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Memory effects and nonequilibrium transport in open many-particle quantum systems

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Full understanding of the relaxation mechanisms and far-from-equilibrium transport in modern mesoscopic structures requires that such systems be treated as open. We therefore generalize some of the core elements of the Kadanoff-Baym-Keldysh nonequilibrium Green's function formalism, inherently formulated for closed systems, to treatment of an open system, coupled with its environment. We define the two-time correlation functions and analyze the influence of the memory effects on the open-system transport. In the transient regime, the two-time correlation functions clearly show four distinct terms: a closed-system-like term, an entanglement term, and two memory terms that depend explicitly on the initial state of the environment. We show that it is not possible to completely eliminate the influence of the environment by a fortunate choice of the initial state, and approximating the system as closed is valid only in the limit of negligible system-environment coupling, which is never the case in the transient regime. We derive the transport equations for transients that properly account for the system-environment coupling. On the other hand, we address the important issue of transport in a far-from-equilibrium steady state. We show that, once a steady state is reached, the balance between the driving and relaxation forces implies that the two-time correlation functions regain a closed-system-like form, but with an effective, modified system Hamiltonian, and with the *system statistical operator unrelated to that of the initial state*. We emphasize that the difference between the transient and the far-from-equilibrium steady-state regimes, crucial for theoretical investigation of nonequilibrium quasiparticle transport, effectively lies within the different relative magnitude of the combined entanglement and memory terms with respect to the closed-system-like term in two-time correlation functions.

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I. INTRODUCTION

The past few decades have brought much activity in the fields of mesoscopic and nanoscale physics [1–3]. Today, conventional silicon-based semiconductor devices are smaller than ever, typical dimensions being only a few to a few tens of nanometers [4], and low-dimensional semiconductor structures offer a variety of exciting features, both fundamentally interesting (e.g., conductance quantization in quantum point contacts [5,6], Coulomb blockade, and single-electron tunneling in quantum dots [7,8], etc.), and technologically applicable (e.g., high-mobility two-dimensional electron gas in semiconductor heterostructures [9]). On the other hand, ultrashort laser pulse excitations are finally providing us with experimental insight into the femtosecond relaxation properties of materials [10]. Consequently, our present understanding of electronic transport is being challenged in multiple ways, and it has become evident that the typical time and space scales of modern condensed matter physics have dramatically shrunk. Today, a plausible transport theory ought to describe small, very inhomogeneous structures, and be able to adequately address the fast relaxation processes, as well as far-from-equilibrium steady states [2,11–13].

The Kadanoff-Baym-Keldysh nonequilibrium Green's function (NEGF) formalism [14,15] is known to be a very general and powerful technique for theoretical treatment of the evolution of nonequilibrium interacting many-particle systems. Variants of this technique have been used in virtually all disciplines of theoretical physics [1,2,16,17]. The appeal of the NEGF formalism lies in the perturbation expansion, which enables one to elegantly obtain results by partial summation of the diagrams that are dominant within a certain approximation, provided that the initial state admits Wick's decomposition (this important question was addressed in detail by Danielewicz [18]). However, the NEGF formalism is, above all, formulated for closed systems. The state of the environment, if important, is assumed known and unaffected by the feedback from the system. The environment influences the system through a correction to the Hamiltonian, but no degrees of freedom besides the system's are present. Thus, the essence of the NEGF formalism is that the many-body system of interest obeys Hamiltonian dynamics. The evolution is perfectly reversible, and one has the well-defined Heisenberg and interaction pictures, and, consequently, the definitions of the Green's functions and the perturbation expansion. Finally, for the analysis of transport, evaluation of the first few lowest-order Green's functions is usually quite sufficient to obtain quantities such as the current density, etc.

Here we see a principal constraint for the use of the NEGF formalism in the treatment of far-from-equilibrium transport in mesoscopic structures. A far-from-equilibrium steady state of the system of interest is achieved through a balance between the driving and relaxation forces, and cannot be uniquely related to the initial system microstate [19]. This irreversibility in the behavior is due to the fact that the system of interest (the current-carrying electrons) is not a

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closed system, but rather an open subsystem of a larger, interacting closed system (containing phonons, etc.). The environment is indeed affected by the system, especially in the transient regime (e.g., nonequilibrium phonons [20]), and the memory effects become important—the dynamics of an open system is non-Hamiltonian. Full treatment of open systems traditionally relies on the calculation of the system reduced density matrix, but such an approach is feasible only in fairly small systems, such as molecules [21]. In many-body systems, the reduced density matrix is not only impossible to calculate, but is actually unnecessary to analyze transport, as, from experience with closed systems, we know that the first few lowest-order Green's functions should suffice. However, the non-Hamiltonian dynamics makes it impossible to straightforwardly define the open system's counterparts of the Heisenberg and interaction pictures: the memory term in the equation of motion is a crucial element that has no counterpart in closed systems, and thus requires a complete reassessment of many notions lying at the very core of the NEGF formalism as we know it.

In this paper, motivated by the need to deepen the understanding of transport in mesoscopic structures, we generalize some of the core elements of the nonequilibrium Green's function formalism to treatment of transport in open quantum systems; namely, we first generalize the two-time correlation functions to open systems, in such a way that their physical meaning is retained, and their form tends to that of the closed system when the system-environment coupling is turned off. Haake [22] addressed the evaluation of an open system's correlation functions, but his approach requires information about the entire evolution of the environment, which is precisely what we wish to avoid here. Thus, our generalization of the two-time correlation functions is based on the use of the so-called partial-trace-free approach [23], which enables one to avoid calculation of the full system $+$environment quantities when one is interested only in the system. Definition of the two-time correlation functions is at the very core of theoretical analyses of quasiparticle transport (we show how other single-particle Green's functions are easily defined). In this way, we are able to calculate the functions with as little information about the environment as necessary. At this point, we are equipped to analyze the impact of the system-environment coupling on the transport of the open system, and we focus our attention on two extremely distinct regimes: the transient regime and the far-from-equilibrium regime. In the transient regime, we clearly demonstrate that there are four different terms appearing in the two-time-correlation functions. In addition to the closed-system-like term, there are two memory terms, containing the information on the initial state of the environment. In addition, there is an entanglement term, which we show cannot be lost through any manipulation of the initial state of the environment. This term relates the initial state of the system to the present state of the system, sampling the state of the environment at one point in the meantime. This analysis is complemented by the equations of motion for the two-time correlation functions for transients, and by some specific illustrative examples. On the other hand, we analyze the behavior of the two-time correlation functions in a far-from-equilibrium steady state. We point out that one can rigorously arrive at the fundamental, intuitively plausible qualities of the far-from-equilibrium steady state, which are the facts that a balance between the relaxation and the driving forces is obtained and that the statistical operator in such a state cannot be uniquely related to the initial state. Due to the gain-loss balance, we assert that the two-time correlation functions for a far-from-equilibrium steady state are akin to those of a closed system, but with an effective, modified Hamiltonian, and with a density matrix that is unrelated to that of the initial state. We conclude that, as far as quasiparticle transport in open systems is concerned, the transient and steady state regimes can be distinguished by the relative magnitude of the combined entanglement and memory terms with respect to the closed-system-like term: memory and entanglement are very important during transients and virtually nonexistent in a steady state.

