Open system evolution and "memory dressing"

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Due to recent advances in quantum information, as well as in mesoscopic and nanoscale physics, the interest in the theory of open systems and decoherence has significantly increased. In this paper, we present an interesting approach to solving a time-convolutionless equation of motion for the open system reduced density matrix beyond the limit of weak coupling with the environment. Our approach is based on identifying an effective, memory-containing interaction in the equations of motion for the representation submatrices of the evolution operator (these submatices are written in a special basis, adapted for the "partial-trace-free" approach, in the system+environment Liouville space). We then identify the "memory dressing," a quantity crucial for solving the equation of motion for the reduced density matrix, which separates the effective from the real physical interaction. The memory dressing obeys a self-contained nonlinear equation of motion, which we solve exactly. The solution can be represented in a diagrammatic fashion after introducing an "information exchange propagator," a quantity that describes the transfer of information to and from the system, so the cumulative effect of the information exchange results in the memory dressing. In the case of weak system-environment coupling, we present the expansion of the reduced density matrix in terms of the physical interaction up to the third order. However, our approach is capable of going beyond the weak-coupling limit, and we show how short-time behavior of an open system can be analyzed for arbitrary coupling strength. We illustrate the approach with a simple numerical example of single-particle level broadening for a two-particle interacting system on short time scales. Furthermore, we point out a way to identify the structure of decoherence-free subspaces using the present approach.

I. INTRODUCTION

Evolution of an open system, coupled to its environment and possibly influenced by external driving fields, is an old problem that is of much interest now, due to recent advances in quantum information theory [1–3] and mesoscopic and nanoscale physics [4–6]. Whether it is a problem of manipulating entanglement for the purpose of information processing or cryptography, or trying to analyze decoherence in a nanostructure, the system-environment interaction is the key. The difficulty, however, lies in trying to analyze the evolution of the system without necessarily having to gather too much information about the environment [7,8].

A class of approaches to solving for the evolution of the open system's reduced density matrix is based on the projection operator technique, introduced by Nakajima [9], Zwanzig [10], and Mori [11], and used subsequently, in different versions, in many areas of physics [8,12–17]. In response to the problems arising from the treatment of the memory kernels, Tokuyama and Mori [18] first proposed the time-convolutionless equation of motion for the reduced density matrix in the Heisenberg picture. This work was extended by Shibata *et al.* [19] in the Schrödinger picture, and later used by many [20–24]. The crucial feature of the time-convolutionless approaches is that, instead of a memory kernel, the memory effects are accounted for by introducing special (invertible) operators.

There are two problems that we wish to address here. Generally, many reduced density matrix approaches rely on the approximation of weak coupling between the system and the environment, and essentially perform perturbation expan-

sion in terms of the coupling (see, e.g., Ref. [8], p. 445). Unfortunately, this approximation is often not plausible. So, the first problem is a need for a treatment that goes beyond the weak coupling limit. Secondly, there are a few conceptual and numerical problems with time-convolutionless approaches in general. We have already addressed the problem of reducing the effective dimensions of matrices in calculation with the partial-trace-free approach [25]. Here, we want to address the requirement of invertibility of one of the memory-containing operators, which is a constraint that may be hard to fulfill with some physical approximations and, in addition, the inversion of a large matrix is certainly an undesirable numerical task.

In this paper, we present a modification of a time-convolutionless equation of motion for the reduced density matrix, which relies on our results with the partial-trace-free approach [25]. We present a way to avoid the operator inversion typical for time-convolutionless approaches, and we derive an alternative set of equations. An effective, memory-containing interaction is identified, which enables us to point out a quantity of paramount importance, the so-called "memory dressing." The memory dressing separates the effective from the real physical interaction, and obeys a self-contained nonlinear equation of motion. The memory dressing is also what relieves us of the matrix inversion, and brings robustness to our approach. We solve the equation of motion for the memory dressing in a fashion similar to diagrams known in the Green's function formalism. The diagrams actually address the first problem noted: namely, one can make physical approximations for the memory dressing, and still have all orders of the interaction in the equation of

motion for the reduced density matrix of the open system.

This paper is organized as follows. In Sec. II, we over-view some elements of the partial-trace-free approach introduced in Ref. [25], and become familiar with the concepts of "purely system states" and "entangled states." In Sec. III, we write down the partial-trace-free time-convolutionless equations of motion, and point out a way to avoid operator inversion: we introduce the memory dressing in Sec. III B. In Sec. III C we solve the equation of motion for the memory dressing, and analyze in detail, using diagrams to help our intuition, how exactly the memory dresses the physical interaction. In Sec. IV, we present a few applications of the formalism: in Sec. IV A, a perturbation expansion for the limit of weak coupling up to the third order is presented. In Sec. IV B, we go beyond the limit of weak coupling, and analyze short-time behavior of the system for arbitrary interaction strength (e.g., we easily obtain level broadening from the information in the memory dressing), and illustrate with a simple numerical example. In Sec. IV C, we point out a way to identify the structure of decoherence-free subspaces using the present approach. Finally, we conclude with a brief over-view in Sec. V, where we also highlight the figures of merit of this approach.

II. PARTIAL-TRACE-FREE APPROACH. "PURELY SYSTEM STATES" AND "ENTANGLED STATES"

A. Eigenproblem of a projection operator. Partial-trace-free approach

Consider an open system S, interacting with its environment E, so that the system+environment ($S+E$) is closed, and possibly influenced by external driving fields that are assumed known and unaffected by the feedback from $S+E$. The Hilbert spaces of the environment and the system, $\mathcal{H}_E$ and $\mathcal{H}_S$, are assumed to be of finite dimensions d_E and d_S, respectively, yielding for the $S+E$ Hilbert space $\mathcal{H}_{S+E} = \mathcal{H}_E \otimes \mathcal{H}_S$. Given the $S+E$ Hamiltonian $h(t)$, which consists of the system part $h_{\text{sys}} = 1_E \otimes h_S$, the environment part $h_{\text{env}} = h_E \otimes 1_S$ and the interaction part h_{int}, so that $h = h_{\text{sys}} + h_{\text{env}} + h_{\text{int}}$, the evolution of the total $S+E$ density matrix ρ is given by the quantum Liouville equation (we use units $\hbar = 1$)

$$\frac{d\rho(t)}{dt} = -i[h(t), \rho(t)] \equiv -iL(t)\rho(t), \qquad (1)$$

where $L(t)$ is the Liouville superoperator (superoperators will be denoted by capital letters) corresponding to $h(t)$, and is of the form $L = L_{\text{sys}} + L_{\text{env}} + L_{\text{int}}$. With T^c (T^a) denoting the chronological (antichronological) time ordering, Θ being the Heaviside step function, and t_0 being the initial time at which we assume we know $\rho(t_0)$, the formal solution of Eq. (1) is given by

$$\rho(t) = U(t, t_0)\rho(t_0),$$

$$U(t, t') = \Theta(t - t') T^c \exp\left(-i \int_{t'}^{t} d\tau L(\tau)\right)$$
$$+ \Theta(t' - t) T^a \exp\left(i \int_{t}^{t'} d\tau L(\tau)\right). \qquad (2)$$

Now, the evolution of the open system S is described by the reduced density matrix $\rho_S = \text{Tr}_E(\rho)$, with $\text{Tr}_E(\cdots)$ denoting the partial trace over the environment states. To deduce how ρ_S evolves, we use the projection-operator technique based on the uniform environment density matrix [25]

$$\bar{\rho}_E \equiv (d_E^{-1}) 1_{d_E \times d_E}, \qquad (3)$$

which introduces projection superoperators[1] $\bar{P}$ and $\bar{Q}$ on $\mathcal{H}_{S+E}^2 = (\mathcal{H}_E \otimes \mathcal{H}_S)^2$ (the Liouville space of $S+E$, i.e., the space of all operators on $\mathcal{H}_{S+E}$) by the relations

$$\bar{P}x = \bar{\rho}_E \otimes \text{Tr}_E x, \quad \bar{Q} = 1 - \bar{P}, \quad x \in \mathcal{H}_{S+E}^2. \qquad (4)$$

The projector operators, in general, have been introduced by Nakajima [9], Zwanzig [10], and Mori [11], for obtaining the equation of motion for ρ_S. In the conventional projection-operator approaches, the equation of motion for $P\rho$ is solved, where P is a projector generated by an arbitrarily chosen density matrix ρ_E of the environment, using a relation of type (4), i.e., through $Px = \rho_E \otimes \text{Tr}_E x$, $x \in \mathcal{H}_{S+E}^2$. Then the partial trace over the solution is taken to obtain the system density matrix, as $\text{Tr}_E(P\rho) = \text{Tr}_E(\rho) = \rho_S$. However, we have recently shown [25] that the above choice of $\bar{P}$ is such that the partial trace with respect to the environment becomes unnecessary (so-called "partial-trace-free approach.") Namely, $\bar{P}$ is a projector, thus having eigenvalues 1 and 0, with corresponding eigenspaces being of dimensions d_S^2 and $d_S^2(d_E^2 - 1)$, respectively. The $S+E$ Hilbert space can be represented as a direct sum of these two mutually orthogonal eigenspaces of $\bar{P}$, i.e.,

$$\mathcal{H}_{S+E}^2 = (\mathcal{H}_{S+E}^2)_{\bar{P}=1} \oplus (\mathcal{H}_{S+E}^2)_{\bar{P}=0}. \qquad (5)$$

