

STOCHASTIC PURE STATE REPRESENTATION FOR OPEN QUANTUM SYSTEMS

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We show that the usual master equation formalism of markovian open quantum systems is completely equivalent to a certain state vector formalism. The state vector of the system satisfies a given frictional Schrödinger equation except for random instant transitions of discrete nature. Hasse's frictional hamiltonian is recovered for the damped harmonic oscillator.

The incorporation of damping into the dynamics of quantized open systems is not a trivial task [1]. Actually, the master equation formalism operating with mixed states is being considered as the adequate apparatus in describing damped systems [2,3].

There have been, however, attempts to keep the pure state representation with a certain nonlinear effective Schrödinger equation governing the state vector. For example, Hasse [4] found special solutions to his frictional Schrödinger equation which are physically equivalent to the corresponding density operator solutions of the master equation for the quantized harmonic oscillator with weak damping.

In our paper we propose a general pure state representation for markovian open quantum systems which is completely equivalent to the density operator formalism. Hasse's result [4] will be recovered as a special case.

In the mixed state formalism, the evolution of a given markovian open quantum system is characterized by the master equation:

$$\dot{\rho}(t) = L[\rho(t)], \quad (1)$$

where $\rho(t)$ is the density operator of the system and $L[\rho]$ is an operator-valued linear function of ρ . Since $\rho(t)$ must be normalized and hermitian, L must be traceless and hermitian as well.

For a given pure state $\rho = \psi\psi^+$, where ψ stands for the state vector, it is useful to introduce the total decay rate $w_{\psi \rightarrow}$ by

$$w_{\psi \rightarrow} \equiv -\psi^+ L[\psi\psi^+] \psi \equiv -\langle L[\psi\psi^+] \rangle. \quad (2)$$

Furthermore, the transition rates $w_{\psi \rightarrow \varphi}$ from ψ to another orthogonal state φ can be defined by

$$w_{\psi \rightarrow \varphi} \equiv \varphi^+ L[\psi\psi^+] \varphi, \quad \varphi^+ \psi = 0. \quad (3)$$

If a given set $\{\psi, \varphi_n; n = 1, 2, \dots, N\}$, $N \leq \infty$, forms a complete orthonormal system of state vectors then the identity $\text{Tr} L[\psi\psi^+] = 0$ leads to the following relation:

$$\sum_{n=1}^N w_{\psi \rightarrow \varphi_n} = w_{\psi \rightarrow}, \quad (4)$$

i.e. the partial transition rates to the φ_n sum up to the total decay rate of the state ψ .

Now we turn to develop the pure state equations equivalent to eq. (1).

Let us introduce the frictional Schrödinger equation for the state vector $\psi(t)$:

$$\dot{\psi} = (L[\psi\psi^+] - \langle L[\psi\psi^+] \rangle) \psi \equiv -(i/\hbar) H_{\text{fr}} \psi. \quad (5)$$

Note that the frictional (non-hermitian and non-linear but norm conserving) hamiltonian H_{fr} is not fixed uniquely by the above formula.

Let us assume now that at $t = 0$ the given open system is prepared in a certain pure state $\rho(0) = \psi(0)\psi^+(0)$. By an infinitesimal time $dt \equiv \epsilon$ later the state of the system turns out to be the mixed state

$$\rho(\epsilon) = \psi(0)\psi^+(0) + \epsilon L[\psi(0)\psi^+(0)] \quad (6)$$

according to the master equation (1). If the state $\psi(t)$ of the system satisfied the frictional Schrödinger equation (5) then the density operator $\rho(\epsilon)$ would be equal to

$$\begin{aligned} \psi(\epsilon)\psi^+(\epsilon) &= \psi(0)\psi^+(0) \\ &- (i\epsilon/\hbar)[H_{fr}\psi(0)\psi^+(0) - \psi(0)\psi^+(0)H_{fr}^+] \\ &= \psi(0)\psi^+(0) + \epsilon\{L[\psi(0)\psi^+(0)] \\ &- \langle L[\psi(0)\psi^+(0)] \rangle, \psi(0)\psi^+(0)\}, \end{aligned} \quad (7)$$

which is a pure state of course. Now, the true state (6) can be formally written as

$$\rho(\epsilon) = \psi(\epsilon)\psi^+(\epsilon) + \epsilon W, \quad (8)$$

if we introduce the hermitian operator W as the following function of the actual state ψ :

$$W \equiv L - \{L - \langle L \rangle, \psi\psi^+\}, \quad (9)$$

where the ψ -dependence of $L \equiv L[\psi\psi^+]$ is understood. We shall call W the *transition rate operator* in the given state ψ of the system. Using definition (9), it is trivial to show that the transition rates (3) can equally be expressed by W , too:

$$\begin{aligned} w_{\psi \rightarrow \varphi} &\equiv \varphi^+ L \varphi = \varphi^+ W \varphi, \quad \varphi^+ \psi = 0, \\ w_{\psi \rightarrow} &\equiv -\langle L \rangle = -\langle W \rangle. \end{aligned} \quad (10)$$

