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LETTER TO THE EDITOR

Self-consistent projection-operator method for describing the non-Markovian time-evolution of subsystems

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Abstract. It is pointed out that the usual projection-operator method yields non-positive-definite reduced density operators for subsystems. In order to obtain non-negative probabilities, a new self-consistent projection-operator method for treating non-Markovian behaviour is developed. Finally, the applicability of the method is shown by an example.

The idea of the projection-operator method (POM) is the derivation of a so-called master equation (ME) for a reduced density operator describing the dynamics of a subsystem A being the relevant part of the total system $A+R$ (consisting of two interacting systems A and R). System R usually refers to a large system (reservoir). The POM was developed by Nakajima [1] and Zwanzig [2-4] and was applied to different problems of non-equilibrium statistical mechanics (see, e.g., [5-9] and the references quoted therein).

By applying the POM [1-4, 8] to the Liouville (von Neumann) equation for the statistical density operator $\rho(t)$ in the interaction picture (this picture is used throughout the paper),

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -\mathrm{i}L_{AR}(t)\rho(t) \qquad L_{AR}(t) \equiv [H_{AR}(t), \ldots] \qquad \hbar = 1 \tag{1}$$

the following exact ME can be derived:

$$\frac{\mathrm{d}P\rho(t)}{\mathrm{d}t} = -\mathrm{i}PL_{AR}(t)P\rho(t) - \int_0^t \mathrm{d}t'\, PL_{AR}(t)U(t,t')(I-P)L_{AR}(t')P\rho(t') \tag{2}$$

where we used

$$U(t,t') = \tau \exp\left[-\mathrm{i}\int_{t'}^{t} \mathrm{d}t''\,(I-P)L_{AR}(t'')\right] \tag{3}$$

$$\mathrm{Tr}_{AR}[P(\ldots)] = \mathrm{Tr}_{AR}(\ldots) \tag{4}$$

and the special initial condition of statistically independent systems A and R

$$\rho(0) = P\rho(0) = \rho_A(0) \otimes \rho_R(0). \tag{5}$$

Further, we have introduced the following notation: $I = I_A \otimes I_R$ as the unit operator in the Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_R$ of the total system $A+R$, τ as the Dyson time-ordering operator, Tr_{AR} as the trace over $\mathcal{H}_A \otimes \mathcal{H}_R$, and $\rho_A(0)$ and $\rho_R(0)$ as the initial density operators of systems A and R.

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However, as can be seen from (1.2), the ME is a very complicated integro-differential equation which cannot be solved exactly. In order to obtain a solution, a perturbative series expansion in the strength of interaction between systems A and R in the ME should be carried out.

As long as no approximation is used, the ME (cf (1.2)) is an exact equation of motion for the relevant part of the density operator $P\rho(t)$ and therefore not only the norm

$$\mathrm{Tr}_{AR}[P\rho(t)] = \mathrm{Tr}_{AR}[\rho(t)] = 1 \tag{6}$$

is conserved, but the positive definiteness of the density operator $P\rho(t)$ is also conserved

$$\langle n|P\rho(t)|n\rangle \geqslant 0 \qquad \text{for any } |n\rangle \text{ in } \mathscr{H}. \tag{7}$$

In other words, the diagonal matrix elements of $P\rho(t)$ are probabilities and lie always between zero and unity.

The application of the Born approximation (BA) (which is referred to as second-order perturbative approximation in this letter) leads to the following non-Markovian equation:

$$\frac{\mathrm{d}P\rho^{\mathrm{BA}}(t)}{\mathrm{d}t} = -\mathrm{i}PL_{AR}(t)P\rho^{\mathrm{BA}}(t) - \int_0^t \mathrm{d}t'\, PL_{AR}(t)(I-P)L_{AR}(t')P\rho^{\mathrm{BA}}(t'). \tag{8}$$

One important fact which has been treated extensively in the literature in the case of Markovian ME (see, e.g., [10]), but unfortunately not sufficiently in the case of non-Markovian ME, is the positive definiteness (cf (7)) of the density operator $P\rho^{\mathrm{BA}}(t)$ (cf (8)). This latter is only fulfilled if the ME (8) can be led back to the Liouville equation, i.e. if the integral term vanishes. This, however, means a reduction to the Liouville equation of a subspace which makes the application of the POM superfluous. Moreover, it is obvious that the usually used projection operators (PO) [1-9] cannot fulfil the condition required for the positive-definiteness of the reduced density operator in (8).

