Letter

New results on non-CP dynamics unearthed from urtexts of quantum state diffusion

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Abstract

Thirty years ago, the present author discussed the pure state unraveling (stochastic quantum trajectories) of Markovian open system dynamics. The fact that he considered all positive dynamics, not restricted to the Lindblad–Gorini–Kossakowski–Sudarshan complete-positive subclass, has remained unnoticed so far. We emphasize the importance of the transition-rate-operator W and the merit of the invariant (representation-independent) approach. From the urtexts we point out the condition $W \geqslant 0$ of positive dynamics, the extension of quantum state diffusion for positive dynamics, and as a major new result, the description of all the diffusive unravelings of positive dynamics.

Keywords: open quantum system, Markovian master equation, completely positive dynamics, positive dynamics, quantum trajectory, stochastic unraveling, Stochastic Schrödinger equation

Introduction

In 1986 and 1988, the present author published two papers [1, 2] on what later became known as stochastic quantum trajectories [3] and quantum state diffusion [4], which are now standard methods for open quantum systems [5]. Both papers considered the master equation for the density operator ρ of the Markovian open quantum systems:

$$\dot{\rho} = \mathcal{L}\rho, \tag{1}$$

requiring *positive* dynamics, i.e. that the superoperator $\mathcal{L}$ conserve the positivity of ρ. Then, stochastic Schrödinger equations (SSEs) were constructed to generate pure state solutions (quantum trajectories) ψ, constituting the so-called stochastic *unraveling* dynamics (1). This

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means that the stochastic average of the quantum trajectories must yield the ensemble density operator

$$\mathbb{E}\psi\psi^\dagger = \rho \tag{2}$$

which is the solution of the master equation (1).

The seminal works of Lindblad [6] and Gorini *et al* [7] were mentioned, but the dynamics was not restricted to that of the complete-positive (CP) variety. Hence, the Lindblad–Gorini–Kossakowski–Sudarshan structure

$$\dot{\rho} = -\mathrm{i}[H, \rho] + F_\alpha \rho F_\alpha^\dagger - \frac{1}{2}\{F_\alpha^\dagger F_\alpha, \rho\} \tag{3}$$

was not assumed. (Here and henceforth the Einstein convention of summation for repeated indices is used.) No particular representation of the master equation (1) was introduced at all. All the results were derived and explained in terms of the superoperator $\mathcal{L}$, all results were representation-independent, i.e. *invariant*, and all results were valid for positive, not necessarily CP, dynamics (1).

Since the typical Markovian open quantum systems satisfy the CP master equation (3), all standard works on quantum trajectories in general, and on quantum state diffusion (QSD) [3–5] in particular, have imposed the structure (3). Perhaps the only exception was Gisin's paper in 1990 [8], which determined all the diffusive quantum trajectories for all the positive 2D Markovian dynamics, including those of the non-CP variety. The jump unraveling of a non-CP master equation in 2D appeared next only in [9]. Very recently, a detailed work [10] has extended QSD for non-CP master equations.

Below we are going to recapitulate the cornerstones of the urtexts [1, 2] to emphasize the merit of the invariant approach and to unearth the unnoticed results.

Positive dynamics

Diósi [1] *understands* that the conservation of ρ's positivity is guaranteed if it holds for any pure initial state differentially in time. Hence, in infinitesimal time $\mathrm{d}t$ any pure state must evolve into a non-negative density matrix:

$$0 \leqslant \psi\psi^\dagger + \mathrm{d}t\,\mathcal{L}(\psi\psi^\dagger) \equiv \psi\psi^\dagger + \mathrm{d}tL, \tag{4}$$

where $L = \mathcal{L}(\psi\psi^\dagger)$ is a useful shorthand notation. The central object, related to the superoperator $\mathcal{L}$, is the *transition rate operator*:

$$W = L - \{L, \psi\psi^\dagger\} + \langle L\rangle\psi\psi^\dagger, \tag{5}$$

with the notation $\langle L\rangle = \psi^\dagger L\psi$. The other central object is the *frictional Hamiltonian* satisfying

$$-\mathrm{i}H_{\mathrm{fr}}\psi = (L - \langle L\rangle)\psi. \tag{6}$$

H_{fr} is non-linear and non-Hermitian, but a norm-conserving Hamiltonian. The term to ensure normalization coincides with the total transition rate $w = \mathrm{Tr}W = -\langle L\rangle$, as it follows from equation (5). By substituting equations (5) and (6) on the rhs of the master equation (1), the time-derivative of an initial pure state density operator $\rho = \psi\psi^\dagger$ takes the form

$$\dot{\rho} = -\mathrm{i}H_{\mathrm{fr}}\rho + i\rho H_{\mathrm{fr}}^\dagger + W - w\rho. \tag{7}$$

