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Analysis of the projection-operator method: inconsistencies and their removal

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Abstract. In this paper, it is pointed out that the application of the projectionoperator method leads to the violation of a consistency condition if the so-called Born approximation is made in the non-Markovian master equation. Since only the validity of this consistency condition guarantees obtaining non-negative probabilities, its violation makes the applicability of the whole method in this approximation meaningless. Therefore, it is demonstrated that an additional Markov approximation restores the validity of the consistency condition in the master equation, and thus re-establishes the applicability of the projection-operator method. Furthermore, the possibility of obtaining a self-consistent projection-operator method is also examined.

1. Introduction

We begin with a few words about the idea of the projection-operator method (POM). In the case of open systems (usually systems interacting with a reservoir) perturbative methods based on weak interaction can be applied. As the most powerful and elegant method seems to be the so-called POM developed thirty years ago by Nakajima [1] and Zwanzig [2-4] for time-independent projection operators (POS) and generalized by Robertson [5, 6] and Zubarev [7-9] to time-dependent POS. For successful applications of the POM and its modifications to different problems of non-equilibrium statistical mechanics and quantum optics, we refer to [10-25].

The fundamental idea of the POM is the derivation of a so-called master equation (ME) for a reduced density operator describing the dynamics of the relevant part of some isolated system. This relevant part of the system usually concerns an open system being a subsystem of the total system. However, the ME describing the time evolution of the open system is a very complicated integro-differential equation which cannot be solved exactly. In order to obtain a solution of the ME, a perturbative series expansion as to the strength of interaction between the system of interest and reservoir should be carried out. Nevertheless, this expansion is superior to that of the elementary perturbation theory, since an infinite number of terms of all orders of the usual perturbation expansion have to be summed up in order to recover a given finite-order expansion in the ME. In practice, in the ME approach nobody goes beyond the second-order approximation in the interaction, which is usually the lowest order approximation and, therefore, it is generally referred to as the Born approximation (BA).

As long as no kind of approximation is used, the ME is an exact equation of motion (EM) for the reduced density operator $P\rho(t)$ preserving the norm, $\text{Tr}\left[P\rho(t)\right] = 1$, as well as the positive definiteness of the operator $P\rho(t)$. The problem arises if we make the BA. This leads, namely, to a non-Markovian equation. The fact that from this equation some authors [26, 27] obtained unphysical results (negative probabilities) shows us that the approximation procedure has violated some consistency condition.

It is not an easy task to point out inconsistencies arising from the application of the BA in the POM. Some mutual dependence between the BA and Markov approximation (MA) has been discussed by Grabert *et al* [28]. Furthermore, Davis [29] has shown that the weak-coupling approximation, when carried out consistently, leads to a Markovian semigroup propagator preserving the positivity of the density operator. In spite of these investigations the meaning of the BA and the consequences arising from its application are still obscure. Therefore, the main objective of the present paper is to clarify some of these consequences which were very often overlooked in the literature [26, 27].

In section 2, it will be shown that the POM as well as the Heisenberg EMs lead to identical non-Markovian EMs which, in the BA, violate a consistency condition. In section 3, a new PO leading to a self-consistent POM will be examined.

2. The Argyres-Kelley POM and the Heisenberg EMs

By applying the POM [1-4, 14, 21] to the Liouville (von Neumann) equation for the statistical density operator $\rho(t)$ in the interaction picture,

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -\mathrm{i}L_{AR}(t)\rho(t) \qquad \mathrm{Tr}_{AR}\rho(t) = 1$$

$$L_{AR}(t)(\cdots) := [H_{AR}(t),(\cdots)] \qquad \hbar = 1$$
(2.1)

the following exact ME can be derived:

$$\frac{\mathrm{d}P\rho(t)}{\mathrm{d}t} = -\int_0^t \mathrm{d}t' P L_{AR}(t) T(t,t') L_{AR}(t') P\rho(t')$$
(2.2)

where we used

$$T(t,t') = \mathcal{T} \exp\left[-\mathrm{i} \int_{t'}^{t} \mathrm{d}t'' (\mathbb{I} - P) L_{AR}(t'')\right]$$
(2.3)

$$P(\ldots) = \rho_R(0) \operatorname{Tr}_R(\ldots) \qquad PL_{AR}(t) P = 0 \tag{2.4}$$

$$\rho(0) = P\rho(0) = \rho_A(0) \otimes \rho_R(0)$$
(2.5)

with $\mathbf{I} = \mathbf{I}_A \otimes \mathbf{I}_R$ as the unit operator in the Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_R$ of the total system A + R, Tr_{AR} as the trace over $\mathcal{H}_A \otimes \mathcal{H}_R$, $\rho_A(0)$ and $\rho_R(0)$ as initial density operators of systems A and R, and \mathcal{T} being the Dyson time-ordering operator.

