Projection operators in the theory of open quantum systems

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Abstract. We study different forms of projection operators and their application to open quantum systems. In particular, we show that applying a special class of projection operators to open systems may lead to non-linear dynamical equations, while other projection operators always lead to linear equations. We discuss general features of linear and non-linear dynamical equations. The main properties of different projectors are illustrated by examples of a qubit in a thermal bath and two interacting qubits in a common environment.

1. Introduction

The theory of open quantum systems deals with systems interacting with their environment. This interaction leads to continuous interchange of energy and entropy between a system and its environment and, eventually, to relaxation and decoherence in the system. The general strategy to study open systems is based on an assumption that an open system and its environment together form a closed system. Then, the evolution of the large closed system is investigated with the help of traditional methods of quantum mechanics. Finally, tracing out the degrees of freedom of the environment gives the sought-for time evolution of the open system. Mathematically the evolution of an open quantum system is governed by the following expression

$$\rho_S(t) = \mathrm{Tr}_E \left\{ U(t,t_0)\rho_{SE}(t_0)U^\dagger(t,t_0) \right\}, \tag{1}$$

where ρ_S is the density operator of the open system, $\rho_S E$ is the density operator of the open system and the environment, $U(t,t_0)$ is the evolution operator of the large closed system, and Tr_E is a partial trace over degrees of freedom of the environment.

The Eq. (1) provides comprehensive information about the evolution of an open system. However, the Eq. (1) is hardly satisfactory for the following reasons. First, the environment usually contains infinitely many degrees of freedom and, thus, one has to solve an infinite system of differential equations to find the evolution operator. This is impossible in the most cases. Second, one is often interested only a defined set of observables, characterising an open system, and Eq. (1) brings excessive details of the evolution.

In this paper we study open quantum systems with the help of projection operators and show that the projection operator technique allows to overcome some of the limitations of Eq. (1) mentioned above. The paper is organised as follow. In Sec. 2 we provide necessary information about the projection operator technique. In Sec. 3 we discuss some ideas leading to concrete

forms of projection operators. In Sec. 4 and 5 we apply different projection operators to two models of a qubit in thermal bath and two interacting qubits in a common environment. Finally, in Sec. 6 we conclude.

2. Projection operators and dynamical equation

The main idea behind the use projection operators is to divide a mathematical object, such as the density operator, into several parts and to study each part separately. Usually, in the theory of open quantum systems, the density operator contains some relevant information about the open system itself and irrelevant information about the environment. Of course, one wants to study only the relevant information about the system and ignore irrelevant one. Let $\mathcal{P}$ be a projection operator, $\mathcal{P}^2 = \mathcal{P}$, extracting the relevant part of the density operator,

$$\rho_{\rm rel}(t) = \mathcal{P}\rho(t), \tag{2}$$

where $\rho_{\rm rel}(t)$ is the relevant part of the full density operator $\rho(t)$. Let us assume that the following relation holds

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \mathcal{P}\frac{\partial}{\partial t}\rho(t) = \frac{\partial}{\partial t}\rho_{\rm rel}(t). \tag{3}$$

Under the assumption (3) one can build a fruitful theory and successfully describe the relevant part (2) of the density operator. Indeed, acting the projection operator onto both sides of the Liouville equation $\frac{\partial}{\partial t}\rho(t) = -i[H(t), \rho(t)] = \mathcal{L}(t)\rho(t)$, where $H(t)$ is the system Hamiltonian and $\mathcal{L}(t)$ is the Liouville superoperator, one can proceed in the standard way [1] and derive two different types of master equations, namely, the time-convoluted Nakajima-Zwanzig master equation [2, 3] and the so-called time-convolutionless (TCL) master equation [1].

The celebrated Nakajima-Zwanzig master equation has the following general structure

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \mathcal{P}\mathcal{L}(t)\mathcal{P}\rho(t) + \mathcal{P}\mathcal{L}(t)\mathcal{G}(t,t_0)\mathcal{Q}\rho(t_0) + \mathcal{P}\mathcal{L}(t)\int_{t_0}^{t}\mathcal{G}(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\rho(t)ds, \tag{4}$$

where $\mathcal{G}(t,s) = \exp_{-}\left[\int_s^t \mathcal{Q}\mathcal{L}(s')ds'\right]$, $\mathcal{Q} = 1 - \mathcal{P}$, and $\exp_{\pm}$ is chronological (antichronological) exponent, while the TCL master equation reads

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t) + \mathcal{I}(t)\mathcal{Q}\rho(t_0), \tag{5}$$

where $\mathcal{K}(t) = \mathcal{P}\mathcal{L}(t)[1 - \Sigma(t)]^{-1}\mathcal{P}$, $\mathcal{I}(t) = \mathcal{P}\mathcal{L}(t)[1 - \Sigma(t)]^{-1}\mathcal{G}(t,t_0)\mathcal{Q}$, $\Sigma(t) = \int_{t_0}^{t}\mathcal{G}(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}G(t,s)ds$, and $G(t,s) = \exp_{+}\left[-\int_s^t \mathcal{L}(s')ds'\right]$ is the inverse propagator.

