Non-Markovian Open Quantum Systems: Lorentzian from Markovian

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Abstract

As a general mission, reduced dynamics and master equations are advocated as alternative method and philosophy instead of Green functions, Kubo theory and the like. A smart reduction of the Lorentzian open system to the Ohmic Markovian one (Imamoğlu, 1994) is presented in simple terms.

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1 Introduction: open=reduced

Numerous physical phenomena can be modeled as open dynamical systems. Typically, the very system S under investigation is interacting with a reservoir R and this makes S dynamically open. Its dynamics changes, becomes in general irreversible, dissipative, and non-Markovian. The total composite system S+R can be treated as a closed dynamical system. Its state $\rho_{SR}$ evolves reversibly. In interaction picture, the unitary evolution of $\rho_{SR}$ is generated by the interaction Hamiltonian $\hat{H}_{SR}$:

$$\frac{d}{dt}\rho_{SR}(t) = -i [\hat{H}_{SR}(t), \rho_{SR}(t)].$$

From it, we can derive the so-called reduced state of the system S:

$$\rho_S(t) = \text{tr}_R \rho_{SR}(t),$$

and its reduced dynamics as well. If the reservoir’s self-dynamics and its coupling to the system are of simple structure then the reduced dynamics will be well
calculable. Suppose the system and the reservoir are initially at time $t = 0$ uncorrelated, so the system’s reduced dynamics can be described by a homogeneous non-Markovian master equation [1]:

$$\frac{d}{dt} \rho_S(t) = \int_0^t dt' K(t - t') \rho_S(t'),$$

(3)

which is in principle solvable if we know the initial state $\rho_S(0)$ of the system. However, the closed analytic form of the memory kernel $K(t - t')$ can be found in special cases only. If the self-dynamics of the system is slow compared to the characteristic time of the said memory kernel then the so-called Markovian approximation turns the master equation into the much simpler form:

$$\frac{d}{dt} \rho_S(t) = \mathcal{L} \rho_S(t).$$

(4)

That is a remarkable limit case. It was applied for classical Brownian motion, as well as to quantum physics, for spontaneous atomic emission, nuclear spin-relaxation, transport phenomena, the whole of quantum optics, from quantum electronics to molecules, actually for any quantum system subject to thermal dissipation (or to decoherence, in novel approach) [2].

2 Do we need master equations?

The number and literature of phenomena that we can model by the system-reservoir paradigm is unconceivable. A tendency is, however, seen clearly. Most applications avoid the explicit use of the reduced dynamics and of the master equations (3,4). Rather they concentrate directly on the phenomenon to be described. Typical examples are Kubo’s theory of response functions, the input-output formalism in quantum optics, numerous applications of scattering theory and Green function techniques. These are presumably the optimum methods for the concrete phenomena. Yet, the common divisor of all techniques must be the reduced dynamics, i.e., the master equation that evolves the state $\rho_S(t)$ of the open system. If we point out this explicitly we can deepen our understanding the above techniques and we can remember the common divisor. We help transitions between different applications. We help discovery.

Consider, e.g., the problem of electric conductance in metals. The Markovian master equation (4) of the classical phase space distribution of the electron is the classical Boltzmann-Fokker-Planck equation. If we know its solution in external electric field we can derive Ohm’s Law and the conductance. On the other hand, the widely used modern treatment is based on the Kubo equation. This establishes
a relationship between the external field and the induced current, and it derives conductance directly from the equilibrium correlation function of the current. It circumvents the explicit determination of the reduced dynamics and it only concentrates on the phenomenon of electric conductance in question. Not too often, however, we see the conscious parallel mention of the Boltzmann and Kubo equations [3].

The Markovian approximation of the reduced dynamics and its master equation (4) are well known concerning the mathematical structure [4], the corresponding physics [2], as well as concerning the methods of solutions. The clearest conceptual basis of the Markovian approximation must be the master equation even if in practice some other serviceable techniques are applied. When, however, the Markovian approximation is not justified then we cannot make such a categoric declaration about the credit of master equations. The structure of non-Markovian master equations (3) has not been exhaustively studied. Most non-Markovian master equations are difficult and practically unsolvable. Thus we cannot say that the explicit use of reduced dynamics would always be more advantageous compared to the current techniques of non-Markovian phenomena. In this difficult topic, the goal of this talk will be limited to flash a genuine smart method for the master equation treatment of some special non-Markovian reduced dynamics.