While the above statements about dimensionality of eigenspaces and the existence of decomposition (5) hold for any projection operator P, the choice of $\bar{P}$ has special features. Namely, for any given basis $\{|\alpha\beta\rangle | \alpha, \beta = 1, ..., d_S\}$ in $\mathcal{H}_S^2$ (the Liouville space of the system, i.e., the space of operators acting on the system's Hilbert space $\mathcal{H}_S$), there is a simply constructed basis $\{|\overline{\alpha\beta}\rangle | \alpha, \beta = 1, ..., d_S\}$ in $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$ (see Appendix A) such that, for any $x \in \mathcal{H}_{S+E}^2$,

$$(\text{Tr}_E x)^{\alpha\beta} = \sqrt{d_E}(\bar{P}x)^{\overline{\alpha\beta}}. \qquad (6)$$

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[1] Henceforth, if there is no danger of confusion, we will refer to projection superoperators simply as projection operators, as it is more common in the literature (e.g., the projection-operator technique).

This basis in the unit eigenspace is complemented by an orthonormal basis in the zero eigenspace. According to the decomposition (5), a vector $x \in \mathcal{H}_{S+E}^2$ can be represented in the complete eigenbasis of $\bar{P}$ by a column

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \qquad (7a)$$

and the projectors are represented by

$$\bar{P} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \bar{Q} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \qquad (7b)$$

On the other hand, taking the partial trace with respect to E of any $S+E$ observable x gives what the system sees of this observable. It is important to stress that, from now on, we will make no distinction between a system variable $x_S = \mathrm{Tr}_E x$ and its representation column in the basis $\{|\alpha\beta\rangle\}$ of $\mathcal{H}_S^2$. Therefore, for x_S being the representation column of $x_S = \mathrm{Tr}_E x$ in the basis $\{|\alpha\beta\rangle\}$ of $\mathcal{H}_S^2$, according to Eq. (6) we obtain

$$x_S = x_1 \sqrt{d_E}. \qquad (8)$$

In the eigenbasis of $\bar{P}$, a superoperator A that acts on $\mathcal{H}_{S+E}^2$ is, in general, represented by a block-matrix form

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}. \qquad (9a)$$

If the operator A_{sys} is a system operator, i.e., an operator of the form $A_{\mathrm{sys}} = I_E \otimes A_S$, where A_S acts on $\mathcal{H}_S^2$, then A_{sys} commutes with $\bar{P}$, and is therefore represented by block-diagonal form in the eigenbasis of $\bar{P}$. Furthermore, the block-diagonal form is such that the upper-left block matrix is exactly the one representing A_S in the basis $\{|\alpha\beta\rangle\}$ (see Appendix B of Ref. [26]), namely,

$$A_{\mathrm{sys}} = I_E \otimes A_S = \begin{bmatrix} A_S & 0 \\ 0 & A_2 \end{bmatrix}. \qquad (9b)$$

Returning to the evolution of the system+environment, described by the Liouvuille equation (1) and its solution (2), in the eigenbasis of $\bar{P}$ defined above, the system+environment total density matrix is given by

$$\rho = \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix}, \quad \rho_S = \rho_1 \sqrt{d_E}. \qquad (10a)$$

The Liouville operator and the evolution operator are given by the block forms

$$L(t) = \begin{bmatrix} L_{11}(t) & L_{12}(t) \\ L_{21}(t) & L_{22}(t) \end{bmatrix}, \quad U(t,t') = \begin{bmatrix} U_{11}(t,t') & U_{12}(t,t') \\ U_{21}(t,t') & U_{22}(t,t') \end{bmatrix}, \qquad (10b)$$

where $L_{21} = (L_{12})^+$ (L is Hermitian), and U is unitary. When Eqs. (1) and (2) are written out in their matrix representations, we obtain

$$\frac{d\rho_1}{dt} = -iL_{11}(t)\rho_1(t) - iL_{12}(t)\rho_2(t),$$

$$\frac{d\rho_2}{dt} = -iL_{21}(t)\rho_1(t) - iL_{22}(t)\rho_2(t) \qquad (11a)$$

and

$$\rho_1(t) = U_{11}(t,t')\rho_1(t') + U_{12}(t,t')\rho_2(t'),$$

$$\rho_2(t) = U_{21}(t,t')\rho_1(t') + U_{22}(t,t')\rho_2(t'). \qquad (11b)$$

B. "Purely system states" and "entangled states"

We have established that there are two classes of states in $\mathcal{H}_{S+E}^2$: those from $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$, and those from its orthocomplement $(\mathcal{H}_{S+E}^2)_{\bar{P}=0}$. Due to the isomorphism given by Eq. (6), which reveals that the states from $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$ faithfully represent (within the total Liouville space) what goes on with the system, we will call the states from $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$ "purely system states." Also, we see [Eqs. (9a), (9b)] that the upper-left block matrix of any $S+E$ superoperator can be dubbed the "purely system part" of that superoperator. For instance, the upper-left block matrix L_{11} of the Liouvillian is of the commutator-generated form, i.e., it corresponds to an effective system Hamiltonian $h_{S,\mathrm{eff}}$ given by

$$h_{S,\mathrm{eff}} = h_S + \mathrm{Tr}_E(h_{\mathrm{int}})/d_E, \qquad (12)$$

which accounts for the well-known first-order correction to the system energy spectrum [13,20], due to the coupling with the environment (see Appendix C of Ref. [26]).

States from $(\mathcal{H}_{S+E}^2)_{\bar{P}=0}$, the orthocomplement to $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$, we call "entangled states." The decomposition of $\mathcal{H}_{S+E}^2$ and the isomorphism (6) are depicted in Fig. 1. It is crucial here to clarify what we mean by purely system states and by entangled states. Namely, in quantum information theory, entanglement has a precise definition (see, e.g., Ref. [3]): a composite system ($S+E$) is said to be in a nonentangled (separable) state, if its density matrix can be written as a linear combination of tensor products of subsystems' density matrices (here, density matrices of the system and the environment). Otherwise, the composite system is said to be in an entangled state.

In the present approach, the purely system states are the $S+E$ vectors of the form $x = \bar{\rho}_E \otimes \mathrm{Tr}_E x$, i.e., those which are of a particular separable form. This form is special because all density matrices that are among the purely system states are of such a form that the information entropy of the environment in such states is maximal: in other words, since its density matrix is uniform, the environment has no information to transmit to the system. Therefore

$$s(\rho) \le s(\rho_S) + s(\rho_E) \le s(\rho_S) + s(\bar{\rho}_E), \qquad (13)$$

where s denotes the information (von-Neumann) entropy. Equation (13) means that, among all the $S+E$ states ρ that yield a given reduced density matrix ρ_S, the purely system state corresponding to that ρ_S is the one with the largest

$$(\bar{P}_D x)^{\overline{\alpha\beta}} = (Tr_E x)^{\alpha\beta}/\sqrt{d_E}$$
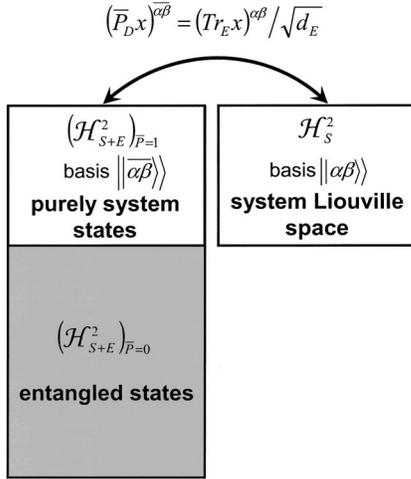

FIG. 1. Decomposition of the total Liouville space into the eigenspaces of the projection superoperator $\bar{P}$ and identification of the purely system states and the entangled states. The purely system states and the states from the system Liouville space are related via the isomorphism given in Eq. (6).

entropy [27]. So, we can think of the purely system states as "the states depleted of environmental information." In a similar fashion, what we call the entangled states should alternatively be thought of as the "states rich in environmental information." In that sense, since the information exchange between the system and the environment is another way of (loosely) stating that the system and environmental states become entangled, we believe that choosing the name "entangled states" for the vectors in $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$ is fairly appropriate, and certainly rolls off the tongue better than, for instance, "states rich in environmental information." We are, however, aware that some might consider the name "entangled states" a misnomer in the present context.