The application of the BA (second-order approximation) to the ME (equation (2.2)) leads to the following non-Markovian equation:

$$\frac{\mathrm{d}\rho_A(t)}{\mathrm{d}t} = -\int_0^t \mathrm{d}t' \operatorname{Tr}_R \left[L_{AR}(t) L_{AR}(t') \rho_R(0) \otimes \rho_A(t') \right].$$
(2.6)

To see whether any consistency condition (leading to non-negative probabilities) is violated in obtaining this ME is almost an unmanagable task.

To prove the positive definiteness of $\rho_A(t)$ we need to define diagonal operators in the Hilbert space \mathcal{H}_A :

$$A_{l} = |l\rangle_{AA} \langle l| \qquad \sum_{l} A_{l} = \mathbf{I}_{A}$$
(2.7)

and prove that the expectation values

$$\langle A_l \rangle_t = \text{Tr}_A[A_l \rho_A(t)] \tag{2.8}$$

which determine the probabilities for finding the open system A in any of the states $|l\rangle_A$, are non-negative.

In order to do this we will change the picture, and derive EMs for A_i in the HP. In our case, for any operator O in the HP it holds that

$$O^{H}(t,t') = U^{+}_{H}(t,0)O(t')U_{H}(t,0) \qquad O^{H}(t) = O^{H}(t,0) = U^{+}_{H}(t,0)O(0)U_{H}(t,0)$$
(2.9)

where the time-development operator $U_H(t,0)$ is given by

$$\frac{\mathrm{d}U_H(t,0)}{\mathrm{d}t} = -\mathrm{i}H_{AR}(t)U_H(t,0). \tag{2.10}$$

Then, the Heisenberg EM reads:

$$\frac{\mathrm{d}O^{H}(t)}{\mathrm{d}t} = -\mathrm{i}[H^{H}_{AR}(t,t),O^{H}(t)] \qquad H^{H}_{AR}(t,t) = U^{+}_{H}(t,0)H_{AR}(t)U_{H}(t,0). \tag{2.11}$$

Quite generally, the interaction Hamiltionian in the interaction picture can be written as

$$H_{AR}(t) = \sum_{j} V_{A,j}(t) \otimes V_{R,j}(t)$$
(2.12)

where $V_{A,j}(t)$ and $V_{R,j}(t)$ are Hermitian operators acting in the Hilbert spaces \mathcal{H}_A and \mathcal{H}_R , respectively. In the case of a reservoir, $V_{R,j}(t)$ reads as

$$V_{R,j}(t) = \sum_{\lambda} \left[g_{j\lambda} b_{\lambda} \mathrm{e}^{-\mathrm{i}\omega_{\lambda}t} + g_{j\lambda}^* b_{\lambda}^+ \mathrm{e}^{\mathrm{i}\omega_{\lambda}t} \right]$$
(2.13)

where $g_{j\lambda}$ are the coupling constants between the system A and the reservoir R, and $b_{\lambda}(t), b_{\lambda}^{+}(t)$ are the boson annihilation and creation operators of the mode λ with the frequency ω_{λ} .

The EMs for our diagonal operators $A_l(t)$ in the HP are given by

$$\frac{\mathrm{d}A_{i}^{H}(t)}{\mathrm{d}t} = -\mathrm{i}L_{AR}^{H}(t,t)A_{i}^{H}(t) = -\mathrm{i}\sum_{j}V_{R,j}^{H}(t,t)L_{A,j}^{H}(t,t)A_{i}^{H}(t) \qquad (2.14)$$

where we used the notation

j

λ

$$L_{A,j}^{H}(t,t)(\cdots) = [V_{A,j}^{H}(t,t),(\cdots)] \qquad L_{R,j}^{H}(t,t)(\cdots) = [V_{R,j}^{H}(t,t),(\cdots)]$$
(2.15)

