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Diffusive Limit of Non-Markovian Quantum Jumps

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We solve two long-standing problems for stochastic descriptions of open quantum system dynamics. First, we find the classical stochastic processes corresponding to non-Markovian quantum state diffusion and non-Markovian quantum jumps in projective Hilbert space. Second, we show that the diffusive limit of non-Markovian quantum jumps can be taken on the projective Hilbert space in such a way that it coincides with non-Markovian quantum state diffusion. However, the very same limit taken on the Hilbert space leads to a completely new diffusive unraveling, which we call non-Markovian quantum diffusion. Further, we expand the applicability of non-Markovian quantum jumps and non-Markovian quantum diffusion by using a kernel smoothing technique allowing a significant simplification in their use. Lastly, we demonstrate the applicability of our results by studying a driven dissipative two level atom in a non-Markovian regime using all of the three methods.

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Introduction.—Deriving and solving the equations of motion for driven dissipative quantum systems is a notoriously hard task, especially in the presence of quantum memory effects. In this Letter, we open new avenues to tackle these problems of broad on-going interest. Currently, state-of-the-art experiments explore driven dissipative open quantum systems [1]; nonequilibrium phase transitions in a Rydberg gas have been observed [2], simulation of general open system dynamics with trapped ions has been reported [3,4]—and even the statistical likelihood of a physical process (a statistical arrow of time) has been experimentally characterized using superconducting qubit systems [5]. Similar types of open quantum systems appear also in the context of photosynthesis [6,7] and, in general, in molecular aggregates [8].

One of the main difficulties in analyzing driven open quantum systems has its origin in the lack of a typical timescale, such as an energy gap of the system Hamiltonian. One possible solution is to try to model the open system and environment dynamics exactly, as in non-Markovian quantum state diffusion [9,10], where a stochastic Schrödinger equation describes the dynamics of the open system and the effects of the environment are contained in the statistical properties of the driving noise. Typically approximation methods are required to solve the resulting equations of motion [11–13]. This type of approach has been successfully used to describe energy [14–16] and charge transport [17,18] in molecular aggregates.

Alternatively, starting from a microscopic model an effective time local master equation can be derived [19] and unraveled, for example, with non-Markovian quantum jumps [20–22]. Quantum jump methods have been used earlier, e.g., to study excitonic energy transport with [23,24] and without driving [25,26] and even to understand singlet fission in molecular crystals, which may help to design more efficient solar panels [27].

On the theoretical side, our motivation is to look for the missing connection between the quantum jump [20] and quantum state diffusion [10] approaches in the non-Markovian regime—and with the help of these results expand significantly their applicability of the former for complex practical problems. First, we formulate both approaches in the projective Hilbert space, thus extending the well known results from the Markov [28] to the non-Markovian regime. Then a diffusive limit of the quantum jumps is taken in such a way that it coincides with quantum

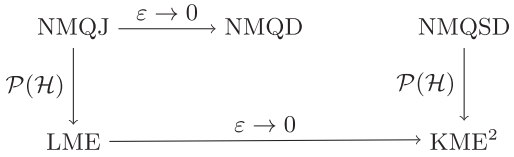

FIG. 1. Relation between non-Markovian quantum jumps (NMQJ), non-Markovian quantum diffusion (NMQD) and non-Markovian quantum state diffusion (NMQSD). In $\mathcal{P}(\mathcal{H})$, NMQJ corresponds to a Liouville master equation (LME), whereas NMQSD is associated with a 2nd order Kramers-Moyal expansion (KME^2) of the LME. In other words, the diffusive limit can be taken in such a way that the LME associated with NMQJ transforms to a KME^2 associated with NMQSD. However, when the very same limit is taken in $\mathcal{H}$, it results in a completely new unraveling, which we call non-Markovian quantum diffusion.

state diffusion in the projective Hilbert space and in the non-Markovian regime. Interestingly, the same limit in Hilbert space results in a completely new unraveling, which we call non-Markovian quantum diffusion (see Fig. 1). We enhance the quantum jumps and quantum diffusion approaches with kernel smoothing techniques [29], which allows us to handle driven dissipative systems with quantum memory effects easily. Lastly, we apply all of the methods to the driven dissipative two level atom.

