

Quantum transport and memory effects in mesoscopic structures

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Abstract

A modern theory of electronic transport in mesoscopic structures needs to non-perturbatively treat the active region of the device as an open subsystem of a larger, interacting closed system, and be able to successfully capture transient processes, as well as a far-from-equilibrium steady state. We present a basis for generalization of the powerful non-equilibrium Green's functions formalism for treatment of open systems. During transient processes and far from equilibrium, we analyze the magnitude and importance of the memory terms, which appear in the two-time correlation functions and are the signatures of the system's openness.

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1. Introduction

The fields of mesoscopic and nanoscale physics have been very active in the past few decades [1–3]. Today, conventional silicon-based semiconductor devices have typical dimensions of a few tens of nanometers (see, e.g., articles in Ref. [4]), and low-dimensional semiconductor structures offer a variety of exciting and useful features [5–7]. On the other hand, ultrashort laser pulse excitations provide us with the experimental insight into the femtosecond relaxation properties of materials [8].

Consequently, our understanding of electronic transport is being challenged in multiple ways, and a modern transport theory needs to be able to fulfill several new requirements. First, it needs to deal with small, very inhomogeneous structures. Not only are

the active regions of the devices small, but so are the contacts. The feedback of the active part of the device (current-carrying electrons) to its environment (contacts, phonons, etc.) may no longer be neglected, or treated in a perturbative fashion—the active part of the device must be treated fully as an open subsystem of a larger, interacting closed system. On the other hand, the enhanced interest in the transient properties of devices implies that a theory must be capable of capturing both the fast relaxation processes in the transient regime and the far-from-equilibrium steady state. Therefore, a *modern electronic transport theory ought to be a real-time theory of open systems*.

Traditionally, open systems are treated using some variant of the reduced density matrix formalism [9,10], which works for small systems, such as molecules. Many-body systems, such as an electron gas, are usually treated with many-body techniques, i.e., with Green's functions. The non-equilibrium Green's function (NEGF) formalism (based on the

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works of Kadanoff and Baym [11], and Keldysh [12]) is attractive because of the perturbation expansion, and usually the first few lowest-order Green's functions are enough to analyze transport. Unfortunately, this formalism is inherently formulated for closed systems, i.e., systems with Hamiltonian dynamics, for which, in the well-known Heisenberg and interaction pictures, respectively, one obtains the definitions of the Green's functions and their diagrammatic expansions. The dynamics of open systems is, however, non-Hamiltonian,¹ since a typical equation of motion for an open system's reduced density matrix in the Schrödinger picture contains an additive term containing information on the evolution of the environment [9,10]. Therefore, a concept of the open-system Heisenberg picture is unclear, and a generalization of NEGF formalism for open systems is not straightforward.

In this paper, we first present an outline of the 'partial-trace-free' approach to treatment of the open system's reduced density matrix [13]. This approach has enabled us to generalize the core elements of the NEGF formalism, i.e., the two-time correlation functions, to open systems [14]. Finally, for two drastically distinct regimes, the transient regime and the far-from-equilibrium steady state, we will discuss the importance and magnitude of different types of terms apparent in the open system two-time correlation functions.

2. Two-time correlation functions for open systems

Given a system S , coupled dynamically to its environment E , so that the system+environment ($S+E$) is closed (and therefore Hamiltonian), the density matrix ρ of $S+E$ evolves according to the Liouville equation

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

where h is the $S+E$ Hamiltonian, and L is the corresponding $S+E$ Liouville superoperator.² The

¹ By non-Hamiltonian, we mean that there are additive terms in the equation of motion for the reduced density matrix that cannot be written in a form of a commutator between an operator and the density matrix.

² Superoperators will be denoted by capital roman characters.

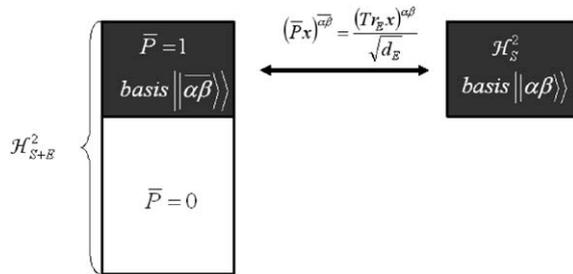


Fig. 1. Decomposition of the system+environment Liouville space into eigenspaces of \bar{P} . The unit-eigenvalue eigenspace is isomorphic to the system Liouville space \mathcal{H}_S^2 , through a simple and useful basis-induced isomorphism (3).