$$\frac{\mathrm{d}b_{\lambda}^{H}(t)}{\mathrm{d}t} = -\mathrm{i}L_{AR}^{H}(t,t)b_{\lambda}^{H}(t) = -\mathrm{i}\sum_{j}V_{A,j}^{H}(t,t)L_{R,j}^{H}(t,t)b_{\lambda}^{H}(t)$$
$$= \mathrm{i}\sum_{j}V_{A,j}^{H}(t,t)\sum_{j}g_{j\lambda}^{*}\mathrm{e}^{\mathrm{i}\omega_{\lambda}t}$$
(2.16)

$$b_{\lambda}^{H}(t) = b_{\lambda}^{H}(0) + \sum_{j} i g_{j\lambda}^{*} \int_{0}^{t} dt' V_{A,j}^{H}(t',t') e^{i\omega_{\lambda}t'}.$$
(2.17)

By inserting this equation (2.17) into equation (2.14) and using the so-called normal ordering (which means that $(b_{\lambda}^{H}(t))^{+}$ appears to the left and $b_{\lambda}^{H}(t)$ to the right of the operators of system A), we obtain

$$\frac{\mathrm{d}A_{i}^{H}(t)}{\mathrm{d}t} = -\mathrm{i}\sum_{j,\lambda} \left\{ g_{j\lambda} \mathrm{e}^{-\mathrm{i}\omega_{\lambda}t} \left[L_{A,j}^{H}(t,t)A_{i}^{H}(t) \right] b_{\lambda}^{H}(0) + g_{j\lambda}^{*}(b_{\lambda}^{H}(0))^{+} \mathrm{e}^{\mathrm{i}\omega_{\lambda}t} \right. \\ \left. \times L_{A,j}^{H}(t,t)A_{i}^{H}(t) \right\} \\ \left. + \sum_{j,j',\lambda} g_{j\lambda}g_{j'\lambda}^{*} \left[L_{A,j}^{H}(t,t)A_{i}^{H}(t) \right] \int_{0}^{t} \mathrm{d}t' \, \mathrm{e}^{-\mathrm{i}\omega_{\lambda}(t-t')} V_{A,j'}^{H}(t',t') \right. \\ \left. - \sum_{j,j',\lambda} g_{j\lambda}^{*}g_{j'\lambda} \int_{0}^{t} \mathrm{d}t' \, \mathrm{e}^{\mathrm{i}\omega_{\lambda}(t-t')} V_{A,j'}^{H}(t',t') L_{A,j}^{H}(t,t) A_{i}^{H}(t). \right.$$
(2.18)

As is well known, the equal-time commutator properties of operators of systems A and R are preserved in the HP:

$$[O_A^H(t), O_R^H(t)] = [O_A^H(0), O_R^H(0)] = 0$$
(2.19)

$$[O_{A,\alpha}^{H}(t), O_{A,\beta}^{H}(t)] = [O_{A,\alpha}^{H}(0), O_{A,\beta}^{H}(0)]$$
(2.20)

$$[b_{\lambda}^{H}(t), (b_{\lambda'}^{H}(t))^{+}] = \delta_{\lambda,\lambda'}$$
(2.21)

where $O_A^H(t), O_{A,\alpha}^H(t), O_{A,\beta}^H(t)$ and $O_R^H(t)$ are arbitrary operators of systems A and R, respectively.

As was pointed out by Ackerhalt and Eberly [30], in order to get consistent results the validity of (2.19)-(2.21) must be preserved in the approximate Heisenberg EMs as well. If the application of the commutator relationships (2.19)-(2.21) in the approximate Heisenberg EMs leads to the violation of any of these relationships, the inconsistency is proved.

The question about the kind of the consistency relationship, which should be fulfilled in order to get non-negative probabilities in the subsystem A, can be easily answered. Namely, the preservation of the validity of the relationship

$$A_{l}^{H}(t)A_{l}^{H}(t) = A_{l}^{H}(t)$$
(2.22)

for diagonal operators of subsystem A by the Heisenberg EMs guarantees the existence of only non-negative probabilities:

$$\langle A_i \rangle_t = \langle \psi(0) | A_i^H(t) | \psi(0) \rangle = \langle \psi(0) | A_i^H(t) A_i^H(t) | \psi(0) \rangle \ge 0$$
(2.23)

since the norm of a vector $A_i^H(t)|\psi(0)\rangle$ is always positive in the Hilbert space.