In Sec. II A, we introduce the elements of the partial-trace-free approach, which allow us to define the open-system two-time correlation functions in Sec. II B. In Sec. III, transport in the transient regime is addressed, and the equations of motion for the two-time correlation functions are derived. In Sec. IV, a far-from-equilibrium steady state is analyzed. We conclude with a summary and outlook in Sec. V.

II. TWO-TIME CORRELATION FUNCTIONS FOR OPEN SYSTEMS

Our principal goal in this section is to generalize the closed system's two-time correlation functions of the type $\mathrm{Tr}[\rho_H a_H(t')b_H(t)]$, where ρ is the (closed) system density matrix, and a and b are two system operators, all given in the Heisenberg picture, as indicated by the subscript H (no subscript indicates the Schrödinger picture). A definition of the correlation functions has been attempted previously by Haake [22], but, in his work, one was required to use the full evolution of the open system$+$environment, which is precisely what we wish to avoid as best we can. A generalization of the two-time correlation functions will eventually enable us to define the core transport variables: the "greater than" and "less than" single-particle Green's functions, given for closed systems by

$$iG^{>}(1,1')=\mathrm{Tr}[\rho_H\psi_H(t)\psi_H^{+}(t')],$$

$$\pm iG^{<}(1,1')=\mathrm{Tr}[\rho_H\psi_H^{+}(t')\psi_H(t)], \qquad (1)$$

where the upper sign refers to bosons and the lower sign to fermions. The field operators, at this point, can be the creation or annihilation operators at a point in space or in a single-particle state. The following approach can easily be generalized to higher-order Green's functions.

For a closed system with Hamiltonian $h(t)$, which may be time dependent due to external driving forces, the density matrix ρ in the Schrödinger picture obeys the quantum Liouville equation [24–26]

$$\frac{d\rho(t)}{dt} = -i[h(t),\rho(t)] \equiv -iL(t)\rho(t), \tag{2}$$

where L is the Liouville superoperator (superoperators will be denoted by capital letters). With T^c (T^a) denoting the chronological (antichronological) time ordering, and Θ being the Heaviside step function,

$$\rho(t) = U(t,0)\rho(0),$$

$$U(t,t') = \Theta(t-t')T^c \exp\left(-i\int_{t'}^{t} d\tau L(\tau)\right) + \Theta(t'-t)T^a \exp\left(i\int_{t}^{t'} d\tau L(\tau)\right). \tag{3}$$

If a and b are time-independent operators in the Schrödinger picture, it is easily shown that the two-time correlation functions can be written as

$$\mathrm{Tr}[\rho_H a_H(t')b_H(t)] = \mathrm{Tr}\{aU(t',t)[b\rho(t)]\}. \tag{4}$$

That is, when written in the Schrödinger picture, the desired expectation value actually means that, at time t, b acts on ρ (actually, b acts on the "ket" part of ρ); then $b\rho(t)$ evolves under the quantum Liouville equation [i.e., is the argument of $U(t',t)$], until a acts on the result at time t'. We will see that the form on the right-hand side of Eq. (4) is actually the form that allows for a generalization to open systems, while keeping the proper physical meaning. So we first need to investigate how exactly the density matrix of an open system evolves.

A. Open-system reduced density matrix and the 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 $\mathcal{H}_{S+E} = \mathcal{H}_E \otimes \mathcal{H}_S$. The evolution of the total $S+E$ density matrix ρ is given by the quantum Liouville equation (2), with the Hamiltonian h consisting of the system part $h_{\mathrm{sys}} = 1_E \otimes h_S$, the environment part $h_{\mathrm{env}} = h_E \otimes 1_S$, and the interaction part h_{int}, so that $h = h_{\mathrm{sys}} + h_{\mathrm{env}} + h_{\mathrm{int}}$. Obviously, the corresponding Liouville operator is of the form $L = L_{\mathrm{sys}} + L_{\mathrm{env}} + L_{\mathrm{int}}$. Now, the evolution of the open system S is described by the reduced density matrix $\rho_S = \mathrm{Tr}_E(\rho)$, with $\mathrm{Tr}_E(\cdots)$ 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 [23]

$$\overline{\rho_E} \equiv d_E^{-1} \cdot 1_{d_E \times d_E}, \tag{5a}$$

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

$$\overline{P}x = \overline{\rho_E} \otimes \mathrm{Tr}_E x, \quad \overline{Q} = 1 - \overline{P}, \quad x \in \mathcal{H}^2_{S+E}. \tag{5b}$$

The projector operators, in general, were introduced by Nakajima [24], Zwanzig [25], and Mori [26], for obtaining the equation of motion for ρ_S. In the conventional projection-operator approach, 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 (5b), i.e., through $Px = \rho_E \otimes \mathrm{Tr}_E x$, $x \in \mathcal{H}^2_{S+E}$. Then the partial trace over the solution is taken to obtain the system density matrix, as $\mathrm{Tr}_E(P\rho) = \mathrm{Tr}_E(\rho) = \rho_S$. However, we have recently shown [23] that the above choice of $\overline{P}$, Eq. (5b), is such that the partial trace with respect to the environment becomes unnecessary (the so-called *partial-trace-free approach*); namely, $\overline{P}$ 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 $\overline{P}$, i.e.,

$$\mathcal{H}^2_{S+E} = (\mathcal{H}^2_{S+E})_{\overline{P}=1} \oplus (\mathcal{H}^2_{S+E})_{\overline{P}=0}. \tag{6}$$