Knowing these difficulties, the application of the POM to the Schrödinger equation, instead of the Liouville equation, seems to be a logical consequence. The restriction of the initial condition to the pure states may be removed by applying the POM to each of the initial states appearing in the statistical mixture, and afterwards weighting the results with the probabilities for the occurrence of the corresponding initial states.

In the Hilbert space of the total system $\mathscr{H}_A \otimes \mathscr{H}_R$, the Schrödinger equation in the interaction picture reads as

$$\frac{\mathrm{d}|\psi(t)\rangle}{\mathrm{d}t} = -\mathrm{i}H_{AR}(t)|\psi(t)\rangle \qquad \langle\psi(t)|\psi(t)\rangle = 1. \tag{9}$$

By introducing a time-independent PO P, it is possible to divide the state vector $|\psi(t)\rangle$ into a relevant part $P|\psi(t)\rangle$ and an irrelevant part $(I-P)|\psi(t)\rangle$. The application of the PO P to the Schrödinger equation (9) leads to two coupled equations:

$$\frac{\mathrm{d}P|\psi(t)\rangle}{\mathrm{d}t} = -\mathrm{i}PH_{AR}(t)(P|\psi(t)\rangle + (I-P)|\psi(t)\rangle) \tag{10}$$

$$\frac{\mathrm{d}(I-P)|\psi(t)\rangle}{\mathrm{d}t} = -\mathrm{i}(I-P)H_{AR}(t)P|\psi(t)\rangle - \mathrm{i}(I-P)H_{AR}(t)(I-P)|\psi(t)\rangle. \tag{11}$$

In order to integrate (11), we have to introduce an integrating operator $U(t, t')$ (a kind of time-development operator) satisfying the equation:

$$\frac{\partial U(t, t')}{\partial t'} = \mathrm{i}U(t, t')(I - P)H_{AR}(t') \tag{12}$$

$$U(t, t) = I. \tag{13}$$

The formal solution for $U(t, t')$ is given by

$$U(t, t') = \tau \exp\left(-\mathrm{i}\int_{t'}^{t} \mathrm{d}t''(I - P)H_{AR}(t'')\right). \tag{14}$$

By applying the integrating operator $U(t, t')$ to (11), we obtain a connecting equation between $|\psi(t)\rangle$ and $P|\psi(t)\rangle$:

$$(I - P)|\psi(t)\rangle = U(t, 0)(I - P)|\psi(0)\rangle - \mathrm{i}\int_0^t \mathrm{d}t'(U(t, t')(I - P)H_{AR}(t')P|\psi(t')\rangle. \tag{15}$$

In order to make the first term on the RHS of (15) vanish, we choose special PO satisfying the initial condition

$$P|\psi(0)\rangle = |\psi(0)\rangle = |\psi(0)\rangle_A \otimes |\psi(0)\rangle_R. \tag{16}$$

By inserting (15) and (16) into (10), we get a closed exact EM for the relevant part of the state vector $P|\psi(t)\rangle$:

$$\frac{\mathrm{d}P|\psi(t)\rangle}{\mathrm{d}t} = -\mathrm{i}PH_{AR}(t)P|\psi(t)\rangle - \int_0^t \mathrm{d}t'\, PH_{AR}(t)U(t, t')(I - P)H_{AR}(t')P|\psi(t')\rangle. \tag{17}$$

The use of the second-order approximation for the interaction Hamiltonian H_{AR} (in the present letter referred to as BA) in (17) means that all terms higher than second order are to be set to zero. That is to say, in order to be able to make a self-consistent BA in (17), the following relation should be fulfilled:

$$(I - P)H_{AR}(I - P) = 0 \tag{18}$$

(which can be obtained by inserting (14) into (17)). This relation reflects a self-consistent truncation condition of the series expansion in H_{AR} of (17), since it means that the action of the Hamiltonian H_{AR} is restricted to a subspace $\mathscr{H}^{S(N)}$ and is given by

$$H_{AR}^{S(N)}(t) = P_{N-1}H_{AR}(t)I^{S(N)} + I^{S(N)}H_{AR}(t)P_{N-1} - P_{N-1}H_{AR}(t)P_{N-1}$$
$$N = 1, 2, \ldots \tag{19}$$

where $I^{S(N)}$ is the unit operator of the subspace $\mathscr{H}^{S(N)}$. This subspace $\mathscr{H}^{S(N)}$ is created in the Nth order of our approximation scheme and is due to the N-fold action of the non-restricted interaction Hamiltonian H_{AR}. That is to say, $\mathscr{H}^{S(N)}$ is defined by the state vectors:

$$\{(H_{AR})^l|\psi(0)\rangle,\ l = 0, 1, \ldots, N;\ N \geqslant 1\}. \tag{20}$$