Open systems and projective Hilbert space.—A typical model for open systems in the interaction picture with respect to environment Hamiltonian $H_B = \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda$ is

$$H(t) = H_S(t) + \sum_\lambda g_\lambda L a_\lambda^\dagger e^{i\omega_\lambda t} + g_\lambda^* L^\dagger a_\lambda e^{-i\omega_\lambda t}, \quad (1)$$

where the creation and annihilation operators $a_\lambda^\dagger$ and a_λ of a bath mode labeled by λ satisfy the bosonic commutation relations $[a_\lambda, a_\mu^\dagger] = \delta_{\lambda\mu}$. We assume that the coupling operator L is traceless, i.e., $\mathrm{tr}\{L\} = 0$. In a projective Hilbert space $\mathcal{P}(\mathcal{H})$, each point is associated with a projector $|\psi\rangle\langle\psi|$ [19,30]. Given a finite dimensional Hilbert space, coordinates $\psi_i \in \mathbb{C}$ on a $\mathcal{P}(\mathcal{H})$ can be easily constructed with respect to a fixed orthonormal basis as $|\psi\rangle = \sum_i \psi_i |i\rangle$. In fact, all physical information obtainable from quantum measurements resides in the projective Hilbert space since global phases are eliminated while computing expectation values. A famous example of a projective Hilbert space is the Bloch vector representation of a qubit. For more information on $\mathcal{P}(\mathcal{H})$, see the Supplemental Material [31].

Non-Markovian quantum state diffusion.—Reduced system dynamics can be represented exactly for a large class of models, even beyond Eq. (1) [36], with the following linear non-Markovian quantum state diffusion equation

$$\partial_t |\psi_t(z^*)\rangle = [-iH_S(t) + z_t^* L]|\psi_t(z^*)\rangle - L^\dagger \int_0^t ds \alpha(t-s) \frac{\delta |\psi_t(z^*)\rangle}{\delta z_s^*}. \quad (2)$$

Here, L is the coupling operator between the system and the bath and $H_S(t)$ is an arbitrary Hamiltonian acting on the open system [9,10]. NMQSD is driven by a complex valued colored Gaussian noise z_t^*, completely characterized by the correlations

$$\mathsf{M}[z_t z_s^*] = \alpha(t-s), \qquad \mathsf{M}[z_t^*] = \mathsf{M}[z_t z_s] = 0, \quad (3)$$

where $\mathsf{M}[\cdot]$ is the average over the noise process z_t^*. Solutions $|\psi_t(z^*)\rangle$ are analytic functionals of the whole noise process z_t^* up to time t.

In the remainder of this Letter, we will make the following restriction. We assume that the functional derivative satisfies, at least approximately [11]

$$\frac{\delta}{\delta z_s^*} |\psi_t(z^*)\rangle = f(t,s) L |\psi_t(z^*)\rangle. \quad (4)$$

Equation (4) guarantees that the reduced state will evolve according to a closed form master equation. However, the NMQSD method itself works perfectly well even if no such master equation exists for the reduced state.

The above stochastic Schrödinger equation (2) satisfies the ordinary rules of calculus since the noise process has a finite correlation time. The dynamics of the average state $\rho(t) = \mathsf{M}[|\psi_t(z^*)\rangle\langle\psi_t(z^*)|]$ described by Eq. (2) with assumption (4) reads

$$\dot\rho(t) = -i[H_S(t) + S(t)L^\dagger L, \rho(t)] + 2\gamma(t) L\rho(t)L^\dagger - \gamma(t)\{L^\dagger L, \rho(t)\}, \quad (5)$$

where $F(t) = \gamma(t) + iS(t)$ and $F(t) = \int_0^t ds \alpha(t-s) f(t,s)$.

To look for a connection between NMQSD and non-Markovian quantum jumps, we first have to derive a representation of the former in the projective Hilbert space. The probability density functional can be expressed as

$$P_Q[\psi, t] = \mathsf{M}[\delta(\psi - \psi_t(z^*))]. \quad (6)$$

We show in Ref. [31], that the probability density functional satisfies the following second order partial differential equation

$$\partial_t P_Q[\psi,t] = \sum_{k=1}^d \partial_{\psi_k} c_k(\psi) P_Q[\psi,t] + \partial_{\psi_k^*} c_k^*(\psi) P_Q[\psi,t] + \sum_{k,l=1}^d \partial^2_{\psi_k \psi_l^*} d_{kl}(\psi) P_Q[\psi,t], \quad (7)$$

where the drift and diffusion coefficients are $c_k(\psi) = \langle k|(-iH - F(t)L^\dagger L)|\psi\rangle$ and $d_{kl}(\psi) = [[F(t) + F^*(t)]\langle k|L|\psi\rangle\langle\psi|L^\dagger|l\rangle$, respectively. NMQSD thus corresponds to a 2nd order Kramers-Moyal expansion in $\mathcal{P}(\mathcal{H})$ [37]. If the diffusion coefficient $[F(t) + F^*(t)] = 2\gamma(t)$ is not negative for any time t the KME^2 equation is, in fact, a proper Fokker-Planck equation [38].