For any given basis $\{|\alpha\beta\rangle | \alpha,\beta = 1,\ldots,d_S\}$ in $\mathcal{H}^2_S$ (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 $\{|\overline{\alpha\beta}\rangle | \alpha,\beta = 1,\ldots,d_S\}$ in $(\mathcal{H}^2_{S+E})_{\overline{P}=1}$ (see Appendix A) such that, for any $x \in \mathcal{H}^2_{S+E}$,

$$(\mathrm{Tr}_E x)^{\alpha\beta} = \sqrt{d_E}(\overline{P}x)^{\overline{\alpha\beta}}. \tag{7}$$

This basis in the unit eigenspace is complemented by an orthonormal basis in the zero eigenspace. According to the decomposition (6), a vector $x \in \mathcal{H}^2_{S+E}$ can be represented in the complete eigenbasis of $\overline{P}$ by a column

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \tag{8a}$$

and the projectors are represented by

$$\overline{P} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \overline{Q} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \tag{8b}$$

On the other hand, taking the partial trace with respect to E of any $S+E$ observable x gives what the system experiences 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 $\mathcal{H}^2_S$. Therefore, for x_S being the representation column of $x_S = \mathrm{Tr}_E x$ in the basis $\{|\alpha\beta\rangle\}$ of $\mathcal{H}^2_S$, according to Eq. (7) we obtain

$$x_S = x_1\sqrt{d_E}. \tag{9}$$

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

$$A=\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}. \tag{10}$$

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 $\overline{P}$, and is therefore represented by a block-diagonal form in the eigenbasis of $\overline{P}$. 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), namely,[1]

$$A_{\mathrm{sys}}=I_E\otimes A_S=\begin{bmatrix} A_S & 0 \\ 0 & A_2 \end{bmatrix}. \tag{11}$$

Returning to the evolution of the system+environment, described by the Liouvuille equation (2) and its solution (3), in the eigenbasis of $\overline{P}$ defined above, the system +environment total density matrix is given by

$$\rho=\begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix}, \quad \rho_S=\rho_1\sqrt{d_E}. \tag{12}$$

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

$$L(t)=\begin{bmatrix} L_{11}(t) & L_{12}(t) \\ L_{21}(t) & L_{22}(t) \end{bmatrix},$$

$$U(t,t')=\begin{bmatrix} U_{11}(t,t') & U_{12}(t,t') \\ U_{21}(t,t') & U_{22}(t,t') \end{bmatrix}, \tag{13}$$

where $L_{21}=(L_{12})^{\dagger}$ (L is Hermitian), and U is unitary. When Eqs. (2) and (3) are written out in their matrix representations, we obtain

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

$$\frac{d\rho_2}{dt}=-iL_{21}(t)\rho_1(t)-iL_{22}(t)\rho_2(t), \tag{14}$$

and

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

$$\rho_2(t)=U_{21}(t,t')\rho_1(t')+U_{22}(t,t')\rho_2(t'). \tag{15}$$

There are several very important features of Eqs. (13)–(15). First, L_{11} is of the commutator-generated form, i.e., it corresponds to an effective system Hamiltonian $h_{S,\mathrm{eff}}$ given by

$$h_{S,\mathrm{eff}}=h_S+\mathrm{Tr}_E(h_{\mathrm{int}})/d_E, \tag{16}$$

which accounts for the well-known first-order correction to the system energy spectrum [11,27], due to the coupling with the environment (see Appendix C). Secondly, it is clear that the upper-left block matrix of any $S+E$ superoperator can be dubbed the "purely system part" of that operator. The terms in Eq. (13) that effectively account for the system-environment coupling are the off-diagonal terms L_{12} and $L_{21}=(L_{12})^{\dagger}$. In order for the system to evolve as decoupled from the environment, we must have

$$\|L_{12}\rho_2\|\ll\|L_{11}\rho_1\|. \tag{17}$$

This requirement is obviously satisfied when the interaction vanishes ($h_{\mathrm{int}}=0$ implies $L_{12}=0$), but we argue in Sec. IV that, even in the case of appreciable coupling, when a balance between the driving and the relaxation forces is achieved, this criterion is satisfied. This actually defines reaching a far-from-equilibrium steady state.

B. $G^{>}$ and $G^{<}$ for open systems

In the system Liouville space $\mathcal{H}_S^2$, multiplication of the reduced system density matrix ρ_S by the system creation and annihilation operators $\psi_S^{\dagger}$ and ψ_S can be described by superoperators $\Psi^{\dagger}$ and Ψ acting on ρ_S as a vector in $\mathcal{H}_S^2$. It is understood that the Liouville space is constructed to allow for this action, i.e., that, in addition to the states corresponding to a given number of particles (e.g., electrons), which are used to construct ρ_S, at least the states with ±1 electron are included. This is a computational rather than a theoretical requirement, and it suffices when one is interested only in two-time correlation functions, meaning that at most one particle is created (annihilated). Accommodation of higher-order Green's functions will require further augmentation of the system Liouville space during computation.

Now, within the total system+environment, annihilation of a system particle can be described by a superoperator Ψ, of the form $\Psi=I_E\otimes\Psi_S$, which, according to Eq. (11), has the following block-diagonal form in the eigenbasis of $\overline{P}$:

$$\Psi=\begin{bmatrix} \Psi_S & 0 \\ 0 & \Psi_2 \end{bmatrix}. \tag{18}$$

Obviously, the creation operator $\psi_S^{\dagger}$ will be associated with $\Psi^{\dagger}$.

