting the passage from pure to mixed states in a unitary evolution scheme but they proceed differently. One deals with weak dissipation, handling the Hermitian part of the LvNL equation through unitary integration and the dissipative terms through conventional integrators [7]. Because of their focus on numerical integration, both these handlings are for small time steps whereas we aim for integration over arbitrary, finite t. Another work [8] introduces a novel "square root operator" of the density matrix and an associated n^2-dimensional Hilbert space, along with additional constraints that are not in conventional quantum mechanics. Our embedding in a higher dimensional space does not introduce any new elements beyond those already in the density matrix.

We begin with the master equation for the density matrix ρ, sometimes called the Liouville-von Neumann-Lindblad equation [1, 2, 3],

$$\begin{aligned} i\dot{\rho} &= [H,\rho] + \frac{1}{2}i\sum_k \left([L_k\rho, L_k^\dagger] + [L_k, \rho L_k^\dagger]\right) \\ &= [H,\rho] - \frac{1}{2}i\sum_k \left(L_k^\dagger L_k\rho + \rho L_k^\dagger L_k - 2L_k\rho L_k^\dagger\right), \end{aligned} \quad (1)$$

where an over-dot denotes differentiation with respect to time and $\hbar$ has been set equal to unity, H is a Hermitian Hamiltonian, and the second term on the right-hand side is the "Liouvillian super-operator" describing coupling to the environment and the resulting irreversibilities of dissipation and decoherence. The above form in the Markov approximation with an explicitly traceless right-hand side guarantees conservation of $Tr(\rho)$ and positivity of the probabilities. For a more mathematical description in terms of so-called "dynamical semigroups," we refer to [9, 10].

Our aim in this paper is to solve Eq. (1) for fairly general time-dependences of H and the L's contained in it, while keeping as closely as possible to the unitary integration that applies in the absence of the super-operator. This method [4, 5, 6] has been developed when $H(t)$ is a sum of terms, each of which involves a time-independent operator multiplying a classical function of time. In such a case, without any recourse to time-ordered Dyson expansions, one can solve for the evolution operator $U(t)$ satisfying

$$i\dot{U}(t) = H(t)U(t), \quad U(0) = \mathcal{I}, \tag{2}$$

by writing $U(t)$ as a product

$$U(t) = \prod_j \exp[-i\mu_j(t)A_j], \tag{3}$$

where A_j are the operators contained in $H(t)$ together with a sequence of other operators formed out of their mutual commutators in a successive fashion. If this set forms a closed algebra under commutation, then upon substitution, Eq. (3) can be shown to satisfy Eq. (2) through repeated application of the Baker-Campbell-Hausdorff (B-C-H) identity [4,6]. This results in a well defined set of coupled first-order, generally nonlinear, equations for the functions $\mu_j(t)$. Thereby the quantal problem is reduced to the classical one of solving this set of equations, following which $\rho(t)$ is obtained as

$$\rho(t) = U(t)\rho(0)U^\dagger(t). \tag{4}$$

In extending this procedure, consider first retaining only the first two terms in the superoperator so as to have Eq. (1) take the form

$$i\dot{\rho} = V\rho - \rho W. \tag{5}$$

Even with V and W non-Hermitian, it is simple to extend Eq. (4) by using two different products $U_L(t)$ and $U_R(t)$ so that $\rho(t) = U_L(t)\,\rho(0)\,U_R^\dagger(t)$, with correspondingly different functions $\mu_{Lj}(t)$ and $\mu_{Rj}(t)$ in Eq. (3). Once again, upon calculating $i\dot{\rho}$ with such a form, the B-C-H identity can be used to cast it in the form of the right-hand side of Eq. (5), that is, having all operators standing on the left or right of $\rho(t)$. From Eq. (5) there then follow a well-defined set of equations for the μ_L and μ_R. However, the last term in the superoperator in Eq. (1), wherein $\rho(t)$ occurs between operators multiplying it both on the right and from the left, no longer permits easy generalization. Note that this last term is the so-called "quantum jump" in interpretations of the LvNL equation as conventional continuous evolution albeit with a non-Hermitian Hamiltonian ($V = H, W = H^\dagger$) plus a jump [11].

For the full master equation, we proceed by separating the invariant $Tr(\rho)$ from the n^2 elements $\rho_{ij}(t)$. Eq. (1) then reduces for the remaining $n^2 - 1$ elements to the Liouville-Bloch form

$$i\dot{\eta}(t) = \mathcal{L}(t)\eta(t), \tag{6}$$

where one convenient choice for the $(n^2 - 1)$ elements of η is $\rho_{11} - \rho_{ii}$, $i = 2, 3, ...n$; $\rho_{ij} + \rho_{ji}$, $\rho_{ij} - \rho_{ji}$, $i > j$. The first $(n - 1)$ of these describe the diagonal elements of the density matrix, the other $(n^2 - n)$ $i \neq j$, describe, respectively, in-phase dispersive and out-of-phase absorptive components of polarization. Even though $\mathcal{L}$ may not be Hermitian, the form of Eq. (6) is now the same as in Eq. (2) with all operators to the left of η so that the same procedure of a product exponential form for $\eta(t)$ as in Eq. (3) can be carried out now in the $(n^2 - 1)$-dimensional space. Thereby, the LvNL equation for ρ has been embedded in a higher-dimensional Liouville-Bloch equation.