In equation (2.23), for the sake of simplicity, we have chosen the special initial condition of pure states, since all initial conditions can be written as

$$\rho(0) = \sum_{m} p_m |\psi_m(0)\rangle \langle \psi_m(0)| \qquad 0 \le p_m \le 1$$
(2.24)

and

$$\langle A_i \rangle_t = \text{Tr}_{AR}[A_i^H(t)\rho(0)] = \sum_m \langle \psi_m(0) | A_i^H(t) | \psi_m(0) \rangle p_m.$$
(2.25)

To see whether the consistency condition (2.22) is fulfilled by the *approximate* Heisenberg EMs, we have to write it in the form:

$$\frac{\mathrm{d}A_i^H(t)}{\mathrm{d}t}A_i^H(t) + A_i^H(t)\frac{\mathrm{d}A_i^H(t)}{\mathrm{d}t} = \frac{\mathrm{d}A_i^H(t)}{\mathrm{d}t}.$$
(2.26)

Now, we turn to the *approximate* Heisenberg EMs. It is easy to see that the BA (second-order approximation in the interaction) in the exact equation (2.18) leads to a non-Markovian equation:

$$\frac{dA_{i}^{H}(t)}{dt} = -i \sum_{j,\lambda} \left\{ g_{j\lambda} e^{-i\omega_{\lambda}t} \left[L_{A,j}^{H}(t,t) A_{l}^{H}(t) \right] b_{\lambda}^{H}(0) + g_{j\lambda}^{*}(b_{\lambda}^{H}(0))^{+} e^{i\omega_{\lambda}t} \right. \\ \left. \times L_{A,j}^{H}(t,t) A_{l}^{H}(t) \right\} \\ \left. + \sum_{j,j',\lambda} g_{j\lambda} g_{j'\lambda}^{*} \int_{0}^{t} dt' e^{-i\omega_{\lambda}(t-t')} \left[L_{A,j}^{H}(t',t) A_{l}^{H}(t') \right] V_{A,j'}^{H}(t',t') \right. \\ \left. - \sum_{j,j',\lambda} g_{j\lambda}^{*} g_{j'\lambda} \int_{0}^{t} dt' e^{i\omega_{\lambda}(t-t')} V_{A,j'}^{H}(t',t') L_{A,j}^{H}(t',t) A_{l}^{H}(t'). \right. \tag{2.27}$$

It is clear that the consistency equation (2.26) leading to non-negative probabilities is violated by equation (2.27). Namely, if one inserts equation (2.27) into equation (2.26), because of the appearance of operators $A_l^H(t)$ and $A_l^H(t')$ at different times t and t', the left-hand side of equation (2.26) does not equal the right-hand side anymore. In other words, the appearance of the operator $A_l^H(t')$ at times t', t' < t in equation (2.27) is in contradiction to the exact equation (2.18) where the time rate change of the operator $A_l^H(t)$ does not depend on $A_l^H(t')$ at previous times t' < t. This means, in contrast to equation (2.27), the exact equation (2.18) is a Markovian equation. Therefore, as will be shown in the following, the inclusion of the MA (neglecting memory effects) into the BA, leads to the preservation of the consistency relationship (2.26). Namely, as was demonstrated by other authors [30], the BA including the MA can be performed by replacing $V_{A,j}^H(t', t')$ by $V_{A,j}^H(t, t')$ in the integrands in equation (2.18), or doing this in equation (2.17) directly. This new Markovian equation immediately fulfils the

consistency relationship (2.26) if the equal-time commutation relationship between the operators of systems A and R, equation (2.19), (whose validity must be demanded in the approximate EMs as well, as was pointed out by Ackerhalt and Eberly [30]) are applied.