Accordingly, the inequality (4) takes this form:

$$0 \leqslant \psi\psi^\dagger - \mathrm{i}H_{\mathrm{fr}}\psi\psi^\dagger\mathrm{d}t + i\psi\psi^\dagger H_{\mathrm{fr}}^\dagger\mathrm{d}t + W\mathrm{d}t - w\psi\psi^\dagger\mathrm{d}t. \tag{8}$$

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Since $W\psi = \psi^\dagger W = 0$ by construction (5), the above inequality is equivalent to the non-negativity of the transition rate operator:

$$W \geqslant 0, \tag{9}$$

which is *understood* in [1]—where the non-negativity of W is taken for granted—as the necessary and sufficient condition on the superoperator $\mathcal{L}$ to conserve the positivity of ρ. This theorem is explicitly stated and derived in [10], starting from the oldest conditions of Kossakowski [11], which were mentioned in [2] in the following invariant form. The dynamics (1) is positive if the operator $L = \mathcal{L}(\psi\psi^\dagger)$ satisfies

$$\psi^\dagger L \psi \leqslant 0, \quad \psi_\perp L \psi_\perp \geqslant 0 \tag{10}$$

for any pair of orthogonal pure states $\psi, \psi_\perp$. As pointed out correctly in [10], these conditions are equivalent to the positivity (9) of the transition rate operator.

Quantum state diffusion

Based on the decomposition (7) of the master equation (1), a jump (piece-wise deterministic) process was constructed in [1], unraveling the generic CP as well as all positive dynamics both for the first time. Below we concentrate on the diffusive unravelings.

When the state vector ψ is subject to diffusion, it turns out from (7) that a correct unraveling can be obtained if the drift velocity of ψ is $-(iH_{\mathrm{fr}}\psi + \frac{1}{2}w)\psi$ and the matrix of diffusion is W. In a given basis numbered by lower-case Latin indices running from 1 to N, the probability distribution p of the complex amplitudes $\{\psi_n, \psi_n^\star\}$ satisfies the following Fokker–Planck equation, as shown in [2]:

$$\dot{p} = \frac{\partial}{\partial \psi_n}(iH_{\mathrm{fr},nm} + \frac{1}{2}w\delta_{nm})\psi_m\, p + \text{c.c.}$$
$$+ \frac{\partial^2}{\partial \psi_n \partial \psi_m^\star} W_{nm}p. \tag{11}$$

Now we digress from the urtexts [1, 2]. As is well known from mathematics, a Fokker–Planck equation is always equivalent to a stochastic differential equation. Percival and Gisin considered the CP subclass (3) of master equations and proposed the following Ito-SSE [4]:

$$d\psi = \left(-iH + \langle F_\alpha\rangle F_\alpha - \frac{1}{2}F_\alpha^\dagger F_\alpha - \frac{1}{2}\langle F_\alpha^\dagger\rangle\langle F_\alpha\rangle\right)\psi dt$$
$$+ (F_\alpha - \langle F_\alpha\rangle)\psi d\xi_\alpha^\star, \tag{12}$$

where each ξ_α is a standard Hermitian white-noise process with the correlations

$$d\xi_\alpha d\xi_\beta^\star = \delta_{\alpha\beta}dt, \quad d\xi_\alpha d\xi_\beta = 0, \tag{13}$$

and with $\mathbb{E}d\xi_\alpha = 0$. One can inspect that the drift part on the rhs of (12) is indeed $-(iH_{\mathrm{fr}}\psi + \frac{1}{2}w)\psi$, while the correlation of the diffusive part yields

$$(F_\alpha - \langle F_\alpha\rangle)\psi d\xi_\alpha^\star[(F_\alpha - \langle F_\alpha\rangle)\psi d\xi_\alpha^\star]^\dagger$$
$$= (F_\alpha - \langle F_\alpha\rangle)\psi\psi^\dagger(F_\alpha^\dagger - \langle F_\alpha^\dagger\rangle)dt = W dt \tag{14}$$

as it should do.

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The equations (12) and (13) became the standard representation of QSD. The Fokker–Planck representation (11), valid beyond CP dynamics, went forgotten for several reasons. First, visualization of the stochastic quantum trajectories is more direct in terms of SSEs. Second, the SSEs serve directly for Monte-Carlo to simulate the solutions of the CP master equation (3). Third, SSEs treat diffusion in finite and infinite dimensions equally well mathematically. Nonetheless, we emphasize the merit of the Fokker–Planck representation, which only depends on the superoperator $\mathcal{L}$ and is thus explicitly invariant against the equivalence transformations of the CP structure. This invariance is less obvious on the standard equations (12) and (13), although one can directly prove it [4].