We are now almost fully equipped to define the two-time correlation functions for open systems. Following the discussion of the introductory part of this section, a definition of $G^{>}(1,1')$ for the open system requires that, first, a system particle is created at time t' [i.e., $\Psi^{\dagger}$ acts on $\rho(t')$]; then $\Psi^{\dagger}\rho$ evolves until t, when a particle is annihilated. However, *we need only the system's point of view of this action*, not the full system+environment's. So, we define two auxiliary variables $\rho^{\Psi^{\dagger},t'}(t)$ and $\rho^{\Psi,t'}(t)$ such that

$$\rho^{\Psi^{\dagger},t'}(t')=\Psi^{\dagger}\rho(t'),\quad \rho^{\Psi^{\dagger},t'}(t)=U(t,t')\rho^{\Psi^{\dagger},t'}(t'),$$

$$\rho^{\Psi,t'}(t')=\Psi\rho(t'),\quad \rho^{\Psi,t'}(t)=U(t,t')\rho^{\Psi,t'}(t'). \tag{19}$$

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[1] We will make no distinction between a system superoperator A_S on $\mathcal{H}_S^2$ and its representation matrix in $\{|\alpha\beta\rangle\}$. The relations that we obtain later are essentially basis independent, since, for any chosen basis $\{|\alpha\beta\rangle\}$ in $\mathcal{H}_S^2$, there is a unique basis $\{|\overline{\alpha\beta}\rangle\}$ in $(\mathcal{H}_{S+E}^2)_{\overline{P}=1}$ such that Eqs. (7)–(11) hold.

We then define the open system's "greater than" and "less than" Green's functions as

$$iG_S^{>}(1,1')\equiv \mathrm{Tr}_S[\Psi_S\rho_S^{\Psi^\dagger,t'}(t)],$$
$$\pm iG_S^{<}(1,1')\equiv \mathrm{Tr}_S[\Psi_S^\dagger\rho_S^{\Psi,t}(t')]. \tag{20}$$

These definitions have exactly the required physical meaning. The information provided by these functions is clear after writing Eqs. (20) as

$$iG_S^{>}(1,1')=\mathrm{Tr}_S[\Psi_S U_{11}(t,t')\Psi_S^\dagger\rho_S(t')] + \sqrt{d_E}\,\mathrm{Tr}_S[\Psi_S U_{12}(t,t')\Psi_2^\dagger\rho_2(t')],$$
$$\pm iG_S^{<}(1,1')=\mathrm{Tr}_S[\Psi_S^\dagger U_{11}(t',t)\Psi_S\rho_S(t)] + \sqrt{d_E}\,\mathrm{Tr}_S[\Psi_S^\dagger U_{12}(t',t)\Psi_2\rho_2(t)]. \tag{21}$$

There are two terms on the right-hand side of Eqs. (21). But, before proceeding with the analysis of Eq. (21), it is important to recall that there are two classes of states in $\mathcal{H}_{S+E}^2$: the first ones belong to the $(\mathcal{H}_{S+E}^2)_{\overline{P}=1}$, and due to the isomorphism given by Eq. (7) we call them the *pure system states*. States from $(\mathcal{H}_{S+E}^2)_{\overline{P}=0}$, the orthocomplement to $(\mathcal{H}_{S+E}^2)_{\overline{P}=1}$, we dubbed *entangled states*, as they contain the information on the entanglement of the system and environment states; namely, by entanglement one usually considers any deviation of the $S+E$ density matrix from a tensor product of the subsystems' density matrices. Here, however, we are interested in whether or not the total $S+E$ density matrix deviates from $\overline{\rho_E}\otimes\rho_S$, i.e., whether $\rho_2\neq 0$. In Sec. III B, we will see that this particular form has special features from the information-entropy standpoint.

We now see that each of the equations (21) contains two terms: one that describes propagation between pure system states and pure system states, and one that describes *the transfer of information between the entangled and pure states*. In Fig. 1, we have depicted the contributions from the two terms to $G^{>}$. It is important to note that, if we were to neglect the system-environment coupling, i.e., if the system were treated as closed, only the first term [Fig. 1(a)] would survive, so propagation between pure system states and pure system states is *closed-system-like*.

An illustration of the solidity of our definition (21) is the form of the average density at a given point; namely,

$$\langle n_S(\mathbf{r},t)\rangle=\pm iG_S^{<}(\mathbf{r}t,\mathbf{r}t)=\mathrm{Tr}_S[\Psi_S^\dagger(\mathbf{r})\Psi_S(\mathbf{r})\rho_S(t)]$$
$$=\mathrm{Tr}_S[\psi_S^\dagger(\mathbf{r})\psi_S(\mathbf{r})\rho_S(t)]=\mathrm{Tr}_S[n(\mathbf{r})\rho_S(t)], \tag{22}$$

since, from Eq. (3), $U(t,t)=1$, so $U_{11}(t,t)=1$, $U_{12}(t,t)=0$, and the result above is exactly what is expected.

Having properly defined $G^{>}$ and $G^{<}$, we can now define the chronological and antichronological Green's functions G^c and G^a as

$$G_S^c(1,1')=\Theta(t-t')G_S^{>}(1,1')+\Theta(t'-t)G_S^{<}(1,1'),$$
$$G_S^a(1,1')=\Theta(t'-t)G_S^{>}(1,1')+\Theta(t-t')G_S^{<}(1,1'). \tag{23}$$

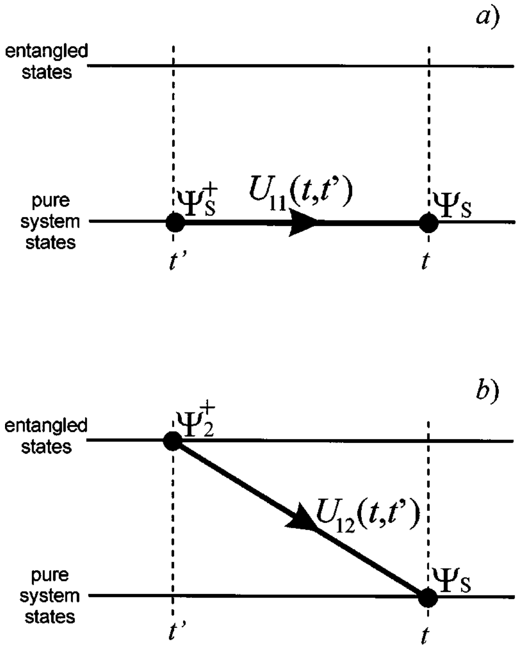

FIG. 1. Illustration of the two terms in the definition of $G_S^{>}$, from Eq. (21). (a) A particle is created at t' among the pure system states, and annihilated at t, also among the pure system states. (b) A particle is created among the entangled states at t', and due to this event the information about the state of the environment becomes apparent at t, when the particle is annihilated.