The terms in Eq. (13) that effectively account for the system-environment coupling are the off-diagonal terms of the Liouvillian, L_{12} and $L_{21} = (L_{12})^+$. In order for the system to evolve as decoupled from the environment, we must have

$$\|L_{12}\rho_2\| \ll \|L_{11}\rho_1\|. \tag{14}$$

This requirement is obviously fulfilled when the interaction vanishes ($h_{\text{int}} = 0$ implies $L_{12} = 0$), but we have argued [26] that, even in the case of appreciable coupling, when a balance between the driving and the relaxation forces is achieved, this criterion is fulfilled. (This actually defines reaching a far-from-equilibrium steady state in nonequilibrium transport.)

III. MEMORY DRESSING AND THE REDUCED DENSITY MATRIX

A. Time-convolutionless equation of motion—an overview

A class of approaches based on projection operators yield the so-called "time-convolutionless equation" (TCE) of motion for the projection $P\rho$ of the total $S + E$ density matrix ρ, where P is a projector generated by an arbitrary environment

density matrix, as described in the previous section [8,18–26]. The term "time-convolutionless" means that the differential equation for $P\rho(t)$ at a time t formally depends only on $P\rho(t)$ and on $Q\rho(t_0)$ at the initial time t_0. Instead of the notorious integral with the memory kernel, which requires knowing $Q\rho(\tau)$ at all times τ in the past ($t_0 \leqslant \tau \leqslant t$), special (invertible) operators are introduced, which account for the system's memory of the environment's evolution.[2]

For the chosen projector $\bar{P}$, the equations of motion for ρ_1 and ρ_2 can be written as

$$\frac{d\rho_1(t)}{dt} = -i[L_{11}(t) - L_{12}(t)K_{22}^{-1}(t;t_0)K_{21}(t;t_0)]\rho_1(t)$$

$$-iL_{12}(t)K_{22}^{-1}(t;t_0)H_{22}(t,t_0)\rho_2(t_0),$$

$$\rho_2(t) = -K_{22}^{-1}(t;t_0)K_{21}(t;t_0)\rho_1(t)$$

$$+ K_{22}^{-1}(t;t_0)H_{22}(t,t_0)\rho_2(t_0), \tag{15}$$

where operators H_{22}, K_{21}, and K_{22} satisfy

$$H_{22}(t,t_0) = T^c \exp\left(-i\int_{t_0}^{t} d\tau L_{22}(\tau)\right),$$

$$\frac{dK_{21}(t;t_0)}{dt} = -iL_{22}(t)K_{21}(t;t_0) + iK_{21}(t;t_0)L_{11}(t)$$

$$+ iK_{22}(t;t_0)L_{21}(t),$$

$$\frac{dK_{22}(t;t_0)}{dt} = -iL_{22}(t)K_{22}(t;t_0) + iK_{22}(t;t_0)L_{22}(t)$$

$$+ iK_{21}(t;t_0)L_{12}(t),$$

$$K_{21}(t_0;t_0) = 0, \quad K_{22}(t_0;t_0) = 1. \tag{16}$$

The second time variable in the argument of submatrices $K_{12}(t;t_0)$ and $K_{22}(t;t_0)$ is not exactly a variable. Namely, t_0 denotes the fixed initial time, which defines the initial conditions for K's, and is separated from the first time variable t by a semicolon instead of a comma to indicate that it is not a variable, but a fixed parameter.

According to Eq. (15), the equations of motion for the evolution submatrices, with the second time argument fixed to t_0, are given by

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[2]We have recently shown [25] that the very existence of time-convolutionless approaches, in general, relies on the invertibility of one of these operators, which is synonymous with the assumption of reversibility in $S + E$ evolution; in principle, this is not a problem, as evolution given by Eqs. (1) and (2) is indeed reversible. However, in practical evaluations of $P\rho$, if an approximation yielding irreversibility is employed, time-convolutionless approaches fail.

$$\frac{dU_{11}(t,t_0)}{dt} = -i[L_{11}(t) - L_{12}(t)K_{22}^{-1}(t;t_0)$$
$$\times K_{21}(t;t_0)]U_{11}(t,t_0),$$

$$\frac{dU_{12}(t,t_0)}{dt} = -i[L_{11}(t) - L_{12}(t)K_{22}^{-1}(t;t_0)$$
$$\times K_{21}(t;t_0)]U_{12}(t,t_0)$$
$$- iL_{12}(t)K_{22}^{-1}(t;t_0)H_{22}(t,t_0),$$

$$U_{21}(t,t_0) = -K_{22}^{-1}(t;t_0)K_{21}(t;t_0)U_{11}(t,t_0),$$

$$U_{22}(t,t_0) = K_{22}^{-1}(t;t_0)[H_{22}(t,t_0) - K_{21}(t;t_0)U_{12}(t,t_0)]. \tag{17}$$

The above are generic time-convolutionless equations of motion,[3] generally well known (maybe not necessarily in this particular form, which is valid for any choice of the projection operator P as long as we are writing the equations in P's eigenbasis). If we are to solve equations (17), we first have to solve the very unpleasant equations (16), among which the equations for K_{21} and K_{22} are coupled. Even if we were to solve Eq. (16), in order to obtain a solution to Eq. (17) we need to perform an additional unappealing task of inverting K_{22}. With the increasing dimension of the $S+E$ Hilbert spaces, K_{22} becomes large [the largest matrices we deal with are H_{22}, K_{22}, U_{22}, of dimension $d_S^2(d_E^2-1) \times d_S^2(d_E^2-1)$; needless to say, one would not want to unnecessarily invert one of them].

B. A way out: memory-containing effective interaction and memory dressing

Luckily, there is a way out of this unpleasant situation. If we examine Eq. (17) more closely, we will notice that we do not actually need all three matrices H_{22}, K_{21}, K_{22} from Eq. (16). The quantities we do need for the equations of motion (17) are actually

$$R(t) = K_{22}^{-1}(t;t_0)K_{21}(t;t_0),$$

$$S(t;t_0) = K_{22}^{-1}(t;t_0)H_{22}(t,t_0). \tag{18}$$

Notice that we have omitted the time quasivariable t_0 in defining R. It does not mean that this information is not present or important; on the contrary, choosing t_0 defines the initial condition for R. But, it will become apparent below why keeping R with one time variable only is in the service of transparency and intuitive plausibility.

It is easily shown, by using Eq. (16), that these quantities satisfy the following equations of motion:

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[3]Note that U_{21} and U_{22} can be written in terms of U_{11} and U_{12}, which is a typical feature of the time-convolutionless approaches.

$$\frac{dR(t)}{dt} = -iL_{22}(t)R(t) - iR(t)L_{12}(t)R(t) + iR(t)L_{11}(t)$$
$$+ iL_{21}(t), \quad R(t_0) = 0,$$

$$\frac{dS(t;t_0)}{dt} = -i[L_{22}(t) + iR(t)L_{12}(t)]S(t;t_0), \quad S(t_0;t_0) = 1. \tag{19}$$

Therefore, if one is to solve for the evolution of the reduced density matrix ρ_S, starting from a given initial $S+E$ density matrix $\rho(t_0) = [\rho_1(t_0) \ \rho_2(t_0)]^T$, one only needs to solve the following equations (with corresponding initial conditions):

$$\frac{dR(t)}{dt} = -iL_{22}(t)R(t) - iR(t)L_{12}(t)R(t) + iR(t)L_{11}(t)$$
$$+ iL_{21}(t), \quad R(t_0) = 0,$$

$$\frac{dS(t;t_0)}{dt} = -i[L_{22}(t) + R(t)L_{12}(t)]S(t;t_0), \quad S(t_0;t_0) = 1,$$

$$\frac{dU_{11}(t,t_0)}{dt} = -i[L_{11}(t) - L_{12}(t)R(t)]U_{11}(t,t_0),$$
$$U_{11}(t_0,t_0) = 1,$$

$$\frac{dU_{12}(t,t_0)}{dt} = -i[L_{11}(t) - L_{12}(t)R(t)]U_{12}(t,t_0)$$
$$- iL_{12}(t)S(t;t_0), \quad U_{12}(t_0,t_0) = 0. \tag{20}$$

(Again, these equations hold for any projection operator, provided that we are writing equations in that projection operator's eigenbasis.) Also, the remaining two submatrices evolve according to

$$U_{21}(t,t_0) = -R(t)U_{11}(t,t_0),$$

$$U_{22}(t,t_0) = S(t;t_0) - R(t)U_{12}(t,t_0),$$

but we have no interest in them presently. Their evolution is of interest when calculating, for instance, two-time correlation functions in electronic transport [26,28], which requires $U(t,t'), t' \neq t_0$. We are interested here only in deducing how the evolution of the reduced density matrix proceeds after t_0, for which we need the initial $S+E$ density matrix $\rho(t_0)$, and submatrices $U_{11}(t,t_0)$ and $U_{12}(t,t_0)$.