Non-Markovian quantum jumps.—Master equations of the form

$$\dot\rho(t) = -i[H_S(t) + \sum_k s_k(t) L_k^\dagger L_k, \rho(t)] + \sum_k 2\gamma_k(t) L_k \rho(t) L_k^\dagger - \gamma_k(t)\{L_k^\dagger L_k, \rho(t)\}, \quad (8)$$

can be unraveled with non-Markovian quantum jumps (NMQJ) [20–22], [39]. It is a piecewise deterministic process in the Hilbert space of the open system. Here we present a linear version of the process (LNMQJ) given by the following Ito stochastic differential equation:

$$|d\psi\rangle = -iG(t)|\psi\rangle dt + \sum_k \Big((L_k - \mathbb{1})|\psi\rangle dN^k_+(t) + \int d\psi' (|\psi'\rangle - |\psi\rangle) dN^k_{-,\psi'}(t) \Big), \quad (9)$$

where $G(t) = H_S(t) + \sum_k s_k(t) L_k^\dagger L_k - i\gamma_k(t)[L_k^\dagger L_k - \mathbb{1}]$. Increments of the Poisson processes, $dN^k_+(t)$ and $dN^l_{-,\psi'}(t)$, are mutually independent $dN^k_+(t)dN^l_+(t) = \delta_{kl} dN^k_+(t)$, $dN^k_{-,\psi'}(t)dN^l_{-,\psi''}(t) = \delta_{kl}\delta(\psi' - \psi'')dN^k_{-,\psi'}(t)$ and $dN^k_+(t)dN^l_{-,\psi'}(t) = 0$. The mean values of the increments are $\mathsf{E}[dN^k_+(t)] = 2\gamma^k_+(t)dt$ and $\mathsf{E}[dN^l_{-,\psi'}(t)] = 2\gamma^l_-(t)(P[\psi',t]/P[\psi,t])\delta(\psi - L_l\psi')dt$, where $\gamma_k(t) = \gamma^+_k(t) - \gamma^-_k(t)$. It is easy to see that the average evolution reproduces Eq. (8).

In NMQJ, the memory effects reside in the jump probability from a source state ψ to a target state ψ' via channel k when $\gamma_k(t) < 0$. In particular, a "reverse jump" can occur from ψ to ψ' iff $L_k|\psi'\rangle = |\psi\rangle$. The probability of such jumps depends on the ratio $P[\psi',t]/P[\psi,t]$. In order to compute the jump probability, the knowledge of the whole ensemble is required [20]. This poses a serious challenge since a state $|\psi\rangle\langle\psi|$ has measure zero in $\mathcal{P}(\mathcal{H})$. We describe later a method to overcome this.

Now, Eq. (5) is equivalent to Eq. (8) with $2m(1 \le k \le 2m)$ time dependent rates and time independent jump operators defined as

$$s_k(t) = \frac{s(t)}{2m|\xi_k|^2\varepsilon^2}, \qquad \gamma_k(t) = \frac{\gamma(t)}{2m|\xi_k|^2\varepsilon^2}, \qquad L_k = \mathbb{1} + \varepsilon\xi_k L, \qquad \text{s.t.} \quad \xi_k + \xi_{k+m} = 0, \quad (10)$$

where $\xi_k \in \mathbb{C}$, $|\xi_k| = |\xi|$ and $\varepsilon > 0$ [40]. The deterministic part $G(t)$ of the quantum jump process in Eq. (9) transforms under Eq. (10) to $G'(t) = H_S(t) + s(t)L^\dagger L - i\gamma(t)L^\dagger L + \Theta(t)\mathbb{1}$. The last term $\Theta(t) = \sum_{k=1}^{2m}[s(t)/(2m|\xi_k|^2\varepsilon^2)]$ is a global phase factor, which can be neglected. If $||\varepsilon L|| < 1$, then operators L_l are invertible [41]. In this case, the transformed statistics of the Poisson increments eventually become

$$\mathsf{E}[dN^k_+(t)] = \frac{\gamma_+(t)}{m\varepsilon^2|\xi_k|^2}dt,$$
$$\mathsf{E}[dN^l_{-,\psi'}(t)] = \frac{\gamma_-(t)}{m\varepsilon^2|\xi_k|^2}\frac{P[\psi',t]}{P[\psi,t]}\frac{\delta(L_l^{-1}\psi - \psi')}{|\det L_l||\det L_l^\dagger|}dt. \quad (11)$$

Remarkably, after the transformation the increment $dN^l_{-,\psi'}(t)$ does not depend on the target state of the jump, $|\psi'\rangle$, anymore. This arises because a reverse jump corresponds to a mapping $|\psi\rangle \mapsto L_l^{-1}|\psi\rangle = |\psi'\rangle$, i.e., the target state of the jump is given by the action of the inverse operator on the source state $|\psi\rangle$.