3 Non-Markovian

Let the reservoir R consist of harmonic modes with spectral density \( D(\omega) \), with emission and absorption operators \( b_\omega, b_\omega^\dagger \), respectively. Let R couple linearly to a certain quantity \( V \) of the system S:

\[
H_{SR} = \int g_\omega \left( V^\dagger b_\omega + V b_\omega^\dagger \right) D(\omega) \frac{d\omega}{2\pi}.
\]

Assume the uncorrelated initial state:

\[
\rho_{SR}(0) = \rho_S(0)\rho_R(0),
\]

where the system’s initial state is arbitrary while the reservoir’s is the canonical Gibbs equilibrium state. For the sake of simplicity, we follow up the case of zero temperature. We are looking for the reduced dynamics, i.e., the exact master equation, to evolve \( \rho_S(t) \). Consider the field quantity \( F = \int g_\omega b_\omega D(\omega) d\omega/2\pi \) of the reservoir, that couples linearly to the system’s quantity \( V \). In interaction picture this field reads

\[
F(t) = \int g_\omega b_\omega e^{-i\omega t} D(\omega) \frac{d\omega}{2\pi}.
\]
Its expectation value vanishes in the reservoir’s initial state. The following correlation function will, however, play a role:

$$\alpha(\tau - s) = \text{tr}_R \left( F(\tau) F^\dagger(s) \rho_R(0) \right).$$  

(8)

It is known that the reduced dynamics in interaction picture will depend but on this correlation function! We can add that this correlation function is the Fourier transform of $g_\omega^2 D(\omega)$, i.e., of the reservoir spectral density weighted by the coupling strengths.

In general, the above correlation function is complicated and the explicit form it determines the requested dynamics (3) requires approximate methods. An exception is when the system $S$ is simple, e.g., a two state system or being itself, too, a harmonic oscillator. In such cases the master equation (3) takes tractable analytic forms. The most relevant special case is the Markovian one, of course.

4 Markovian

Often the spectrum of the reservoir $R$ is broad, smooth and flat compared to the relevant transition frequencies of the system $S$. In other words: the reservoir correlation function (8) is characterized by a memory time and this is much shorter than the characteristic time scales of the system’s self-dynamics. That is the Markovian limit. In this case therefore the spectrum (weighted by coupling strengths) will be considered flat and the correlation function of the field will be considered delta-function:

$$g_\omega^2 D(\omega) = f^2 = \text{const}, \quad \alpha(\tau - s) = f^2 \delta(\tau - s).$$  

(9)

Note that the spectral energy density $\omega D(\omega)$ can alternatively be used, the form $g_\omega^2 D(\omega) = f^2 \omega$, linear in frequency, is called the Ohmic spectrum with a reference to the pioneering theory of electric conductance. It is known that in the Markovian limit (9) the master equation (4) becomes:

$$\frac{d}{dt} \rho_S = f^2 \left( V \rho_S V^\dagger - \frac{1}{2} V^\dagger V \rho_S - \frac{i}{2} \rho_S V^\dagger V \right).$$  

(10)

Many times, the solution of such a simple equation is analytically possible. If not, then a peculiar Monte-Carlo method applies [5], particularly suitable for solutions of Markovian master equations.

Let us consider an elementary Markovian example which we need later. Let the system $S$ itself be an $\omega_0$-frequency harmonic oscillator and let its emission operator $V = a$ couple to a Markovian (Ohmic) reservoir. If the coupling constant is $f$ then
we get the master equation of the damped oscillator which in interaction picture reads:

\[
\frac{d}{dt} \rho_A = f^2 \left( a \rho_S a^\dagger - \frac{i}{2} a^\dagger \rho_S - \frac{i}{2} \rho_S a^\dagger a \right).
\] (11)

The ground state \( \rho_A = |0; A\rangle\langle 0; A| \) is stationary. In it the expectation value of the emission and absorption operator vanish. We can determine the ground state correlation function of \( a(t) \) and \( a^\dagger(t) \) in interaction picture:

\[
\exp[-i\omega_0(\tau - s) - \frac{i}{2} f^2 |\tau - s|].
\] (12)

5 Reducing Non-Markovian to Markovian

Now, we tear ourselves away from the Markovian limit and consider a definitely non-Markovian case which keeps, nonetheless, an intrinsic relationship with the Markovian ones. Let the spectrum be Lorentzian:

\[
g_\omega^2 D(\omega) = g^2 \frac{\gamma}{(\omega - \omega_0)^2 + (\gamma/2)^2}.
\] (13)

The corresponding correlation function is exponentially damped:

\[
\alpha(\tau - s) = g^2 \exp[-i\omega_0(\tau - s) - \frac{i}{2} \gamma |\tau - s|].
\] (14)

It can be shown that the reduced dynamics of the system in the Lorentzian reservoir is exactly identical with the reduced dynamics of a fictitious system in a Markovian reservoir [6].