At this point, it is useful to note several features of Eq. (20). First, R has a self-contained nonlinear equation of motion, which should obviously be the starting point of a calculation. This equation is a matrix Riccati equation, whose general properties and solutions are the subject of active research, especially in control systems theory [29]. In Sec. III C, we will solve this equation exactly, for the particular initial condition $R(t_0) = 0$. Secondly, evolution of U_{11} obeys a Liouville-like equation, with a generally non-Hermitian "quasi-Liouvillian" $L_{11}(t) - L_{12}(t)R(t)$, with $L_{12}R$ obviously playing the role of an effective, memory-containing interaction. Since we have already identified L_{12} as the term

accounting for the real physical interaction, it is then clear that $R(t)$ plays the role of a "memory dressing" of the interaction, and this is what we will call it henceforth. In the evolution of U_{12}, we see an effective driving term $-iL_{12}S$ in addition to the quasi-Liouvillian $L_{11}(t)-L_{12}(t)R(t)$.

C. Evaluation of the memory dressing $R(t)$

Since the memory dressing R apparently plays an important role in calculation of the evolution operators' time dependence, we will now solve its equation of motion

$$\frac{dR}{dt} = -iL_{22}R - iRL_{12}R + iRL_{11} + iL_{21}. \tag{21}$$

(We will omit the time arguments for brevity.) Regardless of the interaction strength (i.e., the magnitude of L_{12}), this equation is complemented by the initial condition $R(t_0) = 0$. We will thus solve it by forming a power expansion in terms of L_{12} (or L_{21}, which is the adjoint of L_{12},), i.e., by assuming the form

$$R(t) = \sum_{n=0}^{\infty} R^{(n)}(t),$$

$$R^{(n)} = (L_{12})^n \times [\text{function of } (L_{11}, L_{22})]. \tag{22a}$$

(The right-hand side of the last equation is a symbolic expression, because L_{12} is not a square matrix, so its powers are not defined. Rather, $R^{(n)}$ is a product of generally nonsquare matrices, so that L_{12} and its adjoint appear a total of n times in the product, whereas the other matrices in the product depend only on L_{11} and/or L_{22}.) In addition, for all n, the following initial condition holds:

$$R^{(n)}(t_0) = 0, \quad n \geq 0. \tag{22b}$$

For the zeroth order term, the equation of motion is obtained from Eq. (21) as

$$\frac{dR^{(0)}}{dt} = -iL_{22}R^{(0)} + iR^{(0)}L_{11}. \tag{23a}$$

A general solution of Eq. (23a), for times $t \geq t_0$ (which are the only times meaningful to investigate, as we do not have sufficient knowledge about the system prior to t_0), is given by

$$R^{(0)}(t) = T^c \exp\left(-i\int_{t_0}^{t} d\tau L_{22}(\tau)\right)$$

$$\times R^{(0)}(t_0) T^a \exp\left(i\int_{t_0}^{t} d\tau L_{11}(\tau)\right). \tag{23b}$$

Since $R^{(0)}(t_0) = 0$ for all times t we have

$$R^{(0)}(t) = 0. \tag{23c}$$

The equation of motion for the first-order term $R^{(1)}$ reads

$$\frac{dR^{(1)}}{dt} = -iL_{22}R^{(1)} + iR^{(1)}L_{11} + iL_{21}. \tag{24a}$$

This is an inhomogeneous linear equation, with the general solution

$$R^{(1)}(t) = T^c \exp\left(-i\int_{t_0}^{t} d\tau L_{22}(\tau)\right)$$

$$\times \left[R^{(1)}(t_0) + \int_{t_0}^{t} d\tau T^a \exp\left(i\int_{t_0}^{\tau} d\tau' L_{22}(\tau')\right)\right.$$

$$\times [iL_{21}(\tau)] T^c \exp\left(-i\int_{t_0}^{\tau} d\tau' L_{11}(\tau')\right) \Big]$$

$$\times T^a \exp\left(i\int_{t_0}^{t} d\tau L_{11}(\tau)\right). \tag{24b}$$

With the initial condition $R^{(1)}(t_0) = 0$, we obtain

$$R^{(1)}(t) = \int_{t_0}^{t} d\tau T^c \exp\left(-i\int_{\tau}^{t} d\tau' L_{22}(\tau')\right)$$

$$\times [iL_{21}(\tau)] T^a \exp\left(i\int_{\tau}^{t} d\tau' L_{11}(\tau')\right). \tag{24c}$$

At this point it is useful to recall that, in the absence of coupling (i.e., $L_{12}=0$), the off-diagonal evolution submatrices become zero ($U_{21}^{(0)}=0$, $U_{12}^{(0)}=0$), whereas for $t, t' > t_0$ we obtain the diagonal evolution submatrices

$$U_{11}^{(0)}(t,t') = \Theta(t-t') T^c \exp\left(-i\int_{t'}^{t} d\tau L_{11}(\tau)\right)$$

$$+ \Theta(t'-t) T^a \exp\left(i\int_{t}^{t'} d\tau L_{11}(\tau)\right),$$

$$U_{22}^{(0)}(t,t') = \Theta(t-t') T^c \exp\left(-i\int_{t'}^{t} d\tau L_{22}(\tau)\right)$$

$$+ \Theta(t'-t) T^a \exp\left(i\int_{t}^{t'} d\tau L_{22}(\tau)\right). \tag{25}$$

(As before, Θ denotes the Heaviside step function.) Each of the submatrices $U_{11}^{(0)}$, $U_{22}^{(0)}$ is unitary, and these evolution submatrices, for purely system states and entangled states separately, form groups [note that operator $H_{22}(t,t_0)$ from Eq. (16) is actually just $U_{22}^{(0)}(t,t_0)$]. We can now rewrite Eq. (24c) as

$$R^{(1)}(t) = \int_{t_0}^{t} d\tau U_{22}^{(0)}(t,\tau)[iL_{21}(\tau)]U_{11}^{(0)}(\tau,t), \tag{26}$$

which is the form we will later use frequently. It was important to evaluate the first-order correction explicitly, as the only free term (i.e., term not containing R) in Eq. (21) is of the first order in L_{12} [the iL_{21} term on the right-hand side of Eq. (21)].

For all higher orders n, $n > 1$, it is straightforward to prove, using Eq. (21), that

$$\frac{dR^{(n)}}{dt} = -iL_{22}R^{(n)} - i\sum_{k=0}^{n-1} R^{(k)}L_{12}R^{(n-1-k)} + iR^{(n)}L_{11}.$$

(27)

Lemma 1. All even-order terms in R are zero, i.e.,

$$R^{(2k)}(t) = 0, \quad k \geq 0.$$

(28)

The detailed proof is given in Appendix B.

Lemma 2. Odd-order terms $R^{(2k+1)}$, $k \geq 1$ can be calculated according to

$$R^{(2k+1)}(t) = \int_{t_0}^{t} d\tau_1 \int_{t_0}^{t} d\tau_2 \cdots \int_{t_0}^{t} d\tau_k \mathcal{P}(t,\tau_1)$$

$$\times [-iL_{12}(\tau_1)]\mathcal{P}(\tau_1,\tau_2)$$

$$\times [-iL_{12}(\tau_2)]\mathcal{P}(\tau_2,\tau_3)\cdots$$

$$\times \cdots \mathcal{P}(\tau_{k-1},\tau_k)[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t),$$

(29)

where

$$\mathcal{P}(\tau,\tau') = \begin{cases} \tau > \tau', & U_{22}^{(0)}(\tau,\tau')\mathcal{R}(\tau') \\ \tau < \tau', & \mathcal{R}(\tau)U_{11}^{(0)}(\tau,\tau') \end{cases}, \quad \tau,\tau' \geq t_0.$$

(30a)

$$\mathcal{R}(t) = R^{(1)}(t) = \int_{t_0}^{t} d\tau \, U_{22}^{(0)}(t,\tau)[iL_{21}(\tau)]U_{11}^{0}(\tau,t), \quad t \geq t_0,$$

(30b)

The quantity $\mathcal{P}$ is called "the information-exchange propagator." The detailed proof is given in Appendix C.

Theorem. The solution of Eq. (21), with the initial condition $R(t_0) = 0$, is given by

$$R(t) = \sum_{k=0}^{\infty} R^{(2k+1)}(t) = \mathcal{R}(t) + \sum_{k=1}^{\infty} \int_{t_0}^{t} d\tau_1 \cdots \int_{t_0}^{t} d\tau_k \mathcal{P}(t,\tau_1)$$

$$\times [-iL_{12}(\tau_1)]\mathcal{P} \cdots \mathcal{P}(\tau_{k-1},\tau_k)[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t).$$

(31)

The proof follows a straightforward implementation of lemmas 1 and 2.