Eqs. (4)-(5) encode most types of master equations. Moreover, with an appropriate choice of a projection operator these equations give a powerful tool to study only a relevant part of the density operator. Both above master equations are equivalent. In this paper we deal with the TCL master equation (5).

3. Explicit form of projection operators

There exist several type of the projection operators, which can be divided into two classes, namely, algebraic and functional projection operators. Action of the both type of projection operators extracts only the relevant part of the density operator characterising the system, but the mathematical structure of the relevant density operator (2) is different.

3.1. Functional projection operators

Let us choose a set of relevant dynamical variables or elements of the density operator P_m, characterising the system. This set carries all necessary information about a quantum system. We also assume that the relevant density operator (2) has some specific functional form

$$\rho_{\rm rel}(t) = \mathcal{F}(P_m, t). \tag{6}$$

To avoid contradictions we demand that the following self-consistency condition holds

$$\langle P_m \rangle^t = \langle P_m \rangle^t_{\rm rel} \equiv {\rm Tr}(P_m \rho_{\rm rel}(t)), \tag{7}$$

where the superscript means time-dependence. In other words, we want that the real averages, following from the quantum Heisenberg or Liouville equations, coincide with the averaging with respect to the relevant density operator. Generally, the self-consistency conditions are a system of n algebraic equations, where n is the number of relevant variables, and formally, the real averages $\langle P_m \rangle^t$ are known.

As example, we can form a Gibbs-like relevant density operator in the form

$$\rho_{\rm rel} = \exp[-\sum_m F_m(t) P_m]/{\rm Tr}\exp[-\sum_m F_m(t) P_m], \tag{8}$$

and the parameters $F_m(t)$ are fixed with the help of the self-consistency conditions (7). In this case the parameters F_m have transparent physical meaning as non-equilibrium thermodynamical parameters and the self-consistency conditions (7) connect dynamical and thermodynamical variables.

The Kawasaki-Gunton projection operator which replaces any density operator by the relevant one (6) has the following form

$$\mathcal{P}(t)A = \rho_{\rm rel}(t){\rm Tr}A + \sum_m \Big\{ {\rm Tr}(AP_m) - ({\rm Tr}A)\langle P_m \rangle^t \Big\} \frac{\partial \rho_{\rm rel}(t)}{\partial \langle P_m \rangle^t}. \tag{9}$$

The main properties of the Kawasaki-Gunton projection operator (9) can be found in [4, 5]. Here we notice that the Kawasaki-Gunton projection operator can be used to take into consideration ideas of non-equilibrium thermodynamics. In particular, using the principle of maximal entropy one can choose different types of entropy and build other types of relevant operators distinguished from (8). In such cases, the self-consistency conditions determine another type of generalised thermodynamics.

Notice that Eqs. (4) and (5) with the Kawasaki-Gunton projection operator (9) represent a non-linear system of equations in general. Nevertheless, due to direct connection of dynamics and thermodynamics of quantum systems the method based on the functional projection operator allows to study quantum systems more carefully and to determine more information about the system without additional non-trivial calculation in terms of only relevant variables. This fact may be very useful for some applications.

3.2. Algebraic projection operators

Algebraic projection operators iare used to extract the relevant degree of freedom without any additional assumption about a system. The general form of the algebraic projection operator is

$$\mathcal{P}A = \sum_{ij} {\rm Tr}(E_{ij} A) E^\dagger_{ij} / {\rm Tr} E_{ij} E^\dagger_{ij}, \tag{10}$$

where ${\rm Tr} E_{ij} E^\dagger_{kl} \sim \delta_{ik}\delta_{jl}$ is any set of orthogonal operators.

Particular cases of the projection operator (10) are widely used in different applications, especially in the theory of open quantum system. The most commonly used projection operator [1] has the form

$$\mathcal{P}A = (\mathrm{Tr}_E A) \otimes \rho_E(0), \tag{11}$$

where the partial trace is taken over the environmental degrees of freedom and the $\rho_E(0)$ is some fixed state of the environment. Clearly, that the projection operator (11) is a special case of the general form (10).