Writing down the equations of motion for these time-ordered Green's functions would be the next logical step. However, since we do not wish to specify anything about the interaction, and thus cannot *a priori* expect to obtain a Martin-Schwinger-type hierarchy, we will not proceed along these lines. Rather, we will focus our interest on the importance of the memory effects on transport.

III. TRANSPORT IN THE TRANSIENT REGIME

Transient regimes have, so far, received fairly little theoretical attention, compared to steady-state regimes. First, the transient regime is virtually irrelevant when the main purpose is the description of the steady-state regime, as the system tends to "forget" about the unimportant details of its past. Second, the conceptual difficulties of formulating and solving transport equations within the transient regime have been significant. Third, until the femtosecond laser excitation enabled insight into the short-time behavior of systems, the fine details of transport on these time scales were experimentally unverifiable.

Recently, transients have been receiving enhanced theoretical attention [16,28]. For example, much work on the treatment of initial correlations in nonequilibrium Green's functions has been done recently [29]. Ladder-type diagrams have been obtained as a correction to the diagrammatic expansions due to the initial correlations. However, we believe that the introduction of initial correlations, which are undoubtedly very important, may be insufficient to describe the relaxation. Here, we will try to achieve an understanding of transient processes in general, within the present approach and without necessarily specifying the details of the Hamiltonians. We will investigate how exactly the memory effects influence the near-equilibrium transport; i.e., how the state of the environment and the entanglement between the system and the environment states are observed in the open system's evolution.

During transient processes, the state of $S+E$ can be tracked back to the initial state at time t_0, which is assumed to be given by a known density matrix $\rho(t_0)$. There usually exists a typical relaxation time τ_{relax}, during which the transient may be considered to occur, and after which a steady state is achieved. Consider $G_S^<(1,1')$ in the transient regime, with the initial time set to t_0, and $t_0<t,t'\ll\tau_{\mathrm{relax}}$. Using Eqs. (21) and (15), we obtain

$$\begin{aligned}\pm iG_S^<(1,1') = {} & \mathrm{Tr}_S[\Psi_S^\dagger U_{11}(t',t)\Psi_S U_{11}(t,t_0)\rho_S(t_0)] \\ & + \mathrm{Tr}_S[\Psi_S^\dagger U_{12}(t',t)\Psi_2 U_{21}(t,t_0)\rho_S(t_0)] \\ & + \sqrt{d_E}\,\mathrm{Tr}_S[\Psi_S^\dagger U_{11}(t',t)\Psi_S U_{12}(t,t_0)\rho_2(t_0)] \\ & + \sqrt{d_E}\,\mathrm{Tr}_S[\Psi_S^\dagger U_{12}(t',t)\Psi_2 U_{22}(t,t_0)\rho_2(t_0)]. \end{aligned} \tag{24}$$

Of course, $G_S^<$ measures the probability of ending up in the same system state, after having annihilated a particle at time t at a given position $\mathbf{r}$, and then having created it at a (later) time t' at $\mathbf{r}'$. Apparently, there are four terms that contribute to this correlation function, and they are depicted in Fig. 2. The first term is the *closed-system-like term* [Fig. 2(a)], the only one that survives if the coupling between S and E is turned off (i.e., if $L_{12}\to 0$); the name given to it has to do with the fact that this term describes only the influence that pure system states have on pure systems states, whereas the *information on the state of the environment is never incorporated*. The last two terms [Figs. 2(c) and 2(d)] are the so-called *memory terms*, as they start with the entangled states, so they contain the information on the *initial state of the environment*. These terms are both of first order in the coupling L_{12}. The second term [Fig. 2(b)] is dubbed the *entanglement term*, as it does start and end with pure system states, but in between the information on the state of the environment is sampled. This term is of second order in L_{12}. The classification of terms as closed-system-like, entanglement, and memory terms retains its meaning even in multiple-time correlation functions (for entanglement terms, the requirement will be that the term starts and ends with pure states, but in between *at least once* the state of the environment is sampled). In the attempt to generalize the Kadanoff-Baym-Keldysh equations for open systems, we believe that it will be possible to treat the entanglement terms through a type of correction to the self-energy part, whereas the memory terms will unfortunately remain as additive terms in the equations of motion.

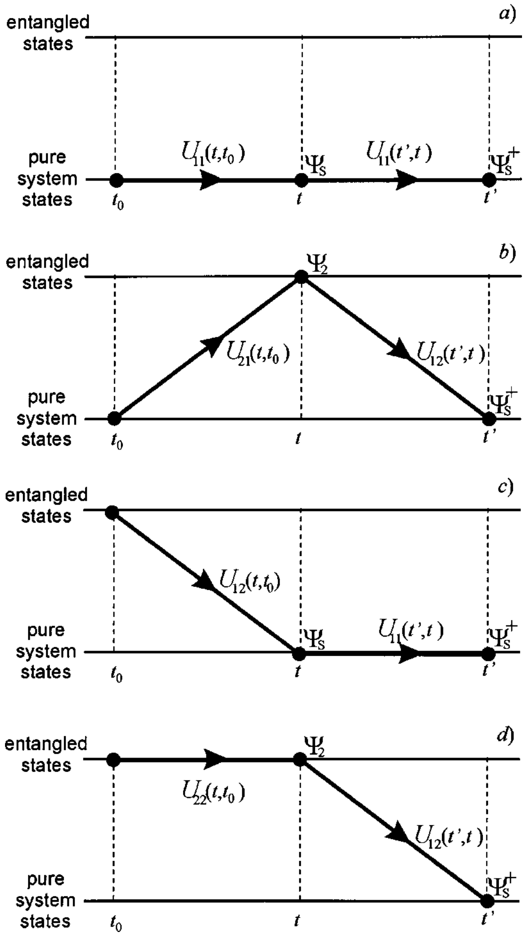

FIG. 2. The four terms in $G_S^<$ for an open system in the transient regime, from Eq. (24). (a) The closed-system-like term; (b) the entanglement term; (c) and (d) the memory terms.