(All lower-order spaces $\mathscr{H}^{S(k)}$ are contained in the higher-order spaces $\mathscr{H}^{S(m)}$, $m > k$, as subspaces.) The PO P_{N-1} is the projector on the subspace $\mathscr{H}^{S(N-1)}$ and is defined by

$$P_{N-1} = I^{S(N-1)}. \tag{21}$$

It should be mentioned that the restriction of the Hamiltonian H_{AR} to a given subspace $\mathscr{H}^{S(N)}$ has the consequence that the whole time evolution as well as the norm conservation of the state vector is restricted to this subspace.

In our approximation procedure, different orders ($N = 1, 2, \ldots$) of the BA exist; each of them results in a restriction to a subspace of the same order N. The order of the BA is given by the choice of the PO, i.e. the order of the BA is always higher by one than that of the corresponding PO (cf (21)).

In the BA of the Nth order, (17) reduces to

$$\frac{\mathrm{d}P_{N-1}|\psi(t)\rangle^{\mathrm{BA}}}{\mathrm{d}t} = -\mathrm{i}P_{N-1}H_{AR}(t)P_{N-1} - \int_0^t \mathrm{d}P_{N-1}H_{AR}(t)[I^{S(N)} - P_{N-1}] \times H_{AR}(t-\tau)P_{N-1}|\psi(t-\tau)\rangle^{\mathrm{BA}} \qquad N = 1, 2, \ldots. \tag{22}$$

Since probability amplitudes in the subspace $\mathscr{H}^{S(N-1)}$ can be calculated from (22), it is obvious that the probabilities, which are the squares of the moduli of probability amplitudes, are always non-negative.

Finally, it should be stressed that within our POM the normalisation is automatically fulfilled, because the BA of the Nth order leads to a restriction to the subspace $\mathscr{H}^{S(N)}$. In other words, as it should be in a self-consistent method, our equation (22) is an exact equation for the restricted Hamiltonian $H_{AR}^{S(N)}(t)$ given by (19), and therefore the norm is always conserved in the corresponding subspace $\mathscr{H}^{S(N)}$.

In conclusion, to illustrate our new POM, we apply it to the case of spontaneous emission from a two-level hydrogen atom. In this case the interaction Hamiltonian, which neither implies the rotating-wave approximation nor ignores the retardation effects (dipole approximation), is [11]

$$H_{AR}(t) = \int_0^\infty \mathrm{d}\omega[g(\omega)a^-(\omega)\,\mathrm{e}^{-\mathrm{i}\omega t} - g^*(\omega)a^+(\omega)\,\mathrm{e}^{\mathrm{i}\omega t}] \otimes (S^+\,\mathrm{e}^{\mathrm{i}\omega_0 t} - S^-\,\mathrm{e}^{-\mathrm{i}\omega_0 t}). \tag{23}$$

Here $S^\pm$ are the atomic dipole-moment operators given by

$$S^+ = |1\rangle\langle 2| \qquad S^- = |2\rangle\langle 1|$$

where

$$|1\rangle \equiv |n_1 = 2, j_1 = 1, m_1 = 0\rangle \qquad \text{and} \qquad |2\rangle \equiv |n_2 = 1, j_2 = 0, m_2 = 0\rangle$$

are the excited state and the ground state of a hydrogenic atom in the case of the Lyman-α transition (2P$\rightarrow$1S) [11, 12]. The symbols $a^\pm(\omega)$ denote the creation and annihilation operators for a photon with frequency ω and quantum numbers $j = 1$, $m = m_1 - m_2 = 0$ (which follows from the selection rules) and $\tau = 0$ (electric multipole field). The coupling constant $g(\omega)$ includes all the retardation effects and is given by [12]

$$g(\omega) = \left(\frac{\lambda}{2\pi}\right)^{1/2} \frac{(-\mathrm{i})\omega^{1/2}}{[1 + (\omega/\Omega)^2]^2} \qquad \lambda = \frac{\gamma}{\omega_0} \qquad \Omega = \frac{3c}{2a_0} \tag{24}$$

where $\gamma \simeq 10^8\ \mathrm{s}^{-1}$ is the Einstein coefficient for spontaneous Lyman-α radiation, $\omega_0 \simeq 10^{16}\ \mathrm{s}^{-1}$ is the energy separation of the two atomic levels and $a_0 \simeq 10^{-9}$ cm is the Bohr radius.