Below we show two examples how to use the projection operator formalism.

4. Two-level system in external field

We study this model with the help of the functional projection operator. The Hamiltonian of the system is $H = \omega_0\sigma_z + (\Omega(t)\sigma_+ + \Omega^*(t)\sigma_-) + \sum_j \omega_j b_j^\dagger b_j + \sum_j g_j(\sigma_- b_j^\dagger + \sigma_+ b_j)$, where $\Omega(t) = \frac{\Omega}{2}e^{-i\omega_L t}$ is monochromatic classical field with frequency ω_L and Rabi frequency Ω, $\sigma_\pm = (\sigma_x \pm i\sigma_y)$, and the σ_i are spin matrices. In this case the open system has a finite number of degrees of freedom. As relevant variables we can choose the components of the Bloch vector $\sigma_-, \sigma_+, \sigma_z$. The relevant distribution has the form

$$\rho_{\mathrm{rel}} = \frac{1}{Z_1 Z_2}\exp[-F_1(t)\sigma_+ - F_2(t)\sigma_z - F_3(t)\sigma_-]\exp[-\beta\sum_j \omega_j b_j^\dagger b_j], \tag{12}$$

where $Z_1 = \mathrm{Tr}\exp[-F_1(t)\sigma_+ - F_2(t)\sigma_z - F_3(t)\sigma_-] = 2\cosh(\frac{1}{2}\sqrt{4F_1(t)F_3(t) + F_2(t)^2})$ and $Z_2 = \mathrm{Tr}\exp[-\sum_j \omega_j b_j^\dagger b_j]$. The solution of the self-consistency conditions (7) is [5]

$$F_1(t) = -\langle\sigma_-\rangle^t R(t),\ F_2(t) = -2\langle\sigma_z\rangle^t R(t),\ F_3(t) = F_1^*(t), \tag{13}$$

where we introduced the functions $R(t) = \mathrm{arctanh}(2X)/X$, and $X = \sqrt{|\langle\sigma_-\rangle^t|^2 + (\langle\sigma_z\rangle^t)^2}$. Thus, the non-equilibrium entropy $S = \mathrm{Tr}\rho\log\rho$ of the system has the form

$$S(t) = -2X^2 R(t) + \ln 2 - 1/2\ln(1 - 4X^2) + S_{\mathrm{eq}}, \tag{14}$$

where S_{eq} is the equilibrium entropy of the bath.

The dynamics of the two-level system is governed by the master equation (5). For the considering model the equations up to the second order in the coupling constant are written as [5]

$$\frac{\partial\langle\sigma_z\rangle^t}{\partial t} = i(\Omega\langle\sigma_-\rangle^t - \Omega\langle\sigma_+\rangle^t) - \langle\sigma_z\rangle^t\left(f(t,\beta) + f^*(t,\beta)\right) - \frac{1}{2}\left(f(t) + f^*(t)\right), \tag{15}$$

$$\frac{\partial\langle\sigma_+\rangle^t}{\partial t} = -2i\Omega\langle\sigma_z\rangle^t - f(t,\beta)\langle\sigma_+\rangle^t. \tag{16}$$

In the above equations we introduced the following correlation functions

$$f(t,\beta) = \int_0^t dt' \int_0^\infty d\omega J(\omega)\coth\left(\frac{\beta\omega}{2}\right)e^{i(\omega-\omega_0)t},$$

$$f(t) = f(t,\infty) = \int_0^t dt' \int_0^\infty d\omega J(\omega)e^{i(\omega-\omega_0)t},$$

The dynamical equations (15)-(16) are identical to the usual result derived with the help of the TCL master equation [1] with traditional projection operator (11). For this model the two approaches give the same results. Nevertheless, due to the self-consistency conditions we have additional information about the thermodynamics of the open quantum system.