In this way we have shown that only the BA including the MA preserves the validity of the consistency relationship (2.26) leading to non-negative probabilities (2.23), whereas in the case of the BA without the MA this relationship is not valid any more and negative probabilities may arise (see e.g. [26, 27]). In order to make these statements valid in the case of the POM as well, we have to show that in the BA from both equation (2.27) and the ME (2.6) the same EM for the expectation value of any operator O_A follow. Namely, from (2.6) it follows that

$$\frac{\mathrm{d}\langle O_A\rangle_t}{\mathrm{d}t} = -\int_0^t \mathrm{d}t' \operatorname{Tr}_{AR} \left\{ \left[L_{AR}(t') L_{AR}(t) O_A \right] \rho_R(0) \otimes \rho_A(t') \right\}.$$
(2.28)

Using (2.12) and (2.15) we get

$$L_{AR}(t')L_{AR}(t)O_{A} = \sum_{j,j'} \{V_{A,j'}(t')[L_{A,j}(t)O_{A}] \otimes V_{R,j'}(t')V_{R,j}(t) - [L_{A,j}(t)O_{A}]V_{A,j'}(t') \otimes V_{R,j}(t)V_{R,j'}(t')\}.$$
(2.29)

By inserting (2.29) and (2.13) into (2.28) we obtain

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$$\frac{\mathrm{d}\langle O_A \rangle_t}{\mathrm{d}t} = -\sum_{j,j'} g_{j\lambda}^* g_{j'\lambda} \int_0^t \mathrm{d}t' \,\mathrm{e}^{\mathrm{i}\omega_\lambda(t-t')} \langle V_{A,j'}(t') [L_{A,j}(t)O_A] \rangle_{t'} + \sum_{j,j'} g_{j\lambda} g_{j'\lambda}^* \int_0^t \mathrm{d}t' \,\mathrm{e}^{-\mathrm{i}\omega_\lambda(t-t')} \langle [L_{A,j}(t)O_A] V_{A,j'}(t') \rangle_{t'}$$
(2.30)

where we used the special initial condition of a reservoir at T = 0 (bosonic vacuum):

$$\rho_R(0) = |\{0\}\rangle\langle\{0\}| \tag{2.31}$$

and the relation

$$\operatorname{Tr}_{R}\left[V_{R,j'}(t')V_{R,j}(t)\rho_{R}(0)\right] = \sum_{\lambda} g_{j'\lambda}g_{j\lambda}^{\bullet} \mathrm{e}^{\mathrm{i}\omega_{\lambda}(t-t')}.$$
(2.32)

We now sketch the derivation of the EM for the expectation value $\langle O_A \rangle_t = \text{Tr}_{AR}[\rho_A(0) \otimes \rho_R(0) O_A^H(t)]$ by using the Heisenberg EMs in the BA. It is clear that (2.27) is valid for any operator $O_A^H(t)$ of the system A if $A_i^H(t)$ is replaced by $O_A^H(t)$ throughout the equation. Then by multiplying this equation by $\rho_A(0) \otimes \rho_R(0)$, afterwards carrying out the trace over it, and taking into account (2.31), (2.30) of the POM follows.

3. Special POs and a new self-consistent POM

In this section, in order to clarify entirely the consequnces arising from the application of the BA in the POM, we introduce new special POs which will make the invention of a new self-consistent POM possible.

For the sake of simplicity, we restrict our initial conditions to the pure states $|\psi(0)\rangle$:

$$\rho_{PS}(0) = |\psi(0)\rangle\langle\psi(0)| \tag{3.1}$$

without restricting the generality. Namely, as is well known, a generalization to a statistical mixture is always possible by weighting the different initial pure states $|\psi_m(0)\rangle$ with the corresponding probabilities p_m .

In contrast to the Argyres-Kelley PO which projects onto a subsystem, here we define POs of different order N projecting onto subspaces $\mathcal{H}^{S(N)}$ of the same order. The subspace $\mathcal{H}^{S(N)}$ is created by the N-fold action of the non-restricted interaction Hamiltonian H_{AR} , i.e. $\mathcal{H}^{S(N)}$ is defined by the state vectors:

$$\{(H_{AR})^{l}|\psi(0)\rangle, l = 0, 1, \dots, N\}.$$
(3.2)

