

Evolution of the reduced density matrix: a generalized projection-operator approach

Irena Knezevic*, David K. Ferry

*Department of Electrical Engineering and Center for Solid State Electronics Research, Arizona State University,
Box 876206, Tempe, AZ 85287-6206, USA*

Abstract

A convolutionless equation of motion for the reduced density matrix of a system coupled to its environment, where the system + environment is closed, may be obtained using a projection-operator technique. We show that, when both the system and the environment Hilbert spaces are finite-dimensional, it is possible to eliminate the need for the partial trace over the environment states by constructing a simple and transparent basis-induced isomorphism between the system Liouville space and the unit-eigenspace of a special projection operator. Consequently, an equation of motion for the reduced density matrix is derived by a mere basis transformation within the system + environment Hilbert space and the explicit dependence of the reduced density matrix on the matrix elements of the Hamiltonian is uncovered, in a form well suited for numerical calculation. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Density matrix; Time-convolutionless equation; Memory effects; Quantum Liouville equation

1. Introduction

One approach to far-from-equilibrium systems relies upon the reduced density matrix formalism, which involves an equation of motion with a memory kernel [1]. In response to difficulties with the memory kernel, a memoryless (or time-convolutionless) equation of motion, based on the projection operator technique [1–3], has been proposed [4–6], and used successfully for a wide range of physical systems [7–10]. This approach relies upon the equations of motion for two mutually orthogonal projections of the system + environment density matrix. A partial trace over the environment states uncovers the evolution of the system reduced density matrix, in a form that bears a seemingly artificial dependence on the projection operators. In this paper, for finite-dimensional Hilbert spaces of both the system and its environment, we present a generalized projection-operator approach, which enables us

*Corresponding author. Fax: +1-480-965-8058.
E-mail address: irenak@asu.edu (I. Knezevic).

to obtain a partial-trace-free differential equation of motion for the reduced density matrix [11]. We discuss the integrability of the equation of motion, conditions for the steady-state solutions, decoherence, a possible failure of the approach, and how our approach behaves when describing the evolution of initially uncoupled system and environment.

2. Equation of motion for the reduced density matrix

Consider a system S (with Hilbert space \mathcal{H}_S of dimension d_S), which interacts with its environment E (space \mathcal{H}_E , dimension d_E), so that the system and the environment together (S+E) constitute an isolated physical system ($\mathcal{H} = \mathcal{H}_E \otimes \mathcal{H}_S$, $d = d_E d_S$). The total Hamiltonian h is written as $h(t) = h_S(t) + h_E(t) + h_{\text{int}}(t)$, where h_S , h_E and h_{int} are the system, environment, and interaction Hamiltonians, respectively. Driving fields, provided by applied potentials, are included as part of the system. Since S+E is isolated, the total density matrix ρ evolves according to the quantum Liouville equation

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

with L being the Liouville superoperator corresponding to the Hamiltonian h . The reduced system density matrix ρ_S is defined by $\rho_S = \text{Tr}_E(\rho)$. If we choose an arbitrary environment density matrix ρ_D , which acts on \mathcal{H}_E and is constant in time, we can introduce time-independent projection operators P_D and Q_D , associated with ρ_D , and acting on \mathcal{H}^2 (the space of all operators on \mathcal{H}), such that $P_D x = \rho_D \otimes \text{Tr}_E x$, $Q_D = 1 - P_D$, for $x \in \mathcal{H}^2$. In particular, since $\text{Tr}_E(\rho_D) = 1$ (ρ_D is a density matrix), it follows that $\text{Tr}_E(P_D \rho) = \rho_S$. The equation of motion for $P_D \rho$ can be written as [5–11]

$$\frac{dP_D \rho(t)}{dt} = -iP_D L(t)K(t)^{-1}P_D \rho(t) - iP_D L(t)K(t)^{-1}H(t,0)Q_D \rho(0) \quad (2)$$

where

$$H(t, t') = T^c \exp \left(-i \int_{t'}^t d\tau Q_D L(\tau) Q_D \right), \quad G(t', t) = T^a \exp \left(i \int_{t'}^t d\tau L(\tau) \right)$$

$$K(t) = 1 + i \int_0^t d\tau H(t, \tau) Q_D L(\tau) P_D G(\tau, t)$$

and T^c and T^a denote the time-ordering and the anti-time-ordering operators, respectively. Eq. (2) exists if $K(t)$ is invertible. Usually, by taking a partial trace over the environment states in (2), an equation of motion for ρ_S is obtained. It, however, bears a dependence on ρ_D , which is an artifact and makes the equation nontransparent. Here, we will use the density matrix $\bar{\rho}_D \equiv d_E^{-1} \cdot 1_{d_E \times d_E}$, which is inherent to any finite-dimensional space. In a particularly chosen orthonormal eigenbasis of \bar{P}_D [11], with the bold characters denoting the representation matrices in this eigenbasis, we obtain

$$\rho = \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix}, \quad \bar{P}_D = \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \quad \bar{Q}_D = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{bmatrix}, \quad \rho_S = \sqrt{d_E} \cdot \rho_1 \quad (3)$$