Now that we have formally solved the equation of motion for the memory dressing R, and introduced the information-exchange propagator $\mathcal{P}$, let us try to develop an intuitive feeling of what these results actually mean. In Fig. 2, $\mathcal{R}(t)$ is depicted. We see that $\mathcal{R}(t)$ calculates a cumulative effect that the purely system states have on the entangled states, provided that at any given time the information exchange is due to the first order in coupling. Note how, to obtain $\mathcal{R}(t)$, we go backwards in time among the purely system states (which evolve as if there were no coupling, according to $U_{11}^{(0)}$), then the interaction occurs, and afterwards the entangled states evolve forward in time, again as if there were no coupling.

Figure 3 presents a diagrammatic representation of $\mathcal{P}(t,t')$ for two different orderings of t and t'. Note how
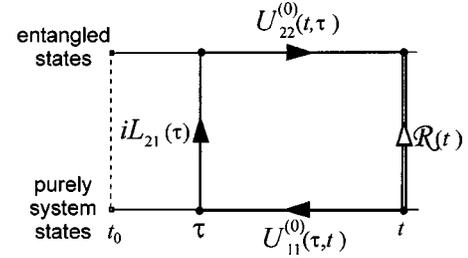

FIG. 2. Diagrammatic representation of $\mathcal{R}(t)$, the first-order contribution to the memory dressing.

$\mathcal{R}(t)$ is always present at the later of the times. In Fig. 4, the third-order correction to the memory dressing R is depicted. Note how, if one uses the result for $\mathcal{P}(t,t')$ depicted in Fig. 3, we see that this third-order correction contains a cumulative effect that the purely system states have on the entangled states, provided that at any given time the information exchange is due to the third order in coupling $[iL_{21}(\tau)L_{12}(\tau)L_{21}(\tau)$ at time τ in the figure]. In Fig. 5, we see two topologically nonequivalent contributions to the fifth-order correction.

IV. APPLICATIONS

A. Perturbation expansion in the limit of weak coupling

In the limit of weak coupling with the environment, a perturbation expansion in terms of L_{12} can be performed. The following statement is easily proven, in a fashion similar to the proof of lemma 1 in Appendix B.

Lemma 3. When expanding the submatrices of Eq. (20) into a power series in terms of L_{12} (or L_{21}), the following are found to be true:

$$U_{11}^{(2k+1)} = 0, \quad S^{(2k+1)} = 0, \quad U_{12}^{(2k)} = 0, \quad k \geq 0.$$

(32)

In other words, U_{11} and S have even-order terms only, whereas the U_{12} and R have only odd-order terms. Here are the results for the first few orders of the perturbation theory.
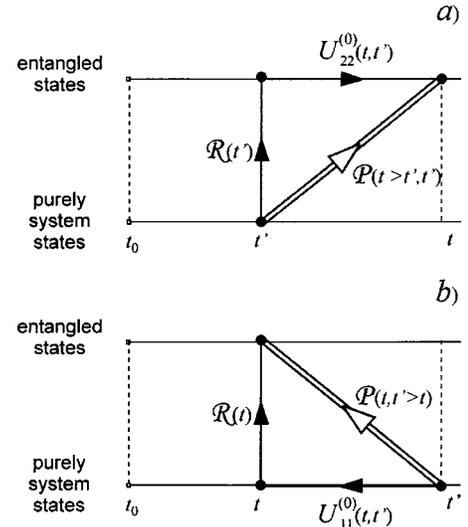

FIG. 3. The information-exchange propagator $\mathcal{P}(t,t')$ for different orderings of t and t'. (a) $t > t'$. (b) $t' > t$.
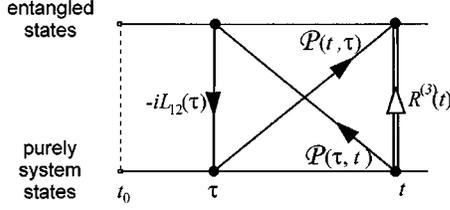
FIG. 4. Diagrammatic representation of $R^{(3)}(t)$, the third-order contribution to the memory dressing.

Zeroth order. For $U_{11}^{(0)}$, we already have the result in Eq. (25). Also, it is easily proven $S^{(0)} = U_{22}^{(0)}$. So, the zeroth-order equation of motion for the reduced density matrix reads

$$\rho_S^{(0)}(t) = U_{11}^{(0)}(t,t_0)\rho_S(t_0). \tag{33}$$

First order. We already have the solution for $R^{(1)}$, and the equation for the first-order correction to $U_{12}^{(1)}$ is given by

$$\frac{dU_{12}^{(1)}(t,t_0)}{dt} = -iL_{11}(t)U_{12}^{(1)}(t,t_0) - iL_{12}(t)S^{(0)}(t;t_0),$$

$$U_{12}^{(0)}(t_0,t_0) = 0, \tag{34a}$$

with the solution

$$U_{12}^{(1)}(t,t_0) = \int_{t_0}^{t} d\tau U_{11}^{(0)}(t,\tau)[-iL_{12}(\tau)]U_{22}^{(0)}(\tau,t_0)$$

$$= \mathcal{R}^+(t)U_{22}^{(0)}(t,t_0), \tag{34b}$$

so the first order correction to the reduced density matrix is obtained in the form

$$\rho_S^{(1)}(t) = (\sqrt{d_E})U_{12}^{(1)}(t,t_0)\rho_2(t_0)$$

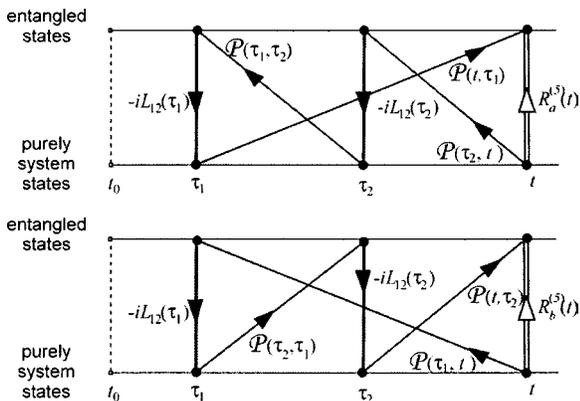$$= (\sqrt{d_E})\mathcal{R}^+(t)U_{22}^{(0)}(t,t_0)\rho_2(t_0). \tag{34c}$$

Second order.

FIG. 5. Diagrammatic representation of the two topologically nonequivalent contributions to $R^{(5)}(t)$, the fifth-order term in the memory dressing.

$$\frac{dU_{11}^{(2)}(t,t_0)}{dt} = -iL_{11}(t)U_{11}^{(2)}(t,t_0) + iL_{12}(t)R(t)$$

$$\times U_{11}^{(0)}(t,t_0), \quad U_{11}^{(2)}(t_0,t_0) = 0,$$

$$\frac{dS^{(2)}(t;t_0)}{dt} = -iL_{22}(t)S^{(2)}(t;t_0) - iR^{(1)}(t)L_{12}(t)$$

$$\times S^{(0)}(t;t_0); \quad S^{(2)}(t_0;t_0) = 0. \tag{35a}$$

The solutions are given by

$$U_{11}^{(2)}(t,t_0) = \int_{t_0}^{t} d\tau U_{11}^{(0)}(t,\tau)[iL_{12}(\tau)]\mathcal{R}(\tau)U_{11}^{(0)}(\tau,t_0),$$

$$S^{(2)}(t;t_0) = \int_{t_0}^{t} d\tau U_{22}^{(0)}(t,\tau)\mathcal{R}(\tau)[-iL_{12}(\tau)]U_{22}^{(0)}(\tau,t_0), \tag{35b}$$

so the second-order contribution to the reduced density matrix is actually

$$\rho_S^{(2)}(t) = U_{11}^{(2)}(t,t_0)\rho_S(t_0)$$

$$= \int_{t_0}^{t} d\tau U_{11}^{(0)}(t,\tau)$$

$$\times [iL_{12}(\tau)]\mathcal{R}(\tau)U_{11}^{(0)}(\tau,t_0)\rho_S(t_0). \tag{35c}$$

Third order.

$$\frac{dU_{12}^{(3)}(t,t_0)}{dt} = -iL_{11}(t)U_{12}^{(3)}(t,t_0) + iL_{12}(t)R^{(1)}(t)U_{12}^{(1)}(t,t_0)$$

$$- iL_{12}(t)S^{(2)}(t;t_0), \quad U_{12}^{(3)}(t_0,t_0) = 0. \tag{36a}$$

The solution is

$$U_{12}^{(3)}(t,t_0) = \int_{t_0}^{t} d\tau U_{11}^{(0)}(t,\tau)[iL_{12}(\tau)\mathcal{R}(\tau)U_{12}^{(1)}(\tau,t_0)$$

$$- iL_{12}(\tau)S^{(2)}(\tau,t_0)]$$

$$= \int_{t_0}^{t} d\tau U_{11}^{(0)}(t,\tau)iL_{12}(\tau)\left\{ \mathcal{R}(\tau)\mathcal{R}^+(\tau) \right.$$

$$+ \int_{t_0}^{\tau} d\tau' U_{22}^{(0)}(\tau,\tau')\mathcal{R}(\tau')$$

$$\times [iL_{12}(\tau')]U_{22}^{(0)}(\tau',\tau) \bigg\} U_{22}^{(0)}(\tau,t_0). \tag{36b}$$