Therefore, we can write the transformed process as

$$|d\psi_t\rangle = -iG'(t)|\psi\rangle dt + \sum_k [(L_k - \mathbb{1})|\psi_t\rangle dM^k_+(t) + (L_k{}^{-1} - \mathbb{1})|\psi_t\rangle dM^k_-(t)], \quad (12)$$

with mutually independent Poisson increments $dM^k_\pm$ with statistics $\mathsf{E}[dM^k_+(t)] = [\gamma_+(t)/m\varepsilon^2|\xi_k|^2]dt$ and $\mathsf{E}[dM^k_-(t)] = \{(P[L_k{}^{-1}\psi,t])/(P[\psi,t]|\det L_k||\det L_k^\dagger|)\}\{[\gamma_-(t)]/(m\varepsilon^2|\xi_k|^2)\}dt$, which are just relabeled increments of Eq. (11). To assert that this equation is still valid, we compute the average evolution of $|\psi\rangle\langle\psi|$ which coincides with the master equation (5) (see the Supplemental Material [31]).

It is worth stressing that when $\gamma_k(t) < 0$, the quantum jumps are given by the inverse jump operator L_k^{-1}. Contrary to the original approach in Ref. [20], the quantum jumps and reverse quantum jumps are exactly inverses of each other. The quantum memory effects are contained in the probability for these jumps which still depends on the ratio $P[L_k^{-1}\psi,t]/P[\psi,t]$.

LNMQJ in projective Hilbert space.—In the projective Hilbert space LNMQJ corresponds to the following Liouville master equation [22]

$$\partial_t P[\psi,t] = i\sum_k \partial_{\psi_k}(\langle k|G'(t)|\psi\rangle P[\psi,t]) - \partial_{\psi_k^*}(\langle\psi|G'^\dagger(t)|k\rangle P[\psi,t]) + \int d\phi (R[\psi|\phi]P[\phi,t] - R[\phi|\psi]P[\psi,t]), \quad (13)$$

where the jump rates $R[\phi|\psi]$ are

$$R[\phi|\psi] = \sum_{k=1}^{2m}\frac{\gamma_+(t)}{m\varepsilon^2|\xi_k|^2}\delta(\phi - L_k\psi) + \frac{\gamma_-(t)}{m\varepsilon^2|\varepsilon_k|^2}\frac{P[\phi,t]}{P[\psi,t]}\delta(\psi - L_k\phi). \quad (14)$$

When comparing the drift terms in Fokker-Planck equation (7) and in the Liouville master equation (13), we see that they are equal. The jump part takes the form $\int d\phi (R[\psi|\phi]P[\phi,t] - R[\phi|\psi]P[\psi,t]) = \sum_{k=1}^{2m}\{[\gamma(t)]/(m\varepsilon^2|\xi_k|^2)\} F_k[\psi] - [2\gamma(t)/\varepsilon^2|\xi|^2]P[\psi,t]$, where

$$F_k[\psi] = \frac{P[L_k^{-1}\psi,t]}{|\det L_k||\det L_k^\dagger|}. \quad (15)$$

After expanding $F_k[\psi]$ to second order in ε and assuming $m > 2$ we find $\int d\phi (R[\psi|\phi]P[\phi,t] - R[\phi|\psi]P[\psi,t]) \to \sum_{k,l=0}^{d}\partial^2_{\psi_k\psi_l^*}(2\gamma(t)\langle k|L|\psi\rangle\langle\psi|L^\dagger|l\rangle P[\psi,t])$, while $\epsilon \to 0$ [42], see Ref. [31]. We thus have proven the validity of the part LME $\overset{\varepsilon\to 0}{\to}$ FPE of the diagram in Fig. 1.

Non-Markovian quantum diffusion.—Next we take the above diffusion limit directly on the piecewise deterministic LNMQJ process in the Hilbert space. Full details can be found in the Supplemental Material [31]. First, Eq. (12) is expanded to first order in ε, resulting in

$$|d\psi_t\rangle = -iG'(t)|\psi\rangle dt + \sum_k [\xi_k L|\psi_t\rangle \varepsilon dM_+^k(t) - \xi_k L|\psi_t\rangle \varepsilon dM_-^k(t)] + \mathcal{O}(\varepsilon^2). \tag{16}$$

We define new processes $dV_\pm^k = \varepsilon dM_\pm^k - \varepsilon E[dM_\pm^k]$ [43] and by using the Ito rules, we have $\mathsf{E}[dV_\pm^k] = 0$, $\mathsf{E}[dV_-^k dV_+^l] = 0$ and $\mathsf{E}[dV_+^k dV_+^l] = \delta_{kl}(\varepsilon dV_+^k + \{[\gamma_+(t)]/[m|\xi_k|^2]\}dt)$. We then define $\lim_{\varepsilon\to 0} dV_\pm^k = dW_\pm^k$, where the increments $dW_\pm^k$ satisfy the following Ito rules

$$\mathsf{E}[dW_\pm^k] = 0, \qquad \mathsf{E}[dW_-^k dW_+^l] = 0,$$
$$\mathsf{E}[dW_+^k dW_+^l] = \delta_{kl}\frac{\gamma_+(t)}{m|\xi_k|^2}dt,$$
$$\mathsf{E}[dW_-^k dW_-^l] = \delta_{kl}\frac{\gamma_-(t)}{m|\xi_k|^2}dt. \tag{17}$$