Hamiltonian h is generally a sum of the system part h_{sys} , the environment part h_{env} , and the system–environment interaction term, h_{int} . Consequently, $L = L_{\text{sys}} + L_{\text{env}} + L_{\text{int}}$. The Liouville space of $S+E$, \mathcal{H}_{S+E}^2 (square of the $S+E$ Hilbert space³ \mathcal{H}_{S+E} , i.e., the space of operators on \mathcal{H}_{S+E}) can be decomposed into a direct sum of eigenspaces of a particular projection operator \bar{P} , whose action is given by

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

where \otimes denotes the tensor product, $\bar{\rho}_E = d_E^{-1} \cdot 1_{d_E \times d_E}$ is a uniform environment density matrix, and d_E is the dimensionality of the environment Hilbert space [13].⁴ This decomposition is depicted in Fig. 1. The unit-eigenvalue eigenspace of \bar{P} , denoted by $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$, is isomorphic to the Liouville space of the system alone, \mathcal{H}_S^2 . If, in the unit eigenspace of \bar{P} ,

³ For many-particle systems, the role of the Hilbert space is commonly played by the particles' Fock space, or some of its relevant subspaces.

⁴ It is important to remark that the choice of what is the system and what is the environment within $S+E$ must be fixed; and consequently, their Hilbert spaces are fixed as well. In that respect, the partial trace with respect to the environment states is always well defined and time-independent. Cases of, for instance, time-dependent boundaries between subsystems cannot, in general, be addressed with the above approach. The same generally holds for treatment of phase transitions: if the nature of the states available for the subsystems before and after the transition is different (e.g. in low-temperature superconductivity: free electrons+phonons before, Bose condensate after), the above approach will not be able to capture the transitions if only one species of states is present in the Hilbert spaces.

a specific basis $\{|\overline{\alpha\beta}\rangle\}$ is chosen (details of construction can be found in [13]), uniquely related to a basis $\{|\alpha\beta\rangle\}$ in \mathcal{H}_S^2 , the isomorphism between $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$ and \mathcal{H}_S^2 becomes very simple and useful. Namely, we find

$$(\text{Tr}_E x)^{\alpha\beta} = \sqrt{d_E} \cdot (\bar{P}x)^{\alpha\bar{\beta}}, \quad (3)$$

for any $x \in \mathcal{H}_{S+E}^2$; i.e., the action of \bar{P} becomes equivalent to taking the partial trace over the environment states, up to a constant, $\sqrt{d_E}$.

Using the decomposition from Fig. 1, $x \in \mathcal{H}_{S+E}^2$ can be represented with a block column $x = [x_1 \ x_2]^T$, and $\text{Tr}_E x \in \mathcal{H}_S^2$ will be represented by x_S in basis $\{|\alpha\beta\rangle\}$, so that, according to Eq. (3), $x_S = x_1 \sqrt{d_E}$. Moreover, choosing the basis $\{|\alpha\beta\rangle\}$ implies that a system superoperator A_{sys} has a simple block-diagonal form that satisfies $A_{\text{sys}} = I_E \otimes A_S = \text{diag}[A_S \ A_2]$. We can apply the last form to the system creation and annihilation superoperators,⁵ $\Psi_{\text{sys}}^+(\mathbf{r}) = I_E \otimes \Psi_S^+(\mathbf{r}) = \text{diag}[\Psi_S^+(\mathbf{r}) \ \Psi_2^+(\mathbf{r})]$ and $\Psi_{\text{sys}}(\mathbf{r}) = I_E \otimes \Psi_S(\mathbf{r}) = \text{diag}[\Psi_S(\mathbf{r}) \ \Psi_2(\mathbf{r})]$, of a system particle at a given position in space \mathbf{r} . We are now able to define the system two-particle correlation functions, $G_S^>$ and $G_S^<$, as