Let us first consider a fictitious reservoir consisting of a single \( \omega_0 \)-frequency oscillator (ancilla). Let us couple the system S to this ancilla instead of the Lorentzian reservoir:

\[
H_{S_A} = g \left( V^\dagger a + V a^\dagger \right).
\] (15)

This, too, is a system-reservoir interaction just the reservoir consists of a single oscillator. Otherwise we can do everything like for the case of S+R, just we use the notation S+A this time. The coupled field (7) is simply \( F = ga \). In interaction picture we calculate the correlation function (8) of the field, it is trivial:

\[
\langle 0; A|F(\tau)F^\dagger(s)|0; A\rangle = g^2 e^{-i\omega_0(\tau - s)}.
\] (16)

If his correlation function were identical with the Lorentzian damped correlation function (14) then, according to our previous consideration, also the reduced dynamics \( \text{tr}_A \rho_{SA}(t) \) would be identical with the reduced dynamics emerging from a Lorentzian reservoir. But the correlation function of the ancilla A is not Lorentzian.
Yet it can easily be made so! Indeed, we saw that if we place the ancilla-oscillator into an Ohmic Markovian reservoir (and choose $f^2 = \gamma$) then the ancilla’s correlation function will obtain exactly the desired exponential damping factor (12). It is thus clear that the influence of the Lorentzian reservoir can exactly be replaced by the influence of an ancilla-oscillator which itself is damped by a Markovian (Ohmic) reservoir.

Let us summarize the method. Consider the composite system $S + A$ with an uncorrelated initial state:

$$\rho_S(0)|0; A\rangle\langle 0; A|.$$  \hspace{1cm} (17)

Assume an interaction $H_{SA}$ (15). Let the ancilla-oscillator $A$ be damped by an Ohmic Markovian reservoir. Hence the composite state $\rho_{SA}(t)$ evolves according to the following Markovian master equation:

$$\frac{d}{dt}\rho_{SA} = -ig\left[V^\dagger a + V a^\dagger, \rho_{SA}\right] + \gamma \left(a\rho_{SA}a^\dagger - \frac{1}{2}a^\dagger a\rho_{SA} - \frac{1}{2}\rho_{SA}a^\dagger a\right),$$  \hspace{1cm} (18)

where $a$ and $V$ are time-dependent operators in interaction picture. If we have solved the above initial value problem then we trace over the ancilla-oscillator $A$ and this way we obtain the system’s current state:

$$\rho_S(t) = \text{tr}_A\rho_{SA}(t).$$  \hspace{1cm} (19)

Using this method, the non-Markovian influence of a Lorentzian reservoir has been reduced to the influence of a Markovian (Ohmic) reservoir - with the insertion of a single ancilla-oscillator.

The relevance of Lorentzian reservoir may perhaps not go much beyond the high-frequency (Drude-) regularization of the Ohmic Markovian one. On the other hand, the above method is not restricted to the Lorentzian reservoir, it has been suggested for the so-called fotonic band gap materials as well since, surprisingly, the method of ancilla-oscillator applies, with minor modification, to an upside-down Lorentzian spectrum as well, i.e., to a Lorentzian forbidden band in the Ohmic flat spectrum.

6 Closing remarks

It was my studying basic quantum structures and phenomena - like the nowadays popular decoherence or the even more fashionable quantum information - which lead me to open quantum systems and master equations. I admittedly miss my overview of the corresponding vast literature. Neither had I felt necessary to disperse the audience’s attention by flashing the investigations where I tried to
contribute myself. Rather I thought to pick up and present a unique smart non-Markovian method. Also the cited references are selective - yet suitable to direct the interested toward the relevant discussions of a few issues on non-Markovian open system dynamics.

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