All lower-order spaces $\mathcal{H}^{S(k)}$ are contained in the higher-order spaces $\mathcal{H}^{S(m)}$, m > k as subspaces. The PO P_N is the projector onto the subspace $\mathcal{H}^{S(N)}$ and is defined by the corresponding unit operator:

$$P_N = \mathbf{I}^{S(N)} \qquad N = 0, 1, \dots \tag{3.3}$$

By applying the PO

$$\tilde{P}_N(\cdots) = P_N(\cdots)P_N \tag{3.4}$$

to the Liouville equation (2.1), the following ME in the BA can be derived:

$$\frac{\mathrm{d}[P_N\rho(t)P_N]}{\mathrm{d}t} = -\mathrm{i}P_N L_{AR}(t)P_N\rho(t)P_N - \int_0^t \mathrm{d}t' \,\tilde{P}_N L_{AR}(t)(\mathbf{I}-\tilde{P}_N)L_{AR}(t')P_N\rho(t')P_N$$
(3.5)

where we used $\rho(0) = P_N |\psi(0)\rangle \langle \psi(0)| P_N = |\psi(0)\rangle \langle \psi(0)|$.

By taking into account the fact that the operators $(H_{AR})^{l} \mathbb{I}^{S(N)}(H_{AR})^{l'}$, $l, l' = 0, 1, \ldots, K$ act in the subspace $\mathcal{H}^{S(N+K)}$, the integrand of (3.5) can be further reduced. In other words, as a consequence of the BA, the action of the Hamiltonian $H_{AR}(t)$ is restricted to the subspace $\mathcal{H}^{S(N+1)}$:

$$H_{AR}^{S(N+1)}(t) = P_N H_{AR}(t) \mathbb{I}^{S(N+1)} + \mathbb{I}^{S(N+1)} H_{AR}(t) P_N - P_N H_{AR}(t) P_N.$$
(3.6)

In the present case it is easy to see whether a consistency relationship has been violated in the ME (3.5) (derived in the BA). Namely, the application of the PO \tilde{P}_N assumes the existence of a special form

$$\bar{P}_{N}\rho(t) = P_{N}|\psi(t)\rangle\langle\psi(t)|P_{N}$$
(3.7)

for the reduced density operator. In other words, the simplest consistency condition which should be fulfilled is the preservation of the special form (3.7) of the reduced density operator in the approximate ME (3.5). On the other hand, the validity of (3.7) implies the existence of a reduced state vector $P_N|\psi(t)\rangle$. From this, it can be concluded that the existence of an EM for the reduced state vector $P_N|\psi(t)\rangle$ is a necessary and sufficient condition for the fulfilment of the consistency condition (3.7) in the approximate ME (3.5). However, it is easy to see that the equation

$$\frac{\mathrm{d}[P_N\rho(t)P_N]}{\mathrm{d}t} = \frac{\mathrm{d}[P_N|\psi(t)\rangle]}{\mathrm{d}t} \langle \psi(t)|P_N + P_N|\psi(t)\rangle \frac{\mathrm{d}[(\psi(t)|P_N]}{\mathrm{d}t}$$
(3.8)

cannot be written in the form of the ME (3.5), because the integration in (3.5) is to be carried out over the whole reduced density operator $\tilde{P}_N \rho(t') = P_N |\psi(t')\rangle \langle \psi(t')| P_N$ and not only over the part corresponding to the reduced state vector. This means that analogously to the Argyres-Kelley POM, the non-Markovian ME violates the consistency condition whose validity would guarantee non-negative probabilities.

Similarly as in the case of Argyres-Kelley PO, if the MA is included into the BA, the consistency condition (3.7) is preserved, because by using (3.6), the ME (3.5) can be written in a form which is reducible to an EM for the reduced state vector

$$\frac{\mathrm{d}P_{N}|\psi(t)\rangle}{\mathrm{d}t} = -\mathrm{i}P_{N}H_{AR}^{S(N+1)}(t)P_{N}|\psi(t)\rangle - \int_{0}^{t}\mathrm{d}t' P_{N}H_{AR}^{S(N+1)}(t)[\mathbb{I}^{S(N+1)} - P_{N}] \times H_{AR}^{S(N+1)}(t')P_{N}|\psi(t)\rangle.$$
(3.9)

Knowing this, it is easy to develop a new *self-consistent* POM. This has been done in [31, 32] where, instead of applying the POM to the Liouville equation, the POM has been applied directly to the Schrödinger equation. In this way an EM for a reduced state vector has been obtained. Since from such an EM probability amplitudes can be calculated, it is clear that the probabilities, which are squares of the moduli of probability amplitudes, are always non-negative.

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