A. Transport equations for the transient regime

The evaluation of the submatrices U_{ij}, needed to calculate the open system's $G^<$ (and $G^>$, in a similar fashion), becomes difficult with increasing size of the system and environment, and direct computation is generally out of the question. However, within the time-convolutionless approach, U_{21} and U_{22} can always be written in terms of U_{11} and U_{12}, but formalization of these relationships requires establishing a time t_0. This approach is therefore ideal for transients, and we present it along the lines of Ref. [23]; namely, the equations of motion for ρ_1 and ρ_2 can be written as[2]

$$\begin{aligned}\frac{d\rho_1(t)}{dt} = {} & -i[L_{11}(t)-L_{12}(t)K_{22}^{-1}(t;t_0)K_{21}(t;t_0)]\rho_1(t) \\ & -iL_{12}(t)K_{22}^{-1}(t;t_0)H_{22}(t,t_0)\rho_2(t_0), \\ \rho_2(t) = {} & -K_{22}^{-1}(t;t_0)K_{21}(t;t_0)\rho_1(t) \\ & +K_{22}^{-1}(t;t_0)H_{22}(t,t_0)\rho_2(t_0), \end{aligned} \tag{25}$$

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[2] This presentation of the equations of motion is somewhat different from the presentation in Ref. [23], but they are easily shown to be equivalent.

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

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

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

$$\frac{dK_{22}(t;t_0)}{dt}=-iL_{22}(t)K_{22}(t;t_0)+iK_{22}(t;t_0)L_{22}(t)+iK_{21}(t;t_0)L_{12}(t),$$

$$K_{21}(t_0;t_0)=0,\quad K_{22}(t_0;t_0)=1. \tag{26}$$

Note that the second time variable in the argument of the 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 boundary conditions for *K*, 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.

Now, according to Eq. (25), when the second time variable in the evolution matrices is fixed to t_0, the equations of motion for the evolution submatrices are given by

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

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

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

$$U_{22}(t,t_0)=K_{22}^{-1}(t;t_0)[H_{22}(t,t_0)-K_{21}(t;t_0)U_{12}(t,t_0)]. \tag{27}$$

After solving Eqs. (26) and (27), and taking into account $U(t',t)=U(t',t_0)U^{+}(t,t_0)$, we can obtain the submatrices needed in the two-time correlation functions and the relevant single-particle quantities. Although Eqs. (25)–(27) are undoubtedly complicated, their main advantage is their enhanced transparency. Since there is no explicit environmental partial trace that obscures the structure of relevant terms, an expansion in terms of L_{12} can be performed. We will now analyze some specific examples.

B. The example of a "randomized environment"

An interesting example is the example of a "randomized environment," i.e., the case in which the state of the system+environment at t_0 is given by $\rho_{\mathrm{rand}}(t_0)=\overline{\rho_E}\otimes\rho_S(t_0)$. We have dubbed this state the case of the "randomized environment" because the initial density matrix of the environment is the uniform density matrix $\overline{\rho_E}$, and it is known that the entropy corresponding to such a density matrix is maximal. One may wonder if such an example has any relation to the real world, and the answer is "yes." Let us assume that the initial state of $S+E$ is of the tensor-product type (indicating that *S* and *E* were, at least approximately, uncoupled in the past), and that the initial environment density matrix $\rho_E(t_0)$ commutes with the environment Hamiltonian h_E (which is the case, e.g., in thermal equilibrium). If the system-environment coupling becomes appreciable, but such that the environment states, which come into play through the matrix elements of the interaction Hamiltonian h_{int}, are virtually equally distributed within $\rho_E(t_0)$, we can reduce the dimension of the environment Hilbert space that is relevant, and within this reduced space the effective initial environment density matrix is uniform, so the "randomized environment" approximation actually is quite plausible. A typical example is found at very high temperatures, when for all the relevant environment energy levels $\varepsilon_{n,E}$, $\varepsilon_{n,E}/k_BT\to 0$.

Since $\rho_E(t_0)=\overline{\rho_E}$, $\rho_2(t_0)=0$. From Eq. (25), we see that the equation for ρ_S becomes

$$\frac{d\rho_S(t)}{dt}=-i[L_{11}(t)-L_{12}(t)K_{22}^{-1}(t;t_0)K_{21}(t;t_0)]\rho_S(t), \tag{28}$$

the form of which indicates that the system evolves as if decoupled from the environment. However, the influence of the environment is contained in the entanglement operators K_{21} and K_{22}—there may not be obvious memory effects (i.e., explicit information on the evolution of the environment all the way from the initial state), but entanglement occurs. Information on the current state of the environment is present, as the second term on the right-hand side of Eq. (28) is clearly related to the term $\rho_2(t)=-K_{22}^{-1}(t;t_0)K_{21}(t;t_0)\rho_1(t)$ [from Eq. (25)]. This feature is also seen when analyzing $G^{<}_{S,\mathrm{rand}}$. That is, among the four terms from Eq. (24), the two memory terms have vanished, but the closed-system-like term and the entanglement term survive, namely,

$$\pm iG^{<}_{S,\mathrm{rand}}(1,1')=\mathrm{Tr}_S[\Psi_S^{\dagger}U_{11}(t',t)\Psi_SU_{11}(t,t_0)\rho_S(t_0)]+\mathrm{Tr}_S[\Psi_S^{\dagger}U_{12}(t',t)\Psi_2U_{21}(t,t_0)\rho_S(t_0)]. \tag{29}$$

So the statement that the system evolves as uncoupled from the environment is not exactly true: the memory terms may be absent, but entanglement is present.

The case of the randomized environment is only one among the class of situations where the initial state can be factorized as $\rho(t_0)=\rho_E(t_0)\otimes\rho_S(t_0)$. As shown in Ref. [23], for any such case, the reduced density matrix at a given time *t* can be related to the initial reduced density matrix according to an equation of the form

$$\rho_S(t)=\mathcal{E}(t,t_0)\rho_S(t_0), \tag{30}$$

where $\mathcal{E}$ is not unitary, but we will not go into details of its structure. One might say that the system *S* is, in this case, evolving as decoupled from the environment, and, according to Lindblad [30], no other type of initial density matrix $\rho(t_0)$ will allow for such evolution. What we want to stress here is that, since the initial state of the environment is contained within $\mathcal{E}$ [23], the memory terms will be important in transport, as the two-time correlation functions will contain them. In the case of a randomized environment, however, one may say that no memory terms are present for the simple reason of the environment having initially *no information to transmit* (its initial density matrix was uniform). All the ordering in the environment (i.e., deviations in the environment's density matrix from the uniform one) can be attributed to the system's influence.