The goal is now to express the stochastic Schrödinger equation (16) in terms of Wiener increments $dW_\pm^k$. After some simplification steps (detailed in the Supplemental Material [31]), we find in the limit $\varepsilon \to 0$

$$|d\psi\rangle = \left(-iG'(t) + 2\gamma_-(t)\sum_{n=0}^{d}\langle\psi|L^\dagger|n\rangle\frac{\partial \ln P[\psi,t]}{\partial\psi_n^*}L\right)|\psi\rangle dt + L|\psi\rangle dZ_+ - L|\psi\rangle dZ_-, \tag{18}$$

where $dZ_\pm = \sum_k \xi_k dW_\pm^k$. The complex noise $dZ_\pm$ satisfies

$$\mathsf{E}[dZ_\pm] = 0, \mathsf{E}[dZ_\pm dZ_\pm] = 0,$$
$$\mathsf{E}[dZ_\pm dZ_\pm^*] = 2\gamma_\pm(t)dt. \tag{19}$$

The average evolution of NMQD equation (18) corresponds to Eq. (8) as we show in the Supplemental Material [31].

Interestingly, both noises $dZ_\pm$ couple to the system via L but with a different phase. Nevertheless, both noise terms produce "sandwich" terms $2\gamma_\pm(t)L\rho L^\dagger dt$ on the average evolution. The drift term with logarithmic derivative compensates the term $2\gamma_-(t)L\rho L^\dagger dt$ on average, such that the correct sandwich term $2[\gamma_+(t) - \gamma_-(t)]L\rho L^\dagger dt$ emerges. The term proportional to the logarithmic derivative can be seen as the change in the stochastic entropy of the system that contributes to the deterministic evolution [44].

Kernel smoothing.—A Gaussian kernel K is defined

$$K[\psi] = \frac{1}{\pi^{d+1}}e^{-||\psi||^2}, \qquad |\psi\rangle \in \mathbb{C}^{d+1}. \tag{20}$$

Given an ensemble of stochastic states $\{|\psi^\nu\rangle\}_{\nu=1}^M$, we estimate the probability density $P[\psi]$ in the projective Hilbert space with

$$P_\sigma[\psi] = \frac{1}{M(\sigma^2\pi^{d+1})}\sum_{\nu=1}^{M} K[(\psi - \psi^\nu)/\sigma], \tag{21}$$

where $\sigma > 0$ is a free parameter. A rule of thumb for choosing the variance is that $\sigma = M^{-1/d+5}$ [29], where d is the real dimension of the underlying Hilbert space. Using the estimated density, we can compute the logarithmic derivative of the density appearing in Eq. (18) as

$$\frac{\partial \ln P_\sigma[\psi]}{\partial\psi_n^*} = -\frac{\sum_{\nu=1}^M e^{-||\psi_n-\psi_n^\nu||^2}\frac{\psi_n-\psi_n^\nu}{\sigma^2}}{\sum_{\nu=1}^M e^{-||\psi_n-\psi_n^\nu||^2}} = -\frac{\psi_n - \langle\!\langle\psi_n\rangle\!\rangle}{\sigma^2}, \tag{22}$$

where the average $\langle\!\langle\cdot\rangle\!\rangle$ is taken with respect to distribution $p_\sigma = \frac{1}{\mathcal{Z}}e^{-|\psi-\psi^\nu||^2/\sigma^2}$, with $\mathcal{Z} = \sum_{\nu=1}^M e^{-||\psi_n-\psi_n^\nu||^2}$. Kernel estimation can be also used to evaluate the ratios $P_\sigma[\psi']/P_\sigma[\psi] = \{\sum_{\nu'=1}^M K[(\psi' - \psi^{\nu'})/\sigma]\}/\{\sum_{\nu=1}^M K[(\psi - \psi^\nu)/\sigma]\}$. Therefore, after performing the transformation (10) on the NMQJ and using the smoothed estimate for $P[\psi, t]$ we can compute the reverse jump probabilities easily. The reason for this simplification is that the target state of the jump is directly given by the inverse jump operator and the ratio of probabilities for the target and the source state to occur can be efficiently evaluated from the estimate.