$$\begin{aligned} iG_S^>(\mathbf{r}, t; \mathbf{r}', t') &= \text{Tr}_S[\Psi_S(\mathbf{r})U_{11}(t, t')\Psi_S^+(\mathbf{r}')\rho_S(t')] \\ &\quad + \sqrt{d_E} \cdot \text{Tr}_S[\Psi_S(\mathbf{r})U_{12}(t, t')\Psi_2^+(\mathbf{r}')\rho_2(t')], \\ \pm iG_S^<(\mathbf{r}, t; \mathbf{r}', t') &= \text{Tr}_S[\Psi_S^+(\mathbf{r}')U_{11}(t', t)\Psi_S(\mathbf{r})\rho_S(t)] \\ &\quad + \sqrt{d_E} \cdot \text{Tr}_S[\Psi_S^+(\mathbf{r}')U_{12}(t', t)\Psi_2(\mathbf{r})\rho_2(t)], \quad (4) \end{aligned}$$

where the upper sign refers to bosons and the lower one to fermions, ρ_2 comes from the representation column of the total $S+E$ density matrix $\rho = [\rho_1 \ \rho_2]^T$ (i.e., ρ_2 is the part of ρ that belongs to the zero-eigenspace

of \bar{P}), and U_{ij} are the submatrices of the evolution operator

$$\begin{aligned} U(t, t') &= \Theta(t - t')T^c \exp\left(-i \int_{t'}^t d\tau L(\tau)\right) \\ &\quad + \Theta(t' - t)T^a \exp\left(i \int_t^{t'} d\tau L(\tau)\right). \end{aligned}$$

It is important to note that there are two classes of states in \mathcal{H}_{S+E}^2 : the first ones belong to the $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$, and due to the isomorphism described above, we call them the *pure system states*. States from $(\mathcal{H}_{S+E}^2)_{\bar{P}=0}$, the orthocomplement to $(\mathcal{H}_{S+E}^2)_{\bar{P}=1}$, we dub *entangled states*, as they contain the information on the entanglement of the system and environment states: i.e., to put it more formally, they indicate whether ρ deviates from a particular non-entangled⁶ form $\rho = \bar{\rho}_E \otimes \text{Tr}_E \rho$. Each of the Eqs. (4) contains two terms: one that describes propagation between system states and system states, and one that describes *the transfer of information between the entangled and pure states*.

3. Transients vs. far-from-equilibrium steady state: importance of memory terms

For closed systems, the influence of the initial preparation of the system on its evolution has been addressed by Prigogine and Balescu [16], Danielewicz [17], and, more recently, others [18]. When analyzing an open system S in the transient regime, the evolution can be tracked back to the initial time t_0 , at which the state of $S + E$ was characterized by the density matrix $\rho(t_0)$ determined by the details of preparation. In this case, the system's two-time correlation function $G_S^<$ becomes of the form

$$\begin{aligned} \pm iG_S^<(\mathbf{r}, t; \mathbf{r}', t') &= \text{Tr}_S[\Psi_S^+(\mathbf{r}')U_{11}(t', t)\Psi_S(\mathbf{r})U_{11}(t, t_0)\rho_S(t_0)] \end{aligned}$$

⁵ One normally thinks of creation and annihilation operators (not superoperators), but their action on other operators is such that one can easily introduce superoperators with the same action, which is convenient for the generalization that we have in mind here.

⁶ We rely on the general definition of an entangled state [15]: a density matrix of $S + E$ is said to describe a non-entangled (separable) state if it can be written as a tensor product of an environment density matrix and a system density matrix, or as a linear combination of such tensor products. Otherwise, it describes an entangled state.