Observe that ψ itself is the eigenvector of W with the eigenvalue $-w_{\psi \rightarrow}$:

$$W\psi = (L - \{L - \langle L \rangle, \psi\psi^+\})\psi = \langle L \rangle\psi = -w_{\psi \rightarrow}\psi. \quad (11)$$

This genuine property of the transition rate operator W is strongly correlated with the actual choice (5) of the frictional hamiltonian equation of motion.

Let us suppose now that the transition rate operator (9) has always a discrete spectrum. If $\{\psi, \varphi_n; n = 1, 2, \dots, N\}$, $N \leq \infty$, is the complete orthonormal system of the eigenvectors of W then we obtain the following orthogonal expansion:

$$W = -w_{\psi \rightarrow}\psi\psi^+ + \sum_{n=1}^N w_{\psi \rightarrow \varphi_n}\varphi_n\varphi_n^+, \quad (12)$$

where the eigenvalues were replaced by the corresponding transition rates (10).

Let us substitute such an orthogonal expansion

into the r.h.s. of eq. (8):

$$\begin{aligned} \rho(\epsilon) &= (1 - \epsilon w_{\psi(0) \rightarrow})\psi(0)\psi^+(0) \\ &+ \epsilon \sum_{n=1}^N w_{\psi(0) \rightarrow \varphi_n(0)}\varphi_n(0)\varphi_n^+(0). \end{aligned} \quad (13)$$

And now, we propose the following statistical interpretation of the above orthogonal expansion of the mixed state $\rho(\epsilon)$: Given the pure state $\psi(0)$ at $t = 0$, for the infinitesimal period $dt \equiv \epsilon$ the state vector $\psi(t)$ satisfies the frictional Schrödinger equation (5) with probability $1 - \epsilon w_{\psi \rightarrow}$ but, alternatively, $\psi(t)$ can decay into a given eigenvector φ_n of the actual transition rate operator (9), with the transition rate $w_{\psi \rightarrow \varphi_n} = \varphi_n^+ W \varphi_n$ (10), for $n = 1, 2, \dots, N$ respectively.

It is well known that for a mixed state like $\rho(\epsilon)$ [eq. (13)] the statistical interpretation by a certain mixture of pure states is never unique [5]. Nevertheless, our choice (13) is distinguished by the mutual orthogonality of the pure states which are the terms of the decomposition. This decomposition is highly preferred from the viewpoint [6] of measurement theory, too.

In practice it will turn out that a slightly modified form W' , instead of the transition rate operator W , will be more convenient to use:

$$W' \equiv L - \{L, \psi\psi^+\} + \langle L \rangle\psi\psi^+. \quad (14)$$

By comparing eq. (14) with eq. (9) one can see that $W' = W - \langle L \rangle\psi\psi^+ = W + w_{\psi \rightarrow}\psi\psi^+$, thus W' will be positive semidefinite with the orthogonal expansion similar to (12):

$$W' = \sum_{n=1}^N w_{\psi \rightarrow \varphi_n}\varphi_n\varphi_n^+. \quad (15)$$

Recalling the statistical interpretation of the continual state mixing expressed by eq. (13) we are going to formulate the stochastic pure state representation.

We propose to characterize the state of the given open quantum system by the state vector $\psi(t)$, which is, in this case, to be taken as stochastic variable with vector values from the Hilbert space of states. Then the density operator $\rho(t)$ is recovered by the stochastic mean of the pure state density operator $\psi(t)\psi^+(t)$:

$$\rho(t) = \langle\langle \psi(t)\psi^+(t) \rangle\rangle, \quad (16)$$

where the symbol $\langle\langle \ \rangle\rangle$ stands for the stochastic mean.