Example: Driven dissipative two level atom.—An open system with $H_S = (\omega/2)\sigma_z + (\Omega/2)\sigma_x$ and $L = \sigma_-$ corresponds to an amplitude damped two level atom with driving and is not solvable in closed form. We assume that the bath correlation function takes the following exponential form:

$$\alpha(t,s) = g\frac{\Gamma}{2}e^{-i\omega_c(t-s)-\Gamma|t-s|}, \tag{23}$$

where Γ is the inverse of the bath correlation time $\tau_c = \Gamma^{-1}$, ω_c is the bath resonance frequency, and $g > 0$ is a dimensionless parameter describing the overall system bath coupling strength. The limit $\Gamma \to \infty$ leads to a singular bath correlation function $\alpha(t,s) \to g\delta(t-s)$ and to a Gorini-Kossakowski-Sudarshan-Lindblad master equation with time independent decay rate g [45,46]. The chosen correlation function can emerge from a microscopic model where the driven two level system is placed inside a leaky cavity near absolute zero temperature such that thermal excitations can be neglected. When the bath correlation time is short, Eq. (4) is approximately true [11]. Within this

approximation the NMQSD equation takes the following form:

$$\partial_t|\psi_t(z^*)\rangle = -iH_S|\psi_t(z^*)\rangle + z_t^*\sigma_-|\psi_t(z^*)\rangle - F(t)\sigma_+\sigma_-|\psi_t(z^*)\rangle, \tag{24}$$

with $\alpha(t,s) = \langle z_t z_s^*\rangle$ being the only nonzero correlation of the complex noise. Then the average state obeys the following master equation:

$$\partial_t\rho = -i\left[\frac{\omega}{2}\sigma_z + \frac{\Omega}{2}\sigma_x + s(t)\sigma_+\sigma_-,\rho\right] + 2\gamma(t)\sigma_-\rho\sigma_+ - \gamma(t)\{\sigma_+\sigma_-,\rho\}, \tag{25}$$

where $\gamma(t) + is(t) = F(t)$. The LNMQJ unraveling (25), in turn, is

$$d|\psi\rangle = -iG(t)|\psi\rangle dt + \sum_{k=1}^{4}\varepsilon\xi_k\sigma_-|\psi\rangle dM_+^k(t) - \sum_{k=1}^{4}\varepsilon\xi_k\sigma_-|\psi\rangle dM_-^k(t), \tag{26}$$

where $\xi_1 = 1$, $\xi_2 = -1$, $\xi_3 = i$, $\xi_4 = -i$, and $G(t) = [H_S - iF(t)]\sigma_+\sigma_-$. The statistics of the Poisson increments are $\mathsf{E}[dM_+^k] = [\gamma_+(t)/2\varepsilon^2]dt$ and $\mathsf{E}[dM_-^k] = \{P[(\mathbb{1} - \varepsilon\xi_k\sigma_-)\psi, t]\}/\{P[\psi, t]\}[\gamma_-(t)/2\varepsilon^2]dt$. Subsequently, the diffusive limit of the LNMQJ process corresponding to the NMQD process for this system can be written as

$$d|\psi\rangle = \left(-iG(t) + 2\gamma_-(t)\langle\psi|\sigma_+|0\rangle\frac{\partial \ln P[\psi,t]}{\partial\psi_0^*}\sigma_-\right)|\psi\rangle dt + \sigma_-|\psi\rangle(dZ_+ - dZ_-), \tag{27}$$

where zero mean complex noises satisfy the Ito rules $dZ_\pm dZ_\pm^* = \gamma_\pm(t)dt$ and $dZ_\pm dZ_\pm = dZ_\mp dZ_\pm^* = 0$. We consider the following parameters in all of the numerical examples $\omega/\Gamma = 2$, $\omega_c/\Gamma = 5.5$, $\Omega/\Gamma = 0.5$, $g = 0.8$ and we plot all dynamical quantities as a function of the dimensionless time Γt. The decay rate $\gamma(t)$ is temporarily negative when $\frac{1}{2} < \Gamma t < 3/2$ for these parameter values. Figure 2 shows a good agreement between the master equation solution and its unravelings. However, we also solved the dynamics exactly using the HOPS approach to NMQSD [12,13]. The minor disagreement shows that the approximations leading to the master equation (25) are fairly consistent with the chosen parameters. Therefore, a word of caution is in place here; within the master equation approach, the quality of the obtained equation is extremely hard to assess [47]. In the bottom panel, we also show examples of single trajectories with LNMQJ for different values of ϵ. The purpose is to demonstrate the agreement of