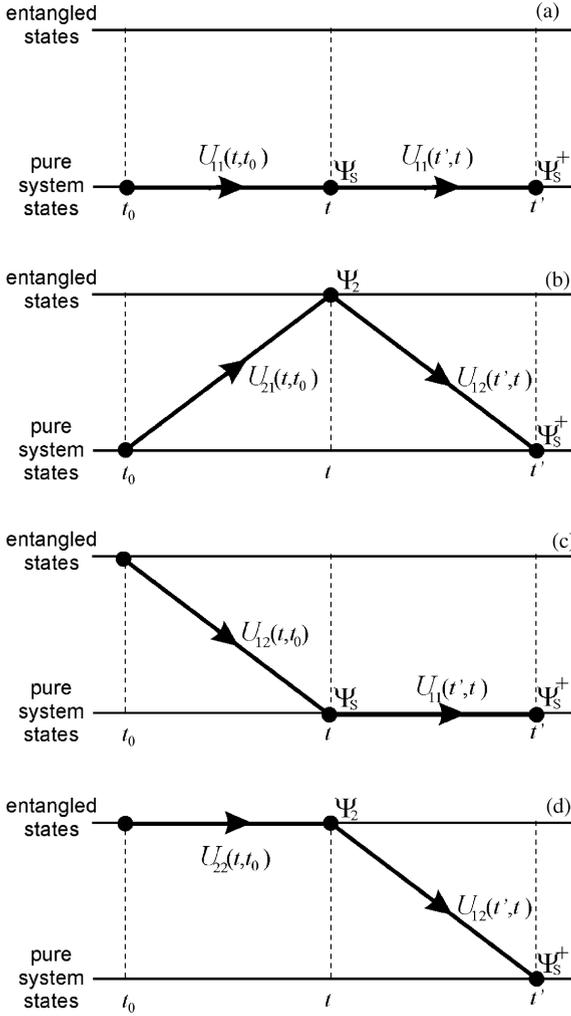


Fig. 2. The four terms in $G_S^<$ for an open system in the transient regime, from Eq. (5). (a) The ‘closed-system-like’ term; (b) the ‘entanglement term’; (c and d) the ‘memory terms’.

$$\begin{aligned}
& + \text{Tr}_S[\Psi_S^+(\mathbf{r}')U_{12}(t', t)\Psi_2(\mathbf{r})U_{21}(t, t_0)\rho_S(t_0)] \\
& + \sqrt{d_E}\text{Tr}_S[\Psi_S^+(\mathbf{r}')U_{11}(t', t)\Psi_S(\mathbf{r}) \\
& \quad \times U_{12}(t, t_0)\rho_2(t_0)] \\
& + \sqrt{d_E}\text{Tr}_S[\Psi_S^+(\mathbf{r}')U_{12}(t', t)\Psi_2(\mathbf{r}) \\
& \quad \times U_{22}(t, t_0)\rho_2(t_0)]. \tag{5}
\end{aligned}$$

The four terms are depicted in Fig. 2. The first term is the *closed-system-like term*, the only one that survives

if the coupling between S and E is turned off (i.e., if $L_{12} \rightarrow 0$), and the nickname given has to do with the fact that this term describes only the influence that the pure system states have on pure systems states, whereas the information on the state of the environment is *never* explicitly incorporated. The last two terms 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 the first order in coupling L_{12} , and are very important in the transient regime. The second term is dubbed the *entanglement term*, as it starts and ends with pure system states, but meanwhile (at time t) the information on the state of the environment is incorporated. This term is of the second order in L_{12} . Equations of motion for the two time correlation functions during transient processes can be found in Ref. [14], but their structure is not our primary interest here. The classification of terms as closed-system-like, entanglement terms, and memory terms retains its meaning even in multiple-time correlation functions. In the light of generalizing the NEGF equations for open systems, we believe that the entanglement terms will be possible to treat through a type of correction to the self-energy. Namely, one may be able to construct a self-energy that contains the system–environment interaction, and that will connect the entanglement and closed-system-like terms in higher order Green’s functions to those of lower order, which holds promise for a Dyson-type equation and a diagrammatic expansion. Again, this is, of course, our belief, as the work is still in progress. On the other hand, the memory terms seem like they will unfortunately remain as additive terms in the equations of motion.

A far-from-equilibrium steady state is, on the other hand, characterized by very different behavior. By a system in a far-from-equilibrium steady state we primarily consider a system driven by an external source (e.g., applied external bias), so that after a sufficiently long time *its relevant output quantities* (e.g., current, conductance, etc.) have reached values that:

- (a) no longer significantly vary with time (steady state);
- (b) are virtually insensitive to the exact preparation of the initial state, and independent of the values that these quantities would have if evaluated in a near-equilibrium state (far-from-equilibrium).