We need to stress here that the inclusion of the interaction Hamiltonian h_{int} will not only change L_{12}, but also L_{11} and L_{22} [we have seen what happens with L_{11}: it is commutator generated, corresponding to an effective system Hamiltonian $h_{S,eff} = h_S + \text{Tr}_E(h_{int})/d_E$]. However, we can treat the changes in L_{22} as negligible, as far as the system is concerned, at least in the first few orders of perturbation, because if L_{21} is neglected, the purely system states have no notion of what is

going on with the entangled states, so the exact magnitude of L_{22} is not important. For example, in electronic transport, when electron-phonon coupling is considered, it is well known that the effects of nonequilibrium phonons are higher-order corrections, and in the first few lowest orders the phonons can be treated as thermal [28], which, in the present approach, corresponds to neglecting changes in L_{22}. As to when exactly one should consider taking into account the effects of interaction on the environment, from Eqs. (35) we see that L_{21} (from purely system states to entangled states) first appears in the second order corrections to the reduced density matrix, so we may safely say that in the first-order approximation we may neglect any changes in the environment dynamics (one can also check that the lowest-order correction in U_{22} is of second order). Of course, one should be advised to check how the eigenvalues of L_{22} really change with the interaction.

B. Beyond the weak coupling limit: short-time evolution for arbitrary coupling strength

However, in real physical situations the coupling between the system and the environment cannot always be assumed to be weak (an example is the electron-electron interaction between the electrons in a quantum dot and those in the reservoirs). In such cases, it is important to be able to go beyond the perturbation expansion.

This is where the strength of the present approach lies. Namely, one can make a physical approximation for R, and cut off the summation (31) at some finite order, and still have all orders of the interaction in the equations of motion for the reduced density matrix. This feature is well known in the Green's function theory, where a set of diagrams is chosen to form a self-energy term, and these diagrams give contributions of all orders to the final Green's function.

Here, we will present a simple approximation that describes the evolution of systems on very short time scales, and which does not involve assuming a weak interaction. Let us first define the short time as

$$t - t_0 \ll \frac{1}{\text{maximal eigenvalue of } (L_{12}L_{21})^{1/2}} \quad (37)$$

(note that $L_{12}L_{21} = L_{12}L_{12}^+$ is a positive operator). In this case, we can keep only the first term in the expression for R, i.e., approximate $R(t) \approx \mathcal{R}(t)$, so Eq. (20) becomes

$$\frac{dS(t;t_0)}{dt} = -i[L_{22}(t) + \mathcal{R}(t)L_{12}(t)]S(t;t_0), \quad S(t_0;t_0) = 1,$$

$$\frac{dU_{11}(t,t_0)}{dt} = -i[L_{11}(t) - L_{12}(t)\mathcal{R}(t)]U_{11}(t,t_0),$$

$$U_{11}(t_0,t_0) = 1, \quad (38)$$

$$\frac{dU_{12}(t,t_0)}{dt} = -i[L_{11}(t) - L_{12}(t)\mathcal{R}(t)]U_{12}(t,t_0)$$

$$- iL_{12}(t)S(t;t_0), \quad U_{12}(t_0,t_0) = 0.$$

One can now solve these equations of motion with a time-dependent non-Hermitian $\mathcal{R}$. But, there are more physics-based simplifications that can be done.

Let us take a closer look at the form of $\mathcal{R}$. If we assume that L_{11}, L_{22} are time independent, or at least only weakly depend on time for the time range of interest (37), and we write $U_{11}^{(0)}$ and $U_{22}^{(0)}$ in their eigenbases $\{|j_1\rangle|j_1 = 1,...,d_S^2\}$ and $\{|i_2\rangle|i_2 = 1,...,d_S^2(d_E^2-1)\}$, we obtain

$$\mathcal{R}(t) = \sum_{j_1=1}^{d_S^2} \sum_{i_2=1}^{d_S^2(d_E^2-1)} \int_{t_0}^{t} d\tau |i_2\rangle\langle i_2| e^{-iE_{i_2}(t-\tau)}$$

$$\times [iL_{21}(\tau)]|j_1\rangle\langle j_1| e^{iE_{j_1}(t-\tau)}$$

$$= \sum_{j_1=1}^{d_S^2} \sum_{i_2=1}^{d_S^2(d_E^2-1)} |i_2\rangle\langle j_1| e^{i(E_{j_1}-E_{i_2})t}$$

$$\times \int_{t_0}^{t} d\tau e^{i(E_{i_2}-E_{j_1})\tau} [iL_{21}(\tau)]_{i_2,j_1}$$

$$\approx \sum_{j_1=1}^{d_S^2} \sum_{i_2=1}^{d_S^2(d_E^2-1)} [iL_{21}(t_0)]_{i_2,j_1}|i_2\rangle\langle j_1|$$

$$\times \frac{1 - e^{-i(E_{i_2}-E_{j_1})(t-t_0)}}{i(E_{i_2}-E_{j_1})}$$

$$= \sum_{j_1=1}^{d_S^2} \sum_{i_2=1}^{d_S^2(d_E^2-1)} [iL_{21}(t_0)]_{i_2,j_1}|i_2\rangle\langle j_1|$$

$$\times \left\{ (t-t_0) - \frac{i}{2}(t-t_0)^2(E_{i_2}-E_{j_1}) + \cdots \right\}$$

$$= iL_{21}(t_0)(t-t_0) + o[(t-t_0)^2]. \quad (39)$$

Hence, we see that, to the first order in $t-t_0$, the resulting equations are

$$\frac{dS(t;t_0)}{dt} \approx [-iL_{22}(t_0) + L_{21}(t_0)L_{12}(t_0)(t-t_0)]S(t;t_0),$$

$$S(t_0;t_0) = 1,$$

$$\frac{dU_{11}(t,t_0)}{dt} \approx [-iL_{11}(t_0) - L_{12}(t_0)L_{21}(t_0)(t-t_0)]U_{11}(t,t_0),$$

$$U_{11}(t_0,t_0) = 1,$$

$$\frac{dU_{12}(t,t_0)}{dt} \approx [-iL_{11}(t_0) - L_{12}(t_0)L_{21}(t_0)(t-t_0)]U_{12}(t,t_0)$$

$$- iL_{12}(t_0)S(t;t_0), \quad U_{12}(t_0,t_0) = 0. \quad (40)$$

S and U evolve under non-Hermitian Liouvillians. While the non-Hermitian part in the quasi-Liouvillian for S, for instance, increases with time, we see that the opposite is true for the U's.

Now, let us consider the situation in which the initial state of $S+E$ was separable, with the environment regarded as a

thermal bath at a temperature high enough, so that it was larger than the energy level spacing between any two environmental levels that are of interest [i.e., that may become involved with the system through the coupling (see discussion in Sec. III B of Ref. [26])]. In that case, we can approximate

$$\rho_E(t_0) = \mathrm{Tr}_S[\rho(t_0)] \approx \bar{\rho}_E \Rightarrow \rho_2(t_0) \approx 0, \qquad (41)$$

which means that the reduced density matrix will evolve according to

$$\rho_S(t) = U_{11}(t,t_0)\rho_S(t_0), \qquad (42)$$

where

$$\frac{dU_{11}(t,t_0)}{dt} = -i[L_{11}(t) - L_{12}(t)R(t)]U_{11}(t,t_0). \quad (43)$$

The Hermitian part of the quasi-Liouvillian $L_{11} - L_{12}R$, given by

$$(L_{11} - L_{12}R)_{\mathrm{Herm}} = \frac{1}{2}[(L_{11} - L_{12}R) + (L_{11} - L_{12}R)^+]$$

$$= L_{11} - \frac{1}{2}[L_{12}R + R^+L_{21}] \qquad (44)$$

defines the system spectrum. On the other hand, the skew-Hermitan part of $L_{11} - L_{12}R$ (up to a minus sign)

$$-(L_{11} - L_{12}R)_{\mathrm{Skew}} = \frac{i}{2}[L_{12}R - R^+L_{21}] \qquad (45)$$

gives level broadening, and, consequently, lifetimes (as pointed out, e.g., in the works of the Brussels school [30]). For short time scales, according to Eqs. (39) and (40), the level broadening increases linearly in $t - t_0$, and, consequently, lifetimes of energy levels decay as

$$\tau_{\min}^{-1}(t) \approx (t - t_0) \times \{\text{max eigenvalue of } (L_{12}L_{21})\}. \qquad (46)$$

A numerical calculation for a simple system is presented. Namely, we start with a two-particle system, each of the particles having two energy levels -10 and $+10$ meV (these are reasonable numbers in the domains of low-temperature mesoscopic physics; for instance, this is the order of magnitude for the charging energy of a Coulomb-blockaded quantum dot). Now a toy model interaction is turned on, such that it does not distinguish between particles, and is characterized by one tuning parameter, which corresponds to a couple of the largest off-diagonal matrix elements of the interaction Liouvillian. How the minimal lifetime for this system changes with time is depicted in Fig. 6.