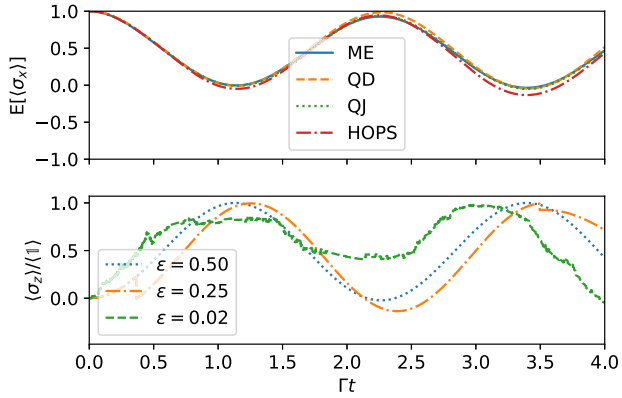

FIG. 2. Top: Ensemble average over 3000 stochastic trajectories of $\langle\sigma_x\rangle$ computed with LNMQJ (dotted), NMQD (dashed) with $\varepsilon = \frac{1}{2}$, and HOPS (dash dotted) with comparison to the master equation solution (ME). HOPS is a numerically exact method and the reasonable agreement shows that the approximations leading to the master equation being unraveled are fairly consistent with the chosen parameters. Bottom: Normalized expectation value for σ_z along a single stochastic trajectory for different values of ε using LNMQJ. The initial state is $|+\rangle = \sqrt{1/2}(|0\rangle + |1\rangle)$.

the ensemble averages with the master equation solution—and that with our new methodological results, even driven systems can be very easily handled with the jump method whenever a reliable master equation is available.

Conclusions.—We have provided a connection between quantum state diffusion and quantum jumps in the non-Markovian regime. As a by-product of these investigations we introduced a linear version of the non-Markovian quantum jumps method and a new type of unraveling which we call non-Markovian quantum diffusion. We combined the non-Markovian quantum jumps and non-Markovian quantum diffusion with kernel smoothing techniques thus extending the applicability of these methods dramatically. Moreover, we also demonstrated the power of our approach with the paradigmatic amplitude damped driven two-level atom model.

When taking the diffusive limit the expectation value of Poisson increments in Eq. (12) are proportional to ε^{-2}. This means that for any finite value of ε, the time step size dt must be adjusted in such a way that "jumps" remain rare events, i.e., $\mathsf{E}[dM_\pm^k] \ll 1$. Most relaxed conditions under which quantum trajectories, either diffusive or piecewise deterministic type, have time a continuous measurement interpretation is currently under active investigation. For recent results on jump type unravelings for P-divisible dynamics; see Ref. [48] and for diffusive trajectories, see Ref. [49].

As an outlook, in addition to applying the methods for various state-of-the art complex driven open quantum systems, it would be interesting to investigate, e.g., what role the stochastic entropy term in non-Markovian quantum diffusion plays in quantum stochastic thermodynamics.

Furthermore, it would be interesting to study the existence of a continuous measurement interpretation for the proposed unravelings in the light of recent results in Refs. [48,49].