But back to the main point: the Fokker–Planck form of QSD is, as we said, valid for all positivity-conserving master equations, even if their CP representation does not exist. The equivalent SSE reads

$$\mathrm{d}\psi_n = -\left(\mathrm{i}H_{\mathrm{fr},nm} + \frac{1}{2}w\delta_{nm}\right)\psi_m\mathrm{d}t + \mathrm{d}\chi_n \tag{15}$$

where χ_n are W-correlated Hermitian white-noise processes:

$$\mathrm{d}\chi_n\mathrm{d}\chi_m^\star = W_{nm}\mathrm{d}t, \quad \mathrm{d}\chi_n\mathrm{d}\chi_m = 0, \tag{16}$$

while $\mathbb{E}\mathrm{d}\chi_n = 0$. As we said, this form is representation-independent, only depending on the invariant operators H_{fr} and W. If we prefer a form with standard Hermitian white-noise processes, resembling standard CP-QSD equations (12) and (13), we decompose W into the mixture of (not necessarily normalized) pure states orthogonal to ψ: $W = \varphi_{\perp\alpha}\varphi_{\perp\alpha}^\dagger$. Then the SSE reads

$$\mathrm{d}\psi = -(\mathrm{i}H + \frac{1}{2}w)\psi\mathrm{d}t + \varphi_{\perp\alpha}\mathrm{d}\xi_\alpha^\star \tag{17}$$

where the ξ_α satisfy (13). It is advisable for the $\varphi_{\perp\alpha}$ to be linearly independent. Caiaffa *et al* [10] took the spectral decomposition of W to define $(N-1)$ states $\{\varphi_{\perp,\alpha}; \alpha = 1, 2, ..., N-1\}$ orthogonal to each other (and to ψ).

All diffusive quantum trajectories

It is straightforward to find all diffusive unravelings of *positive* dynamics (1) if we start from the invariant form of QSD (15, 16). Observe that the ensemble average (2) of the quantum trajectories depends on the Hermitian correlations of the noises, it is independent of $\mathrm{d}\chi_n\mathrm{d}\chi_m$. We can make the χ_n correlate with themselves, generalizing (16):

$$\mathrm{d}\chi_n\mathrm{d}\chi_m^\star = W_{nm}\mathrm{d}t, \quad \mathrm{d}\chi_n\mathrm{d}\chi_m = S_{nm}\mathrm{d}t, \tag{18}$$

although we get diffusive unravelings of the same superoperator $\mathcal{L}$. While QSD corresponds to $S_{nm} \equiv 0$, the matrix S_{nm} uniquely characterizes all diffusive unravelings, under the only constraint that the total correlation matrix of the noises must be non-negative:

$$\begin{pmatrix} \mathrm{d}\chi\mathrm{d}\chi^\dagger & \mathrm{d}\chi\mathrm{d}\chi \\ \mathrm{d}\chi^\dagger\mathrm{d}\chi^\dagger & \mathrm{d}\chi^\dagger\mathrm{d}\chi \end{pmatrix} = \begin{pmatrix} W & S \\ S^\dagger & W \end{pmatrix} \geqslant 0. \tag{19}$$

If we start from the non-invariant representation (17, 13) of QSD, the general diffusive unravelings are characterized by the correlations

Table 1. A summary of the work on different unravelings versus positive or restricted CP dynamics.

	Positive	Complete positive
Jump	[1, 2, 9]	[3]
QSD	[2, 10]	[4]
All diffusive	[8] (present work)	[12, 13]
All jump	?	?

$$\mathrm{d}\xi_\alpha \mathrm{d}\xi_\beta^\star = \delta_{\alpha\beta}\mathrm{d}t, \quad \mathrm{d}\xi_\alpha \mathrm{d}\xi_\beta = s_{\alpha\beta}\mathrm{d}t, \tag{20}$$

with the constraint $\|s\| \leqslant 1$. Note that [12, 13] have obtained this result for the restricted class of CP dynamics. Rigo *et al* [12], citing Gisin's finding of all diffusive unravelings for 2D positive dynamics [8], anticipated that it might be be done in arbitrary dimensions. This has been done now. Wiseman and Diósi [13] had a different merit: they started from the invariant decomposition (7) of the dynamics (1). This decomposition shows explicitly that the only constraint on the stochastic increment $\mathrm{d}\psi$ of a diffusive quantum trajectory reads

$$\mathrm{d}\psi \mathrm{d}\psi^\dagger = W\mathrm{d}t$$

whereas $\mathrm{d}\psi \mathrm{d}\psi$ is free. It is of course possible to derive correct SSEs in many ways, in particular representations, although the invariant method results in shorter calculations and better insights.

Closing remarks

This time we have not intended to discuss the relevance or physical interpretation of the unravelings itemized in table 1. (For CP diffusive SSEs, [13] gave an exhaustive answer in terms of the monitoring and control of ψ, see [14] on the most recent QSD interpretations.) The role of non-CP dynamics in physics is not yet fully understood. The theory of their unraveling might get us closer to an interpretation.

Acknowledgment

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