C. Decoherence

In Sec. III, we have not specified anything about the initial state of the system+environment, in order to keep the discussion as general as possible. However, a special class of
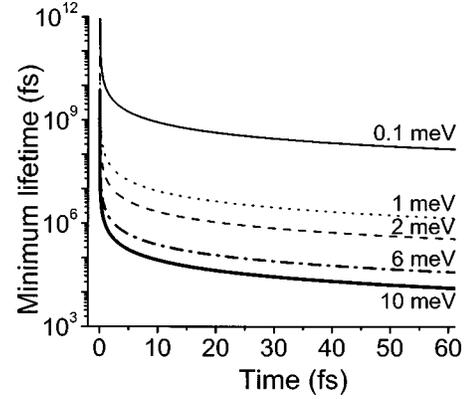

FIG. 6. Short-time evolution of the minimum relaxation time of single-particle levels for a simple two-particle system, for various coupling strengths. In the absence of coupling, each of the particles has two energy levels -10 and $+10$ meV.

initial states have recently been attracting much attention within the quantum information community [8,31–33]: those are separable initial states, of the form $\rho(t_0) = \rho_E(t_0) \otimes \rho_S(t_0)$. As shown by Lindblad [34], such initial states are the only ones allowing for Markovian evolution, i.e., producing an equation of motion for the reduced density matrix of the form $\rho_S(t) = \mathcal{E}(t,t_0)\rho_S(t_0)$ (no free term), where $\mathcal{E}(t,t_0)$ is not necessarily unitary. Special subspaces of the system Liouville space, which are invariant subspaces of $\mathcal{E}(t,t_0)$, and such that the projection of $\mathcal{E}(t,t_0)$ onto them is unitary, are exceptionally interesting, as they are known as the decoherence-free subspaces (DFS's) [31–33]. Namely, the evolution within DFS's is unitary, and considerable effort has recently been directed towards identifying them to optimize error correction procedures for quantum information processing (see, e.g., Ref. [33]).

In Sec. II B, we have seen that the purely system states are a faithful representation of the system Liouville space. Therefore, the identification of the DFS's can be carried out among the purely system states. In an earlier paper [25], we have pointed out how one can obtain $\rho_S(t) = \mathcal{E}(t,t_0)\rho_S(t_0)$ within the partial-trace-free approach, for the initial state given by $\rho(t_0) = \rho_E(t_0) \otimes \rho_S(t_0)$ (see Sec. IV B of Ref. [25]). Namely, the initial density matrix induces its own projection operator, with eigenspaces of the same dimensions as the eigenspaces of $\bar{P}$, so that a unitary transformation M can be constructed that maps from the new projector's eigenbasis to the eigenbasis of $\bar{P}$ (the eigenbases must, of course, be orthonormalized). Then, the equation of motion for the reduced density matrix becomes

$$\rho_S(t) = \underbrace{[U_{11}(t,t_0) - U_{12}(t,t_0)M_{22}^{-1}M_{21}]}_{\mathcal{E}(t,t_0)}\rho_S(t_0),$$

where M_{22}, M_{21} are submatrices of M. Obviously, $\mathcal{E}(t,t_0)$ is, in general, not unitary. The structure of its invariant subspaces, and consequently, identification of decoherence-free subspaces, are dependent on the exact initial state (through M_{22}, M_{21}) and the dynamics (through U_{11}, U_{12}). Here, we briefly point out how the present approach can be used to

identify DFS's; however, a more detailed study will be the subject of a subsequent paper.

V. CONCLUSION

We have presented an approach to solving the time-convolutionless equation of motion for the reduced density matrix of an open system, which is capable of going beyond the limit of weak system-environment coupling. This approach is based on identifying a memory dressing of the physical interaction (Sec. III B), which is a quantity that obeys a self-contained nonlinear equation of motion that we have solved here (Sec. III C). Introduction of the memory dressing supplants the need to invert one of the memory-containing operators present in time-convolutionless approaches, and yields robustness to the approach. We have also introduced a diagrammatic representation of the memory dressing, which makes the approach more intuitively plausible.

In the case of weak coupling, we have presented the expansion of the equations of motion for the reduced density matrix up to the third order in the physical interaction (see Sec. IV A). However, the major strength of our approach is its capability of going beyond the weak-coupling approximation: one can perform physical approximations in the memory dressing expansion, cutting it off at some finite order, and still have all orders of the interaction in the equations of motion for the reduced density matrix. For instance, this approach is well suited for describing short-time behavior of systems, regardless of the interaction strength (see Sec. IV B): we identify how system level broadening, which occurs due to the interaction with the environment, can be tracked approximately on short time scales by calculating the memory dressing to the first order, and then computing the skew-Hermitian part of an effective system quasi-Liouvillian. This feature of the present approach is illustrated by a simple numerical example of single-particle level broadening for a two-particle interacting system on short time scales. Finally, in Sec. IV C, we point out a way to identify the structure of decoherence-free subspaces using the present approach, a further discussion of which will be presented in a subsequent paper.

ACKNOWLEDGMENTS

APPENDIX A

In this Appendix, we give how a basis $\{|\overline{\alpha\beta}\rangle\}$ in $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$ is constructed, and prove Eq. (7) (details can be found in Ref. [23]). Let us choose a basis $\{|\alpha\beta\rangle|\alpha,\beta=1,...,d_S\}$ in $\mathcal{H}_S^2$, and a basis $\{|ij\rangle|i,j=1,...,d_E\}$ in $\mathcal{H}_E^2$, which give rise to the tensor-product basis $\{|i\alpha,j\beta\rangle i,j=1,...,d_E;|\alpha,\beta=1,...,d_S\}$ in $\mathcal{H}_{S+E}^2$. Then, one finds that the vectors defined as

$$|\overline{\alpha\beta}\rangle \equiv \frac{1}{\sqrt{d_E}}\sum_{i=1}^{d_E}|i\alpha,i\beta\rangle \tag{A1}$$

constitute an orthonormal basis within the unit eigenspace of $\bar{P}$, namely,

$$\bar{P}|\overline{\alpha\beta}\rangle=|\overline{\alpha\beta}\rangle, \quad \langle\overline{\alpha\beta}|\overline{\sigma\gamma}\rangle=\delta_{\alpha\sigma}\delta_{\beta\gamma}, \quad (\forall\alpha,\beta,\sigma,\gamma). \tag{A2}$$

$\bar{P}$ can therefore be written as

$$\bar{P}=\sum_{\alpha,\beta=1}^{d_S}|\overline{\alpha\beta}\rangle\langle\overline{\alpha\beta}|, \tag{A3}$$

and it follows that, for any $x\in\mathcal{H}_{S+E}^2$,

$$\bar{P}x=\sum_{\alpha,\beta=1}^{d_S}(\bar{P}x)^{\overline{\alpha\beta}}|\overline{\alpha\beta}\rangle, \tag{A4}$$

where

$$(\bar{P}x)^{\overline{\alpha\beta}}=\langle\overline{\alpha\beta}|x\rangle=\frac{1}{\sqrt{d_E}}\sum_{i=1}^{d_E}\langle i\alpha,i\beta|x\rangle=\frac{1}{\sqrt{d_E}}\sum_{i=1}^{d_E}x^{i\alpha,i\beta}. \tag{A5}$$

Using the fact that $\mathrm{Tr}_E x$, being a vector in $\mathcal{H}_S^2$, is written in terms of the basis $\{|\alpha\beta\rangle\}$ as

$$\mathrm{Tr}_E x=\sum_{\alpha,\beta=1}^{d_S}(\mathrm{Tr}_E x)^{\alpha\beta}|\alpha\beta\rangle=\sum_{\alpha,\beta=1}^{d_S}\left(\sum_{i=1}^{d_E}x^{i\alpha,i\beta}\right)|\alpha\beta\rangle, \tag{A6}$$

from Eq. (A5), we obtain Eq. (6)

$$(\mathrm{Tr}_E x)^{\alpha\beta}=\sqrt{d_E}(\bar{P}x)^{\overline{\alpha\beta}}. \tag{A7}$$

APPENDIX B

Lemma 1. All even order contributions to R are zero, i.e., $R^{(2k)}(t)=0$.