The last equality is a consequence of an especially transparent isomorphism between the unit-

eigenspace of \bar{P}_D and \mathcal{H}_S^2 (the space of all operators on \mathcal{H}_S); ρ_S is the column that represents ρ_S in a basis of \mathcal{H}_S^2 that induces that isomorphism [11]. The block forms of other operators from (2) are readily written as

$$\begin{aligned} L(t) &= \begin{bmatrix} L_{11}(t) & L_{12}(t) \\ L_{21}(t) & L_{22}(t) \end{bmatrix}, \quad G(t', t) = \begin{bmatrix} G_{11}(t', t) & G_{12}(t', t) \\ G_{21}(t', t) & G_{22}(t', t) \end{bmatrix}, \quad H(t, t') = \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & H_{22}(t, t') \end{bmatrix}, \\ K(t) &= \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ K_{21}(t) & K_{22}(t) \end{bmatrix} \end{aligned}$$

so a differential equation of motion for the representation column of the reduced density matrix is obtained as

$$\frac{d\rho_S(t)}{dt} = -i[L_{11}(t) - L_{12}(t)K_{22}^{-1}(t)K_{22}(t)K_{21}(t)]\rho_S(t) + i\sqrt{d_E}L_{12}(t)K_{22}^{-1}(t)H_{22}(t, 0)\rho_2(0) \quad (4)$$

This equation is well-suited for numerical implementation, as one usually starts with a set of the Hamiltonian matrix elements in a tensor-product basis. Additionally, this equation shows that, by merely performing a basis transformation, one can track the evolution of ρ_S in a ‘window’ of \mathcal{H}^2 , rather than in \mathcal{H}_S^2 . An important consequence of this equation is the steady-state condition, which occurs when the following are fulfilled:

$$L_{11}(t) - L_{12}(t)K_{22}^{-1}(t)K_{21}(t) = 0, \quad L_{12}(t)K_{22}^{-1}(t)H_{22}(t, 0)\rho_2(0) = 0 \quad (5)$$

The first equation clearly shows a balance between drive (L_{11}) and system-to-environment loss [$L_{12}(t)K_{22}^{-1}(t)K_{21}(t)$]. This condition is independent of the initial conditions, as expected in far-from-equilibrium situations. The second condition is less understood, it has been suggested to correspond to a ‘random-force’ [12]. If this is the case, then the time-average must vanish, which raises questions about $\rho_2(0)$.

Eq. (4) is integrable, as already mentioned, if K is invertible, which implies $\det K_{22}(t) \neq 0$. If the last condition is fulfilled, it can be shown that the integral equation of motion is given by

$$\rho_S(t) = U(t, 0) \left\{ \rho_S(0) + \int_0^t d\tau [U(\tau, 0)]^{-1} Y(\tau, 0) \right\} \quad (6)$$

where we have defined

$$\begin{aligned} Z(t) &= L_{11}(t) - L_{12}(t)K_{22}^{-1}(t)K_{21}(t), \quad Y(t, 0) = i\sqrt{d_E}L_{12}(t)K_{22}^{-1}(t)H_{22}(t, 0)\rho_2(0), \\ U(t, 0) &= T^c \exp \left[-i \int_0^t d\tau Z(\tau) \right] \end{aligned}$$

Since Z is not necessarily Hermitian, U is consequently not unitary, meaning that the system experiences decoherence, even though its evolution may be reversible [13]. If there are points in time when $\det K_{22}(t) = 0$, solving (4) after those times requires resetting the initial condition. This is virtually impossible in far-from-equilibrium situations: the old and the new initial condition have practically no connection with one another, and deducing the new one requires solving (1) in full, which is often beyond our capabilities for various reasons. On the other hand, such an interpretation is consistent with the second term of (5) being a random-force.

If at $t = 0$ the system and the environment are uncoupled, a standard practice is to choose the initial environment density matrix as the generating matrix for the projection operators. In this way, there is no free term in the differential equation of motion, and the equation ends up being of the form $\rho_S(t) = \mathcal{E}(t, 0)\rho_S(0)$. The same form can actually be obtained from (6), as in the case of initial decoupling the second term in the curly brackets can be written in terms of the first one [11].

3. Conclusions

Using a generalized projection-operator approach, a time-convolutionless, partial-trace free differential equation of motion for the reduced density matrix is derived. The equation holds promise for numerical implementation, as it explicitly involves the Hamiltonian matrix elements. Resulting conditions for a steady-state solution are independent of the initial state and reflect a gain–loss balance, which agrees with intuition for far-from-equilibrium systems. We assert there must be isolated points in time at which the approach fails; these times depend on the projection operator used. In far-from-equilibrium conditions, it is virtually impossible to reset the initial condition and track the evolution further.

Acknowledgements

The authors are grateful to K.M. Indlekofer, J.R. Barker, D. Ahn and D. Vasileska for valuable discussions. The financial support from the Office of Naval Research is gratefully acknowledged.

References

- [1] R. Zwanzig, *J. Chem. Phys.* 33 (1960) 1338.
- [2] S. Nakajima, *Prog. Theor. Phys.* 20 (1958) 948.
- [3] H. Mori, *Prog. Theor. Phys.* 33 (1965) 423.
- [4] M. Tokuyama, H. Mori, *Prog. Theor. Phys.* 55 (1975) 411.
- [5] N. Hashitsume, F. Shibata, M. Shingu, *J. Stat. Phys.* 17 (1977) 155.
- [6] F. Shibata, Y. Takahashi, N. Hashitsume, *J. Stat. Phys.* 17 (1977) 171.
- [7] M. Saeki, *Prog. Theor. Phys.* 79 (1988) 396;
M. Saeki, *Prog. Theor. Phys.* 89 (1993) 607.
- [8] D. Ahn, *Phys. Rev. B* 50 (1994) 8310.
- [9] D. Ahn, J.H. Oh, K. Kimm, S.W. Hwang, *Phys. Rev. A* 61 (2000) 052310.
- [10] D. Ahn, J. Lee, S.W. Hwang, LANL e-print, quant-ph/0105065.
- [11] I. Knezevic, D.K. Ferry, submitted for publication.
- [12] N. Pottier, *Physica A* 117 (1983) 243.
- [13] G.W. Ford, R.F. O'Connell, *Phys. Lett. A* 286 (2001) 87.