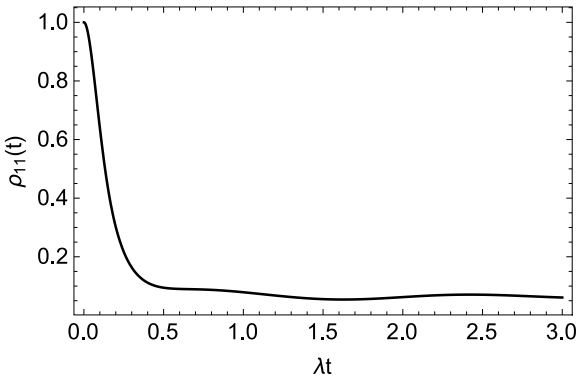

Figure 1. The evolution of the collective excited state $\rho_{11}(t)$ of two interacting qubits in the common thermal bath. Parameters in the system are $V = 0.6\lambda$, $\Omega = 10\lambda$, $\omega = 2\lambda$, $\beta = 0.3$, $\alpha_1 = 0.4 + 0.3i$, $\alpha_2 = 0.5 + 0.2i$

5. Two dipole-dipole interacting qubits

In this section we consider more complicated example. The Hamiltonian for the system is written as

$$H = H_0 + H_{12} + H_B + H_{int}, \tag{17}$$

where $H_0 = \nu \sum_i \sigma_z^i$ is the free qubits Hamiltonian, $H_B = \sum_j \omega_j b_j^\dagger b_j$ is the free Hamiltonian of the bath, $H_{12} = V(\sigma_+^1\sigma_-^2 + \sigma_+^2\sigma_-^1)$ is the Hamiltonian of the qubit interactions and $H_{int} = \sum_i \sum_j g_j b_j \sigma_+^i \alpha_i + \text{h.c.}$ is the qubits-bath interaction Hamiltonian, σ^i is the Pauli matrices for the ith qubit, b_i is the annihilation operator of the jth oscillator in the bath, ν and ω_j are the transition frequency of the qubits and the jth oscillator in the bath, correspondingly, V is the constant of dipole-dipole interaction, g_j is the coupling constant of the qubit and jth oscillator in the bath, α_i are the geometrical factors mark the position of the ith qubit.

First of all transform the Hamiltonian (17) to the interaction picture

$$H_I(t) = e^{i(H_0+H_{12}+H_B)t} H_{int} e^{-i(H_0+H_{12}+H_B)t} = (P_+^1 R(\alpha_2, -\alpha_1) + P_-^1 R(\alpha_2, \alpha_1))\sigma_+^2 B(t) e^{i\nu t} \tag{18}$$
$$+(P_+^2 R(\alpha_1, -\alpha_2) + P_-^2 R(\alpha_1, \alpha_2))\sigma_+^1 B(t) e^{i\nu t} + \text{h.c.} = K(t)e^{i\nu t}B(t) + K^\dagger(t)e^{-i\nu t}B^\dagger(t),$$

where $P_i^+ = \sigma_+^i\sigma_-^i$, $P_i^- = \sigma_-^i\sigma_+^i$ and $R(\alpha, \beta) = \alpha\cos(tV) + i\beta\sin(tV)$, $K(t) = (P_+^1 R(\alpha_2, -\alpha_1) + P_-^1 R(\alpha_2, \alpha_1))\,\sigma_+^2 + (1 \leftrightarrow 2)$, $B(t) = \sum_j g_j b_j$.

The master equation (5) up to the second order with the projection operator (11) for the factorised initial conditions can be written as

$$\dot\rho_S(t) = \int_0^t dt_1 \Big\{ [K^\dagger(t_1)\rho_S(t)K(t) - K(t)K^\dagger(t_1)\rho_S(t)]F$$
$$+ [K(t_1)\rho_S(t)K^\dagger(t) - K^\dagger(t)K(t_1)\rho_S(t)]R + \text{h.c}\Big\}, \tag{19}$$

where $F = \int_0^\infty d\omega J(\omega)(\coth(\beta\omega/2) + 1)/2e^{i(\nu-\omega)(t-t_1)}$ and $R = \int_0^\infty d\omega J(\omega)(\coth(\beta\omega/2) - 1)/2e^{-i(\nu-\omega)(t-t_1)}$.

The dynamics of the collective exited state for the spectral density of the bath $J(\omega) = \lambda\omega\exp[-\omega/\Omega]$ following from the TCL master equations is shown in Fig.1. One can see that the exited state relaxes to the equilibrium quite fast and after that the curve oscillates with small amplitude around the equilibrium. These oscillations may be considered as a signature of the non-Markovian evolution.

6. Conclusion

In this paper we studied different types of projection operators in the context of the theory of open quantum systems. We shown We have shown that general structure of a dynamical equation does not depend on concrete form of a projection operator. There exist two possible forms of the projection operators, which we called algebraic and functional. The functional projection operators lead in general to non-linear dynamical equation and enlighten thermodynamical properties of the system. The algebraic projection operators always lead to linear dynamical equations. We illustrated by two examples use of different types of the projection operators and indicated features given by the corresponding techniques.

References

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