We may conclude that the effects of the system-environment coupling are specified by the dynamics (i.e., the coupling strength) and cannot be *completely* eliminated by a fortunate choice of an initial state, contrary to statements made in some work. Here, we have given only the most general considerations regarding the importance of memory effects in the transient regime. What needs to be done in future work is to obtain a perturbation expansion, in terms of the coupling strength L_{12}, of the memory terms and especially the entanglement term in $G_S^<$ and $G_S^>$, which may result in significant corrections to the fine details of processes such as relaxation of electrons due to scattering with nonequilibrium phonons in semiconductors.

IV. TRANSPORT IN A FAR-FROM-EQUILIBRIUM STEADY STATE

Reaching a well-controlled steady state, independent of initial conditions, is the goal of applying external driving forces in various systems, such as semiconductor devices. Typically, after the characteristic relaxation time τ_{relax}, a far-from-equilibrium steady state is achieved, for which

$$\rho_S \approx \text{const} \quad (t \gg \tau_{\mathrm{relax}}). \tag{31}$$

The relaxation time is sufficiently long to destroy the information about the initial correlations and build up new ones, in agreement with the external driving forces [11]. When the transients have died out, we assert that, since the relaxation forces have adjusted to the driving forces, *no more information from the environment is being passed on to the system*, i.e.,

$$\|L_{12}(t)\rho_2(t)\| \ll \|L_{11}(t)\rho_1\| \quad (t \gg \tau_{\mathrm{relax}}). \tag{32}$$

The system effectively starts to be decoupled from the environment, and ρ_S evolves under L_{11} alone. Together, the decoupling criterion Eq. (32) and the steady-state criterion Eq. (31) imply

$$\frac{d\rho_S}{dt} \approx -iL_{11}(t)\rho_S \approx 0. \tag{33}$$

Since L_{11} is commutator-generated, corresponding to the effective Hamiltonian $h_{S,\mathrm{eff}}$, Eq. (16), we obtain

$$[h_{S,\mathrm{eff}}(t),\rho_S] = [h_S(t) + (1/d_E)\mathrm{Tr}_E h_{\mathrm{int}}(t),\rho_S] \approx 0. \tag{34}$$

This equation is a mathematical way of saying that a balance between the driving forces (h_S) and the relaxation forces $[d_E^{-1}\mathrm{Tr}_E h_{\mathrm{int}}(t)]$ has been achieved. It is important to note that the steady-state influence of the environment is seen *solely* through the *self-consistent relaxation term* $d_E^{-1}\mathrm{Tr}_E h_{\mathrm{int}}(t)$ and no longer through terms that explicitly involve the state of the environment.

As a consequence of the decoupling requirement (32), the far-from-equilibrium steady-state $G_S^<$ takes on the typical form for closed systems, with the effective total system Hamiltonian $h_{S,\mathrm{eff}}$, namely,

$$\begin{aligned} \pm iG_S^<(1,1') &= \mathrm{Tr}_S[\Psi_S^\dagger U_{11}(t',t)\Psi_S\rho_S] \\ &= \mathrm{Tr}_S[\psi_S^\dagger u(t',t)\psi_S\rho_S u(t,t')], \end{aligned} \tag{35}$$

where

$$\begin{aligned} u(t',t) = {} & \Theta(t'-t)T^c \exp\left(-i\int_t^{t'} d\tau\, h_{S,\mathrm{eff}}(\tau)\right) \\ & + \Theta(t-t')T^a \exp\left(i\int_{t'}^{t} d\tau\, h_{S,\mathrm{eff}}(\tau)\right). \end{aligned} \tag{36}$$

The situation seems exceptionally promising, as all the elements of the NEGF formalism could be applied as they are. Unfortunately, there are several major drawbacks. First, we do not really know what the far-from-equilibrium steady-state ρ_S actually is, and, in real systems, one obtains a single far-from-equilibrium state from multiple initial conditions. Furthermore, we are, in general, unable to solve Eq. (34), and, even if we were, the solution may not be unique, and should further be specified by a relevant set of state parameters (such as occupation numbers, average energy, etc.). This could be accomplished by constructing an approximate *relevant statistical operator* [31], which satisfies the self-consistency requirements for the given set of state parameters. However, diagrammatic expansion in terms of the system-environment interaction term $\mathrm{Tr}_E(h_{\mathrm{int}})/d_E$ may not be possible, as the relevant statistical operator does not, in general, admit Wick's decomposition. However, the Dyson equation can be recovered for the so-called *mixed Green's functions* [32].

It is noteworthy that the results of this section actually address an issue well known in semiclassical transport theory. That is, when solving, e.g., the energy-balance equation (a version of the Boltzmann equation [33]) with large energy exchanging terms [which would correspond to the term $d_E^{-1}\mathrm{Tr}_E h_{\mathrm{int}}(t)$ in Eq. (34)], it becomes difficult to integrate over the energy axis, due to noncausality introduced by these terms. An alternative solution starts from an equilibrium distribution that is among the many initial states that would yield a given steady state. In this way, a particular trajectory in the system's evolution is fixed, which makes the integration straightforward and convergent [34].

V. CONCLUSION

Presently, considerable effort is being focused on deepening our understanding of transport in mesoscopic structures, especially on short time scales. In this paper, we have argued that proper treatment of relaxation mechanisms in these systems requires treating the system as open, and we have therefore introduced a basis for generalization of the nonequilibrium Green's functions formalism for analysis of open systems. Using the so-called partial-trace-free approach, we have defined the two-time correlation functions and the time-ordered single-particle Green's functions for an open system. In the transient regime, in addition to the term expected for closed systems, there are additional terms in the two-time correlation functions, which correspond to the entanglement and to the memory effects. The entanglement term is impossible to lose by manipulation of the initial state of the environment. We have also derived the equations of motion for the two-time correlation functions in the transient regime.