One immediate consequence is worth noting. If the operators L_k in Eq. (1) are such that $\mathcal{L}$ in Eq. (6) involves imaginary elements and, consequently, η decays asymptotically, $\eta(t \to \infty) \to 0$, then all coherences vanish (off-diagonal ρ_{ij}) and all diagonal ρ_{ii} become equal, $\rho_{ii}(t \to \infty) \to (1/n)Tr(\rho(0))$. $Tr(\rho^2)$ on the other hand, decreases asymptotically to $(1/n)$ of its initial value. A specific $n = 2$ illustration will be given below of this rather general conclusion.

To demonstrate this method, we turn now to a series of recent papers [12] that discussed phase coherences and transitions in a periodically driven two-level system with a single L in Eq. (1):

$$H = \frac{1}{2}\epsilon(t)\sigma_z + J\sigma_x,\; L = \sqrt{\Gamma}\sigma_z,\; \rho_{ij}(0) = \delta_{ij}\delta_{i1}. \tag{7}$$

Applying our procedure, we have $\rho_{11}(t) + \rho_{22}(t) = 1$, and Eq. (6) for the three remaining elements takes the form

$$i\frac{d}{dt}\begin{pmatrix} \rho_{12} + \rho_{21} \\ \rho_{21} - \rho_{12} \\ \rho_{11} - \rho_{22} \end{pmatrix} = \begin{pmatrix} -i\Gamma & -\epsilon(t) & 0 \\ -\epsilon(t) & -i\Gamma & 2J \\ 0 & 2J & 0 \end{pmatrix} \times \begin{pmatrix} \rho_{12} + \rho_{21} \\ \rho_{21} - \rho_{12} \\ \rho_{11} - \rho_{22} \end{pmatrix}. \tag{8}$$

To solve this as a product of exponentials, we need the eight operators of an SU(3) algebra. Instead, we adopt a simplified variant of Eq. (7) as our model with a symmetric choice for the L_k involving all three Pauli matrices, that is, $L_k = \sqrt{\Gamma/2}\sigma_k$. This modifies Eq. (8) to introduce also a $(-i\Gamma)$ in the third diagonal element of the matrix. With the matrix then expressible as

$$\mathcal{L} = -i\Gamma\mathcal{I} - \epsilon(t)A_z + 2JA_x\;, \tag{9}$$

where A_x, A_y, A_z are the operators of angular momentum in a representation

$$A_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \quad A_y = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix},$$

$$A_z = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{10}$$

the closed Lie algebra of these three suffices to solve Eq. (6) by our unitary integration procedure. Since this procedure rests only on the commutators between A_j, we can use any representation of them as is convenient. We exploit this in choosing Eq. (10) so that $\mathcal{L}$ involves the A_j only linearly. Although, for comparison with [12], only ϵ in Eq. (9) is a function of time, we note that everything that follows applies also to more general time dependences of J and Γ and inclusion of a time-dependent term in A_y as well.

The first term in Eq. (9) leads to a trivial factor $\exp(-\Gamma t)$ and the remaining Hermitian part of $\mathcal{L}$ has been solved before [6]:

$$\begin{aligned} \eta(t) \;&=\; \exp[-\Gamma t] \exp[-i\mu_+(t)A_+] \\ &\times \exp[-i\mu_-(t)A_-] \exp[-i\mu(t)A_z]\eta(0), \end{aligned} \tag{11}$$

with $A_\pm \equiv A_x \pm iA_y$, $\eta(0) = (0, 0, 1)$, and

$$\dot{\mu}_+ - i\epsilon(t)\mu_+ - J(1 + \mu_+^2) \;=\; 0, \tag{12a}$$

$$\dot{\mu} = 2iJ\mu_+ - \epsilon(t), \tag{12b}$$

$$\dot{\mu}_- - i\dot{\mu}\mu_- = J, \qquad \mu_i(0) = 0. \tag{12c}$$

The first of these equations, involving $\mu_+(t)$ alone in Riccati form, is the only non-trivial member of this set. Solutions give through Eq. (11),

$$\begin{aligned} \rho_{11}(t) \;&=\; \frac{1}{2} + \frac{1}{2}\exp(-\Gamma t)\,[1 - 2\mu_+(t)\mu_-(t)], \\ \rho_{22}(t) \;&=\; \frac{1}{2}[1 - \exp(-\Gamma t)] + \mu_+(t)\mu_-(t)\exp(-\Gamma t), \\ \rho_{12}(t) \;&=\; i\mu_-(t)\exp(-\Gamma t), \\ \rho_{21}(t) \;&=\; i\mu_+(t)[\mu_+(t)\mu_-(t) - 1]\exp(-\Gamma t). \end{aligned} \tag{13}$$