The state vector $\psi(t)$ obeys the following markovian stochastic process: $\psi(t)$ satisfies the continuous and deterministic Schrödinger equation (5) with frictional hamiltonian but, at any instant, the state $\psi(t)$ can promptly decay into a certain eigenvector $\varphi_n(t)$ of the actual transition rate operator W' (14) with the transition rate $w_{\psi(t) \rightarrow \varphi_n(t)}$ which is equal to the corresponding eigenvalue of W' (cf. the expansion (15)).

By the construction of this pure state representation (and especially from eq. (13)) it follows that the density operator (16) will obey the original master equation (1) of the given system. Therefore the pure state representation yields identical physical predictions to the density operator formalism.

Finally, we apply our pure state equations to the damped harmonic oscillator. This open system is understood relatively well and the corresponding literature is remarkably wide [1].

The master equation (1) has now the following form:

$$\dot{\rho} = L[\rho] = -(i/\hbar)[H_0, \rho] - (i/\hbar)\lambda[x, \{p, \rho\}] - (1/\hbar^2) \text{Re } D_{ab} [A_a, [A_b, \rho]], \quad (17)$$

where H_0 is the free oscillator hamiltonian. For convenience of notation the vector A stands for the pair of the canonical variables: $A_1 = p$ and $A_2 = x$. Consequently, D is a given 2×2 positive [3,7] hermitian matrix: $D_{11}, D_{22}, \text{Re } D_{12}$ are the diffusion coefficients, $\lambda = (2/\hbar) \text{Im } D_{12}$ is the constant of friction. In eq. (17) and henceforth we use Einstein's convention for summation over repeated indices.

Applying formula (5) we are led to the following frictional Schrödinger equation for the damped harmonic oscillator:

$$\begin{aligned} \dot{\psi} = (L - \langle L \rangle)\psi = & -(i/\hbar)(H_0 - \langle H_0 \rangle)\psi \\ & - (i/\hbar)\lambda(xp + x\langle p \rangle - \langle x \rangle p - \langle xp \rangle)\psi \\ & - (1/\hbar^2) \text{Re } D_{ab} [(A_a - \langle A_a \rangle)(A_b - \langle A_b \rangle) - \sigma_{ab}], \end{aligned} \quad (18)$$

where the positive hermitian 2×2 matrix σ is defined by

$$\sigma_{ab} \equiv \langle A_a A_b \rangle - \langle A_a \rangle \langle A_b \rangle. \quad (18a)$$

The above equation of motion is obviously consistent

with the following choice for the frictional hamiltonian H_{fr} :

$$\begin{aligned} H_{fr} = H_0 + \lambda[\frac{1}{2}\{x, p\} - \frac{1}{2}\langle\{x, p\}\rangle + x\langle p \rangle - \langle x \rangle p] \\ - (i/\hbar) \text{Re } D_{ab} [(A_a - \langle A_a \rangle)(A_b - \langle A_b \rangle) - \sigma_{ab}]. \end{aligned} \quad (19)$$

The antihermitian term of this hamiltonian differs from Hasse's hamiltonian [1,4]. Recall however, that Hasse's derivation requires an additional constraint for the state $\psi(t)$, namely

$$\text{Re } D_{ab} \sigma_{ab} = \frac{1}{2}\hbar^2\lambda. \quad (20)$$

If this condition is fulfilled our hamiltonian (19) will be identical to that of Hasse's theory.

Now, applying the definition (14) to the operator L in the master equation (17), we obtain the modified transition rate operator of the damped oscillator in the following compact form:

$$W' = (2/\hbar^2)D_{ab}(A_a - \langle A_a \rangle)\psi\psi^\dagger(A_b - \langle A_b \rangle), \quad (21)$$

which is explicitly positive semidefinite. The rank of W' is 2, thus its decomposition (15) contains only two states φ_1 and φ_2 which are orthogonal to each other and to the state ψ of the system:

$$W' = w_{\psi \rightarrow \varphi_1} \varphi_1 \varphi_1^\dagger + w_{\psi \rightarrow \varphi_2} \varphi_2 \varphi_2^\dagger. \quad (22)$$

The total decay rate of the actual state ψ is given by the trace of the modified transition rate operator W' :

$$\begin{aligned} w_{\psi \rightarrow} = w_{\psi \rightarrow \varphi_1} + w_{\psi \rightarrow \varphi_2} = (2/\hbar^2)D_{ab} \sigma_{ab} \\ = (2/\hbar^2) \text{Re } D_{ab} \sigma_{ab} - \lambda. \end{aligned} \quad (23)$$

It is interesting to recognize that $w_{\psi \rightarrow}$ vanishes if and only if Hasse's condition (20) is fulfilled for the state ψ of the system. For such states there are no stochastic transitions and thus the frictional Schrödinger equation (18) is satisfied exactly.