Usually, there exists a characteristic relaxation time τ , after which the system is considered to be stationary, at least with respect to a collection of measured average quantities and within a given margin of error. However, if we enhance the number of (independent) measured quantities, and all of them are to be constant in time, then it is reasonable conclusion that the system density matrix ρ_S in a steady state may be considered a constant. On the other hand, the fact that the relaxation processes have died out can be rephrased as “the information between the system and the environment has already been exchanged” (which does *not* imply that they are dynamically decoupled, i.e., that the interaction Hamiltonian vanishes). Mathematically, this means $\|L_{12}\rho_2\| \ll \|L_{11}\rho_1\|$, and the evolution of the system becomes closed-system-like, according to $(d\rho_S/dt) \approx -iL_{11}(t)\rho_S \approx 0$. Bearing in mind that L_{11} is of a commutator-generated form, corresponding to the effective Hamiltonian $h_{S,\text{eff}} = h_S + \text{Tr}_E(h_{\text{int}})/d_E$, we obtain

$$[h_{S,\text{eff}}(t), \rho_S] = \left[h_S(t) + \frac{1}{d_E} \text{Tr}_E h_{\text{int}}(t), \rho_S \right] \approx 0, \quad (6)$$

which is a formal way of writing down the classical notion that a steady state means reaching a balance between the driving and the relaxation forces.⁷ The two-time correlation functions regain their closed system-like form, e.g.,

$$\begin{aligned} & \pm iG_S^<(r, t; r', t') \\ &= \text{Tr}_S [\Psi_S^+(r') U_{11}(t', t) \Psi_S(r) \rho_S] \\ &= \text{Tr}_S [\psi_S^+(r') u(t', t) \psi_S(r) \rho_S u(t, t')], \end{aligned} \quad (7)$$

where

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

and $\psi_S^+(r)$ and $\psi_S(r)$ are the system creation and annihilation operator (not superoperators), respectively. If one were to know the far-from-equilibrium ρ_S , then

the conventional NEGF formalism could be used. Unfortunately, solving (6) for the unknown ρ_S is never easy, and the solution is generally not unique, but should further be specified by a set of state parameters (occupation numbers, average energy, etc.).

4. Concluding remarks

The problem of the connection between the irreversible macroscopic physics and the reversible underlying microscopic equations has been relevant for a long time (for a comprehensive review article of earlier works, see Chester [19]). A description of the relaxation mechanisms in many-body systems and the exact dynamics of transients have been addressed by many, and notable contributions are certainly due to van Hove [20], Prigogine and Balescu [16], Zwanzig [21], and many others. What these approaches have in common is that they rely on the assumption that the system *is indeed closed*. Master equations for special types of systems and for different relevant quantities are solved (e.g., Prigogine and Balescu [16] solve for the diagonal part of the density matrix to analyze irreversible processes in gases, using a diagrammatic expansion).

Here we wish to underline the major differences between the above approaches and what we do. First, we do not wish to calculate the entire density matrices, as they simply contain too much information for our purposes, for which the first few lowest-order Green's functions are sufficient. Secondly, we do not want any more information than absolutely necessary about a special subsystem (i.e., the environment E) of our minimal closed system ($S + E$). We have used a special projection operator to enable us to transparently see the easiest way into disregarding the unimportant parts of the total $S + E$ density matrix, and we have generalized the correlation functions. The terms obtained are intentionally dubbed the closed-system-like term, the entanglement term and the memory terms, as these are common labels, and we certainly wanted them to be intuitively plausible. These terms may look like the terms obtained in various density-matrix formalisms, or in the works of Prigogine and Balescu [16] etc., but how they are calculated is different. They do *not* harbor expansion in terms of some unpleasant non-diagonal two-body interaction; they offer an expansion of relevant quantities of the system S in

⁷ The approximation (6) is insufficient if a description of fluctuations is desired. The interplay of the system and environment dynamics must be taken into account more exactly to treat fluctuations.

terms of the interaction with the irrelevant environment E , so that minimal information on the state of the environment is needed.

To summarize, in this paper we have defined the two-time correlation functions for open systems, which are a basis for the generalization of the non-equilibrium Green's functions formalism for such systems. In the transient regime, we have identified three types of terms in the two-time correlation functions: the closed-system-like term, the entanglement term and memory terms. The entanglement and memory terms may not be neglected in the transient regime, when the coupling between the system and the environment is strong and the information exchange is appreciable. On the other hand, in a far-from-equilibrium state, after the information exchange is finished, the system's evolution becomes closed-system-like, with an effective, modified Hamiltonian. Unfortunately, the far-from-equilibrium density matrix is an unknown, and generally is pretty difficult to obtain. A major difference between the transient regime and the far-from equilibrium steady state is the relative magnitude of the combined memory and entanglement terms with respect to the closed-system-like term: memory and entanglement are very important during transients, and virtually non-existent in a steady state. Further development of the generalized NEGF for open systems is underway.

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