Proof. We will use mathematical induction to prove this statement. It holds $R^{(0)}(t)=0$ [Eq. (23c)]. Let us now assume that there exists $k_0\geq0$, so that the statement holds for all orders $n=2k\leq2k_0$. Then, according to Eq. (27), for $n=2(k_0+1)$, it holds

$$\frac{dR^{(2k_0+2)}}{dt}=-iL_{22}R^{(2k_0+2)}-i\sum_{j=0}^{2k_0+1}R^{(j)}L_{12}R^{(2k_0+1-j)}$$

$$+iR^{(2k_0+2)}L_{11}. \tag{B1}$$

In the second term on the right-hand side, if one of the R's is of odd order, the other one is of even order less than $2k_0$, and therefore zero. Therefore, the entire second term on the right-hand side is zero, reducing the equation to

$$\frac{dR^{(2k_0+2)}}{dt}=-iL_{22}R^{(2k_0+2)}+iR^{(2k_0+2)}L_{11}, \tag{B2}$$

whose solution is of the same for as Eq. (23b), but due to the initial condition $R^{(2k_0+2)}(t_0)=0$, we have $R^{(2k_0+2)}(t)=0$ for all times, which concludes the proof.

APPENDIX C

Lemma 2. Odd-order contributions $R^{(2k+1)}$, $k \geq 1$, can be calculated according to

$$R^{(2k+1)}(t;t_0) = \int_{t_0}^{t} d\tau_1 \int_{t_0}^{t} d\tau_2 \cdots \int_{t_0}^{t} d\tau_k \mathcal{P}(t,\tau_1)[-iL_{12}(\tau_1)]\mathcal{P}(\tau_1,\tau_2)[-iL_{12}(\tau_2)]\mathcal{P}(\tau_2,\tau_3)\cdots$$

$$\times \cdots \mathcal{P}(\tau_{k-1},\tau_k)[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t), \tag{C1}$$

where

$$\mathcal{P}(\tau,\tau') = \begin{cases} \tau > \tau', & U_{22}^{(0)}(\tau,\tau')\mathcal{R}(\tau') \\ \tau < \tau', & \mathcal{R}(\tau)U_{11}^{(0)}(\tau,\tau') \end{cases},$$

$$\mathcal{R}(t) = \int_{t_0}^{t} d\tau\, U_{22}^{(0)}(t,\tau)[iL_{21}(\tau)]U_{11}^{(0)}(\tau,t). \tag{C2}$$

Proof. From Eq. (C1),

$$\frac{dR^{(2k+1)}}{dt} = \frac{d}{dt}\left\{ \int_{t_0}^{t} d\tau_1, \int_{t_0}^{t} d\tau_2 \cdots \int_{t_0}^{t} d\tau_k \mathcal{P}(t,\tau_1)[-iL_{12}(\tau_1)]\mathcal{P}(\tau_1,\tau_2)[-iL_{12}(\tau_2)]\mathcal{P}(\tau_2,\tau_3)\cdots \right.$$

$$\left. \times \cdots \mathcal{P}(\tau_{k-1},\tau_k)[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t) \right\}$$

$$= \int_{t_0}^{t} d\tau_1, \int_{t_0}^{t} d\tau_2 \cdots \int_{t_0}^{t} d\tau_k \left\{ \frac{\partial \mathcal{P}(t,\tau_1)}{\partial t} \right\}[-iL_{12}(\tau_1)]\cdots\mathcal{P}(\tau_{k-1},\tau_k)[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t) + \mathcal{P}(t,t)$$

$$\times [-iL_{12}(t)]\int_{t_0}^{t} d\tau_2 \cdots \int_{t_0}^{t} d\tau_k \mathcal{P}(t,\tau_2)[-iL_{12}(\tau_2)]\cdots[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t)$$

$$+ \sum_{j=2}^{k-1} \left\{ \int_{t_0}^{t} d\tau_1 \int_{t_0}^{t} d\tau_2 \cdots \int_{t_0}^{t} d\tau_{j-1} \mathcal{P}(t,\tau_1)[-iL_{12}(\tau_1)]\cdots\mathcal{P}(\tau_{j-1},t) \right\}[-iL_{12}(t)]$$

$$\times \left\{ \int_{t_0}^{t} d\tau_{j+1} \cdots \int_{t_0}^{t} d\tau_k \mathcal{P}(t,\tau_{j+1})[-iL_{12}(\tau_{j+1})]\cdots\mathcal{P}(\tau_k,t) \right\} + \left\{ \int_{t_0}^{t} d\tau_1 \int_{t_0}^{t} d\tau_2 \cdots \int_{t_0}^{t} d\tau_{k-1}\mathcal{P}(t,\tau_1) \right.$$

$$\left. \times [-iL_{12}(\tau_1)]\cdots\mathcal{P}(\tau_{k-1},t) \right\}[-iL_{12}(t)]\mathcal{P}(t,t) + \int_{t_0}^{t} d\tau_1 \int_{t_0}^{t} d\tau_2 \cdots \int_{t_0}^{t} d\tau_k \mathcal{P}(t,\tau_1)[-iL_{12}(\tau_1)]\cdots\mathcal{P}(\tau_{k-1},\tau_k)$$

$$\times [-iL_{12}(\tau_k)]\left\{ \frac{\partial}{\partial t}\mathcal{P}(\tau_k,t) \right\}. \tag{C3}$$

From Eq. (C2) we see that $\mathcal{P}(\tau,\tau) = \mathcal{R}(\tau)$, and also

$$\frac{\partial}{\partial t}\mathcal{P}(t,\tau<t) = \frac{\partial}{\partial t}U_{22}^{(0)}(t,\tau)\mathcal{R}(\tau) = -iL_{22}(t)U_{22}^{(0)}(t,\tau)\mathcal{R}(\tau),$$

$$\frac{\partial}{\partial t}\mathcal{P}(\tau<t,t) = \frac{\partial}{\partial t}\mathcal{R}(\tau)U_{11}^{(0)}(\tau,t) = +i\mathcal{R}(\tau)U_{11}^{(0)}(\tau,t)L_{11}(t) \tag{C4}$$

so we obtain

$$\frac{dR^{(2k+1)}}{dt} = -iL_{22}(t)\int_{t_0}^t d\tau_1\cdots\int_{t_0}^t d\tau_k \mathcal{P}(t,\tau_1)[-iL_{12}(\tau_1)]\cdots\mathcal{P}(\tau_{k-1},\tau_k)[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t)$$

$$+\underbrace{\mathcal{R}(t)}_{R^{(1)}}[-iL_{12}(t)]\underbrace{\int_{t_0}^t d\tau_2\cdots\int_{t_0}^t d\tau_k \mathcal{P}(t,\tau_2)[-iL_{12}(\tau_2)]\cdots[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t)}_{R^{(2k-1)}}$$

$$+\sum_{j=2}^{k-1}\underbrace{\left\{\int_{t_0}^t d\tau_1\cdots\int_{t_0}^t d\tau_{j-1}\mathcal{P}(t,\tau_1)[-iL_{12}(\tau_1)]\cdots\mathcal{P}(\tau_{j-1},t)\right\}}_{R^{(2j-1)}}[-iL_{12}(t)]$$

$$\times\underbrace{\left\{\int_{t_0}^t d\tau_{j+1}\cdots\int_{t_0}^t d\tau_k \mathcal{P}(t,\tau_{j+1})[-iL_{12}(\tau_{j+1})]\cdots\mathcal{P}(\tau_k,t)\right\}}_{R^{(2(k-j)+1)}}$$

$$+\underbrace{\left\{\int_{t_0}^t d\tau_1\cdots\int_{t_0}^t d\tau_{k-1}\mathcal{P}(t,\tau_1)[-iL_{12}(\tau_1)]\cdots\mathcal{P}(\tau_{k-1},t)\right\}}_{R^{(2k-1)}}[-iL_{12}(t)]\underbrace{\mathcal{R}(t)}_{R^{(1)}}$$

$$+\int_{t_0}^t d\tau_1\cdots\int_{t_0}^t d\tau_k \mathcal{P}(t,\tau_1)[-iL_{12}(\tau_1)]\cdots\mathcal{P}(\tau_{k-1},\tau_k)[-iL_{12}(\tau_k)]\mathcal{P}(\tau_k,t)[iL_{11}(t)]$$

$$\tag{C5}$$

$$\frac{dR^{(2k+1)}}{dt} = -iL_{22}(t)R^{(2k+1)}+R^{(1)}[-iL_{12}]R^{(2k-1)}+\sum_{j=2}^{k-1}R^{(2j-1)}[-iL_{12}]R^{(2k-2j+1)}+R^{(2k-1)}[-iL_{12}]R^{(1)}+iR^{(2k+1)}L_{11}(t)$$

$$= -iL_{22}(t)R^{(2k+1)}+\sum_{j=1}^k R^{(2j-1)}[-iL_{12}]R^{(2k-2j+1)}+iR^{(2k+1)}L_{11}(t). \tag{C6}$$

The above is exactly the equation of motion (27), which concludes the proof.

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