The coherences vanish asymptotically and ρ_{11} and ρ_{22} attain the value $\frac{1}{2}$ as $t \to \infty$. While $Tr(\rho)$ remains always at unity, $Tr(\rho^2)$ decreases to (1/2). Simple numerical integration of Eq. (12a) for an oscillating driving field $\epsilon(t) = A\cos(\omega t)$ are shown in Figs. 1 and 2 for various values of the parameters (ω, J, A, Γ) . They are in agreement with [12]. In Fig. 2(c), we also record the time evolution of the entropy, $S = -Tr(\rho \ln \rho)$. The value of Γ governs the rate of rise as S increases monotonically from 0 to its asymptotic limit of $\ln 2$.

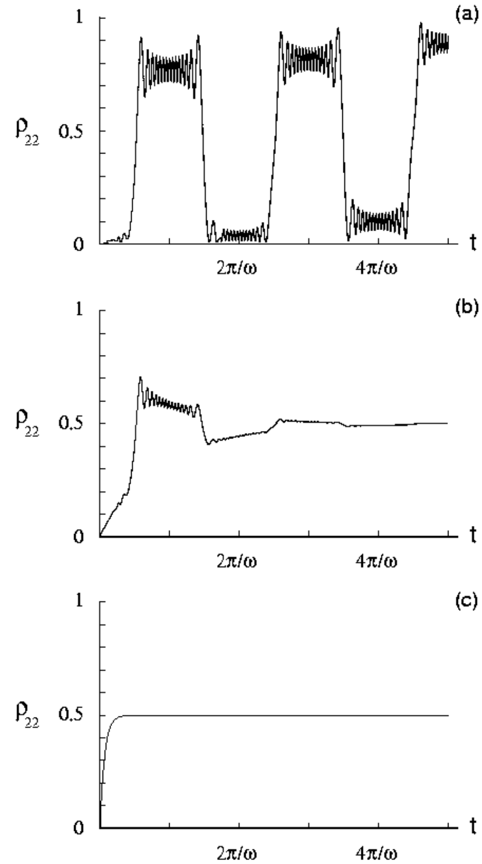

FIG. 1: $\rho_{22}(t)$ for an oscillating driving field with $J/\omega = 3$, $A/\omega = 45$, and damping values (a) $\Gamma/\omega = 0$, (b) $\Gamma/\omega = 0.35$, and (c) $\Gamma/\omega = 5$.

In summary, an n-dimensional LvNL equation describing dissipation and decoherence (or, alternatively, continuous evolution plus a quantum jump) of the density matrix $\rho(t)$ is first embedded into an (n^2-1)-dimensional Liouville-Bloch equation for diagonal and off-diagonal combinations $\eta(t)$ of $\rho(t)$. A unitary integration scheme is then applied to this form of the equation, with $\eta(t)$ expressed as a product of exponentials involving a limited, finite number of factors and operators, often just the three of angular momentum. Through this procedure, all elements of $\rho(t)$ are obtained in terms of solution of a single Riccati equation for a classical function together with ordinary multiplication and integration.

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[*] Email: arau@phys.lsu.edu

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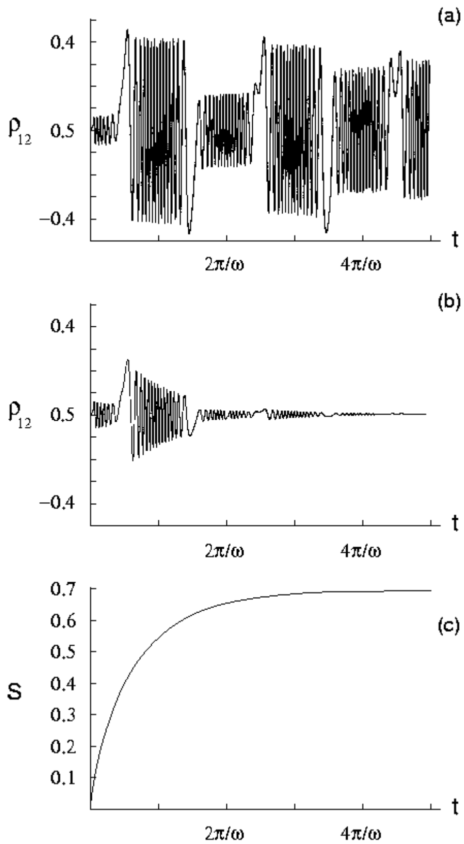

FIG. 2: As in Fig. 1, for $\rho_{12}(t)$ with (a) $\Gamma/\omega = 0$ and (b) $\Gamma/\omega = 0.35$. The entropy S for $\Gamma/\omega = 0.29$ is shown in (c).

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