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[1] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[2] R. Gutiérrez, C. Simonelli, M. Archimi, F. Castellucci, E. Arimondo, D. Ciampini, M. Marcuzzi, I. Lesanovsky, and O. Morsch, Phys. Rev. A **96**, 041602(R) (2017).
[3] J. T. Barreiro, M. Müller, P. Schindler, D. Nigg, T. Monz, M. Chwalla, M. Hennrich, C. F. Roos, P. Zoller, and R. Blatt, Nature (London) **470**, 486 (2011).
[4] M. Müller, K. Hammerer, Y. L. Zhou, C. F. Roos, and P. Zoller, New J. Phys. **13**, 085007 (2011).
[5] P. M. Harrington, D. Tan, M. Naghiloo, and K. W. Murch, Phys. Rev. Lett. **123**, 020502 (2019).
[6] G. S. Engel, T. R. Calhoun, E. L. Read, T.-K. Ahn, T. Mancal, Y.-C. Cheng, R. E. Blankenship, and G. R. Fleming, Nature (London) **446**, 782 (2007).
[7] H. Lee, Y.-C. Cheng, and G. R. Fleming, Science **316**, 1462 (2007).
[8] T. Brixner, R. Hildner, J. Köhler, C. Lambert, and F. Würthner, Adv. Energy Mater. **7**, 1700236 (2017).
[9] L. Diósi, N. Gisin, and W. T. Strunz, Phys. Rev. A **58**, 1699 (1998).
[10] W. T. Strunz, L. Diósi, and N. Gisin, Phys. Rev. Lett. **82**, 1801 (1999).
[11] T. Yu, L. Diósi, N. Gisin, and W. T. Strunz, Phys. Rev. A **60**, 91 (1999).
[12] D. Suess, A. Eisfeld, and W. T. Strunz, Phys. Rev. Lett. **113**, 150403 (2014).
[13] R. Hartmann and W. T. Strunz, J. Chem. Theory Comput. **13**, 5834 (2017).
[14] J. Roden, A. Eisfeld, W. Wolff, and W. T. Strunz, Phys. Rev. Lett. **103**, 058301 (2009).
[15] G. Ritschel, J. Roden, W. T. Strunz, A. Aspuru-Guzik, and A. Eisfeld, J. Phys. Chem. Lett. **2**, 2912 (2011).
[16] V. Abramavicius and D. Abramavicius, J. Chem. Phys. **140**, 065103 (2014).
[17] X. Gao and A. Eisfeld, J. Chem. Phys. **150**, 234115 (2019).
[18] X. Zhong and Y. Zhao, J. Chem. Phys. **138**, 014111 (2013).
[19] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
[20] J. Piilo, S. Maniscalco, K. Härkönen, and K.-A. Suominen, Phys. Rev. Lett. **100**, 180402 (2008).
[21] J. Piilo, K. Härkönen, S. Maniscalco, and K.-A. Suominen, Phys. Rev. A **79**, 062112 (2009).
[22] K. Härkönen, J. Phys. A **43**, 065302 (2010).
[23] Q. Ai, Y.-J. Fan, B.-Y. Jin, and Y.-C. Cheng, New J. Phys. **16**, 053033 (2014).
[24] M.-J. Tao, Q. Ai, F.-G. Deng, and Y.-C. Cheng, Sci. Rep. **6**, 27535 (2016).
[25] P. Rebentrost, R. Chakraborty, and A. Aspuru-Guzik, J. Chem. Phys. **131**, 184102 (2009).
[26] S. A. Oh, D. F. Coker, and D. A. W. Hutchinson, J. Chem. Phys. **150**, 085102 (2019).
[27] N. Renaud and F. C. Grozema, J. Phys. Chem. Lett. **6**, 360 (2015).
[28] H.-P. Breuer and F. Petruccione, Phys. Rev. Lett. **74**, 3788 (1995).
[29] S. Ghosh, *Kernel Smoothing: Principles, Methods and Applications* (Wiley, Hoboken, 2018).
[30] D. Chruscinski and A. Jamiolkowski, *Geometric Phases in Classical and Quantum Mechanics*, Progress in Mathematical Physics (Birkhäuser, Boston, 2004).
[31] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.125.150403 for further information, various mathematical details, proofs and derivations, which includes Refs. [32–35].
[32] P. Busch, P. Lahti, J.-P. Pellonpää, and K. Ylinen, *Quantum Measurement*, 1st ed. (Springer Publishing Company, Inc., Switzerland, 2016).
[33] L. P. Hughston, R. Jozsa, and W. K. Wootters, Phys. Lett. A **183**, 14 (1993).
[34] I. Bengtsson and K. Życzkowski, *Geometry of Quantum States: An Introduction to Quantum Entanglement* (Cambridge University Press, Cambridge, England, 2006).
[35] V. Klyatskin, *Lectures on Dynamics of Stochastic Systems*, Elsevier Insights (Elsevier Science, Amsterdam, 2010).
[36] V. Link and W. T. Strunz, Phys. Rev. Lett. **119**, 180401 (2017).
[37] H. Risken, *The Fokker-Planck Equation: Methods of Solution and Applications*, Springer Series in Synergetics (Springer Berlin Heidelberg, Berlin, Heidelberg, 2012).
[38] C. Gardiner, *Stochastic Methods: A Handbook for the Natural and Social Sciences*, Springer Series in Synergetics (Springer, Berlin, Heidelberg, 2009).
[39] We demand that at time $t = 0$ all of the decay rates $\gamma_k(t)$ have to be non-negative.
[40] We consider a NMQJ unraveling with multiple decay channels and Poisson processes since we anticipate that we will need at least two real valued Poisson processes to obtain one complex valued process in the diffusive limit.
[41] $L_l^{-1} = \sum_{j=0}^{\infty}(-1\xi_l\varepsilon)^j L^j = \mathbb{1} - \varepsilon\xi_l L + \mathcal{O}(\varepsilon^2)$, when $||\varepsilon L|| < 1$.
[42] For the computation we use the results of Ref. [31] to compute the determinant, to expand the probability density, to expand a rational polynomial, and choose $\xi_k = e^{i(\pi/m)(k-1)}$ with $m \geq 2$.
[43] C. Pellegrini and F. Petruccione, J. Math. Phys. (N.Y.) **50**, 122101 (2009).
[44] U. Seifert, Phys. Rev. Lett. **95**, 040602 (2005).
[45] V. Gorini, A. Kossakowski, and E. C. G. Sudarshan, J. Math. Phys. (N.Y.) **17**, 821 (1976).
[46] G. Lindblad, Commun. Math. Phys. **48**, 119 (1976).
[47] HOPS with hierarchy order 1 corresponds closely to the level of approximation we make when using and unraveling the master equation with respect to exact dynamics. In Fig. 2 we have truncated the hierarchy after 8 levels.
[48] A. Smirne, M. Caiaffa, and J. Piilo, Phys. Rev. Lett. **124**, 190402 (2020).
[49] N. Megier, W. T. Strunz, and K. Luoma, arXiv:1912.08662.