On the other hand, we have shown that, in a far-from-equilibrium steady state, due to the balance of the driving and relaxation forces, the system and the environment become virtually independent, as far as information exchange between them is concerned, and the system continues to evolve as if uncoupled from the environment and governed by an effective, modified Hamiltonian. The two-time correlation functions recover their closed-system forms, but the system far-from-equilibrium density matrix remains an unknown. It might be addressed by the relevant statistical operator approach, if a set of measured variables is given. This work rigorously proves that the difference between the transient and the far-from-equilibrium steady-state regimes is that, during transients, the combined memory and entanglement terms are appreciable with respect to the closed-system-like term, while they are virtually nonexistent in a far-from-equilibrium steady state. Further development of the nonequilibrium Green's function formalism for open systems is in progress.

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APPENDIX A

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

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

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

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

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

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

where

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

Using the fact that $\mathrm{Tr}_E x$, being a vector in $\mathcal{H}^2_S$, 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. (7):

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

APPENDIX B

In this appendix, we show that any superoperator of the form $A_{\mathrm{sys}}=I_E\otimes A_S$ commutes with $\overline{P}$, and prove Eq. (11), i.e., we demonstrate that the upper left block matrix of A_{sys} in the eigenbasis of $\overline{P}$ is exactly A_S. First, note that $\overline{P}$ and A_{sys} commute:

$$\begin{aligned}\overline{P}A_{\mathrm{sys}}x&=\overline{\rho_E}\otimes\mathrm{Tr}_E[(I_E\otimes A_S)x]=\overline{\rho_E}\otimes A_S\mathrm{Tr}_E x\\&=(I_E\otimes A_S)(\overline{\rho_E}\otimes\mathrm{Tr}_E x)=A_{\mathrm{sys}}\overline{P}x.\end{aligned} \tag{B1}$$

This result is obviously independent of the choice of the projector, i.e., any environment density matrix can be chosen instead of $\overline{\rho_E}$ to induce the projector. The upper left block-matrix elements of A_{sys} are given by

$$\begin{aligned}(A_{\mathrm{sys}})^{\overline{\alpha\beta}}_{\overline{\sigma\gamma}}&=\frac{1}{d_E}\sum_{i,j=1}^{d_E}\langle i\alpha,i\beta|I_E\otimes A_S|j\sigma,j\gamma\rangle\\&=(A_S)^{\alpha\beta}_{\sigma\gamma}\frac{1}{d_E}\underbrace{\sum_{i,j=1}^{d_E}\delta^i_j}_{d_E}\\&=(A_S)^{\alpha\beta}_{\sigma\gamma}.\end{aligned} \tag{B2}$$

APPENDIX C

We will prove that L_{11} for the Hamiltonian of the form

$$h = 1_E \otimes h_S + h_E \otimes 1_S + h_{\text{int}} \tag{C1}$$

is of the commutator-generated form, corresponding to an effective Hamiltonian given by Eq. (16). That is, the Hamiltonian matrix elements in the basis specified in Appendix A are

$$h^{i\alpha}_{j\beta} = (h_E)^i_j \delta^\alpha_\beta + \delta^i_j (h_S)^\alpha_\beta + (h_{\text{int}})^{i\alpha}_{j\beta}, \tag{C2}$$

yielding the matrix elements of the Liouville operator as

$$L^{i\alpha,j\beta}_{p\sigma,q\gamma} = h^{i\alpha}_{p\sigma} \delta^j_q \delta^\beta_\gamma - h^{q\gamma}_{j\beta} \delta^i_p \delta^\alpha_\sigma . \tag{C3}$$

In particular,

$$\begin{aligned}(L_{\text{sys}})^{i\alpha,j\beta}_{p\sigma,q\gamma} &= \delta^i_p \delta^j_q [(h_S)^\alpha_\sigma \delta^\beta_\gamma - \delta^\alpha_\sigma (h_S)^\gamma_\beta] = \delta^i_p \delta^j_q (L_S)^{\alpha\beta}_{\sigma\gamma},\\ (L_{\text{env}})^{i\alpha,j\beta}_{p\sigma,q\gamma} &= \delta^\alpha_\sigma \delta^\beta_\gamma [(h_E)^i_p \delta^j_q - \delta^i_p (h_E)^q_j] = \delta^\alpha_\sigma \delta^\beta_\gamma (L_E)^{ij}_{pq} .\end{aligned} \tag{C4}$$

According to Eq. (B2), we obtain

$$L^{\overline{\alpha\beta}}_{\overline{\sigma\gamma}} = \langle \overline{\alpha\beta} | L | \overline{\sigma\gamma} \rangle = \frac{1}{d_E} [(\text{Tr}_E h)^\alpha_\sigma \delta^\beta_\gamma - \delta^\alpha_\sigma (\text{Tr}_E h)^\gamma_\beta], \tag{C5}$$

so we see that

$$\begin{aligned}(L_{\text{sys}})^{\overline{\alpha\beta}}_{\overline{\sigma\gamma}} &= (L_S)^{\alpha\beta}_{\sigma\gamma} = [(h_S)^\alpha_\sigma \delta^\beta_\gamma - \delta^\alpha_\sigma (h_S)^\gamma_\beta],\\ (L_{\text{env}})^{\overline{\alpha\beta}}_{\overline{\sigma\gamma}} &= 0,\\ (L_{\text{int}})^{\overline{\alpha\beta}}_{\overline{\sigma\gamma}} &= \left(\frac{1}{d_E}\right) [(\text{Tr}_E h_{\text{int}})^\alpha_\sigma \delta^\beta_\gamma - \delta^\alpha_\sigma (\text{Tr}_E h_{\text{int}})^\gamma_\beta].\end{aligned} \tag{C6}$$

We have already seen from Eq. (C5) that L_{11} is of the commutator-generated form, and we could say that the effective Hamiltonian was $(1/d_E)\text{Tr}_E h$. However, even though $\text{Tr}_E h_{\text{env}} = (\text{Tr}_E h_E) I_S \neq 0$, still $L_{\text{env},11} = 0$, so apparently the influence of the environment is not present in L_{11}. Therefore, we realize that the effective system Hamiltonian, corresponding to L_{11}, should be chosen as

$$h_{S,\text{eff}} = h_S + \frac{1}{d_E} \text{Tr}_E h_{\text{int}} . \tag{C7}$$

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