In order to apply the POM we choose the PO of lowest order:

$$P_0 = I^{S(0)} = \sum_{j=1}^{2} |j\rangle\langle j| \otimes |V\rangle\langle V| \tag{25}$$

$$I^{S(1)} = \sum_{j=1}^{2} |j\rangle\langle j| \otimes \left(|V\rangle\langle V| + \int_0^\infty \mathrm{d}\omega\, |\omega\rangle\langle\omega|\right) \tag{26}$$

where $I^{S(0)}$ and $I^{S(1)}$ are the unit operators in the subspaces of the order $N=0$ and $N=1$, respectively, and $|V\rangle$ and $|\omega\rangle$ are the vacuum and one-photon states of the radiation field, respectively. Furthermore, we assume that the following initial condition holds:

$$\begin{aligned} P_0|\psi(0)\rangle &= |\psi(0)\rangle \\ &= \sum_{j=1}^{2} b_{j,0}(0)|j\rangle\otimes|V\rangle \\ \sum_{j=1}^{2} |b_{j,0}(0)|^2 &= 1 \end{aligned} \tag{27}$$

where $b_{j,0}(t)$ is the probability amplitude for finding the atom in state $|j\rangle$ and no photons in the radiation field. Then, by using the POM in the first-order BA, we obtain for the probability amplitudes

$$b_{j,0}(t) = \langle j|\otimes\langle V|P_0|\psi(t)\rangle$$

two decoupled integro-differential equations:

$$\frac{\mathrm{d}b_{j,0}(t)}{\mathrm{d}t} = -\frac{\lambda}{2\pi}\int_0^\infty \mathrm{d}\omega f(\omega)\int_0^t \mathrm{d}\tau \exp[-\mathrm{i}(\omega_0^{(j)}+\omega)\tau]b_{j,0}(t-\tau) \tag{28}$$

$$\omega_0^{(j)} \equiv (-1)^j\omega_0 \qquad j=1,2$$

and

$$f(\omega) = \frac{\omega\Omega^8}{(\Omega^2+\omega^2)^4}. \tag{29}$$

Equation (28) can be adequately treated by using the Laplace transform and its inverse. A very involved calculation (which was already presented in the case of $j=1$ in [11] and goes quite analogously for $j=2$), yields for the probability amplitude $b_{j,0}(t)$ a Markovian term $R_j(t)$ stemming from the pole u_j and a non-Markovian term $D_j(t)$ describing the deviation from Markovian behaviour [11]:

$$b_{j,0}(t) = R_j(t) + D_j(t) \qquad j=1,2 \tag{30}$$

with

$$R_j(t) = b_{j,0}(0)(1+\Delta_R)\exp(-\mathrm{i}\omega_0^{(j)}t)\exp(-\mathrm{i}u_jt) \tag{31}$$

$$u_j = -\omega_0^{(j)} - \frac{11\lambda\omega_0^{(j)}}{24\pi} - \frac{5\lambda\Omega}{64} + \frac{\lambda\omega_0^{(j)}}{2\pi}\ln\left(\frac{\Omega}{\omega_0}\right) - \mathrm{i}(2-j)\frac{\omega_0\lambda}{2} + \Delta_u \tag{32}$$

$$|\Delta_R| < 10\lambda \qquad \left|\frac{\Delta_u}{u_j}\right| < 4.1\times10^{-13} \tag{33}$$

and

$$D_j(t) = M_j(t) + \Delta_D(t) \qquad M_j(t) = -\frac{\lambda b_{j,0}(0)}{2\pi\omega_0^2t^2}\exp(-\mathrm{i}\omega_0^{(j)}t) \tag{34}$$

$$\left|\frac{\Delta_D(t)}{M_j(t)}\right| < 16.6\times10^{-2} \qquad t \geqslant 10^{-14}\,\mathrm{s} \tag{35}$$

where the error terms: $|\Delta_R|$, $|\Delta_u/u_j|$ and $|\Delta_D(t)/M_j(t)|$ are obtained by a very involved error estimation (for more details see [11]).

The expectation value

$$\langle S^z \rangle_t = |b_{1,0}(t)|^2 - |b_{2,0}(t)|^2 - |b_{1,0}(0)|^2 + \tfrac{1}{2} \tag{36}$$

of the atomic population inversion operator $S^z = \frac{1}{2}(|1\rangle\langle 1| - |2\rangle\langle 2|)$ can be easily obtained from (30), (31) and (34).

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