In general, the diagonalization (22) of W' is trivial, and the eigenvectors are of the form $\varphi_a = C_{ar}(A_r - \langle A_r \rangle)\psi$ with coefficients C depending on the matrices D and σ .

For brevity, however, we shall consider the simplest but still interesting damped oscillator where $D_{11} = D_{12} = D_{21} = 0, D_{22} > 0$. The frictional hamiltonian (19) is then the following:

$$H_{fr} = H_0 - (i/\hbar)D_{22}[(x - \langle x \rangle)^2 - \sigma_{22}]. \quad (24)$$

The transition rate operator (21) is now degenerate and equal to a single diad:

$$W' = 2\hbar^{-2}D_{22}(x - \langle x \rangle)\psi\psi^+(x - \langle x \rangle) = w_{\psi \rightarrow \varphi}\varphi\varphi^+,$$

where

$$\varphi = (\sigma_{22})^{-1/2}(x - \langle x \rangle)\psi \quad (25)$$

is normalized and orthogonal to ψ . The corresponding transition rate is then equal to

$$w_{\psi \rightarrow \varphi} = (2/\hbar^2)D_{22}\sigma_{22}. \quad (26)$$

Now, we claimed that, on the one hand, the state vector $\psi(t)$ satisfies the Schrödinger equation with the frictional hamiltonian (24); on the other hand, $\psi(t)$ can jump stochastically into the state $\varphi(t)$ (25) according to the time-dependent transition rate (26). We are going to prove that the stochastic mean $\rho(t) = \langle\langle\psi(t)\psi^+(t)\rangle\rangle$ (16) satisfies the corresponding master equation (17).

If we suppose $\psi(0) \equiv \psi$ is fixed, then, by $dt \equiv \epsilon$ later, the state $\psi(\epsilon)$ equals $\psi - (i\epsilon/\hbar)H_{fr}\psi$, with probability $1 - \epsilon w_{\psi \rightarrow \varphi}$; and, alternatively, $\psi(\epsilon) = (\sigma_{22})^{-1/2}(x - \langle x \rangle)\psi = \varphi$, with probability $\epsilon w_{\psi \rightarrow \varphi}$. Therefore the density operator is

$$\begin{aligned} \rho(\epsilon)|_{\rho(0)=\psi\psi^+} &= (1 - \epsilon w_{\psi \rightarrow \varphi}) \\ &\times [\psi - (i\epsilon/\hbar)H_{fr}\psi][\psi^+ + (i\epsilon/\hbar)\psi^+H_{fr}^+] \\ &+ \epsilon w_{\psi \rightarrow \varphi}\varphi\varphi^+. \end{aligned} \quad (27)$$

From eqs. (24)–(26) we can substitute H_{fr} , φ and $w_{\psi \rightarrow \varphi}$, respectively, into the r.h.s. of eq. (27). Recalling that ϵ is infinitesimal, eq. (27) can be written as

$$\begin{aligned} \rho(\epsilon)|_{\rho(0)=\psi\psi^+} &= \psi\psi^+ - (i\epsilon/\hbar)[H_0, \psi\psi^+] \\ &- (\epsilon/\hbar^2)D_{22}[x, [x, \psi\psi^+]]. \end{aligned} \quad (28)$$

Remember that this is the density operator at $t = \epsilon$, with the condition that $\rho(0)$ was a given pure state $\psi\psi^+$. It is easy to remove this condition because the r.h.s. of eq. (28) is linear in $\psi\psi^+$. By averaging for all stochastically possible states $\psi(0)$ we can replace $\psi\psi^+$ by $\rho(0)$, via eq. (16); then eq. (28) will be equivalent to the corresponding master equation (17):

$$\begin{aligned} \rho(\epsilon) &= \rho(0) - (i\epsilon/\hbar)[H_0, \rho(0)] \\ &- (\epsilon/\hbar^2)D_{22}[x, [x, \rho(0)]]. \end{aligned} \quad (29)$$

Thus, for the simple damped harmonic oscillator we have directly shown the equivalence of the master equation formalism and the stochastic pure state formalism proposed in the present paper. Note the first simple example was given in our previous work [8] on systems with white-noise potentials. That proposal has now been generalized and extended for all markovian open quantum systems.

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