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.

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 \[1\], non-equilibrium phase transitions in a Rydberg gas has 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 type 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 time scale, 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 unravelled, 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 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

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

where the creation- and annihilation operators $a_\lambda^\dagger$ and $a_\lambda$ of a bath mode labeled by $\lambda$ satisfy the bosonic commutation relations $[a_\lambda, a_\mu^\dagger] = \delta_{\lambda\mu}$. We assume that the coupling operator $L$ is traceless, i.e. $\text{tr} \{L\} = 0$. In a projective Hilbert space $\mathcal{H}$, each point is associated with a projector $|\psi\rangle \langle \psi|$. Given a separable Hilbert space, coordinates $\psi_i \in \mathbb{C}$ on a $\mathcal{H}$ can be easily constructed with respect to a fixed orthonormal basis as $|\psi\rangle = \sum_i \psi_i |i\rangle$. For more information on $\mathcal{H}$, see the Supplementary Material \[31\].
Non-Markovian quantum state diffusion.— Reduced system dynamics can be represented exactly for a large class of models, even beyond Eq. (1), with the following linear non-Markovian quantum state diffusion (NMQSD) equation

$$\dot{\psi}(t, z^*) = -i H_S(t) + \sum_{z} L_z |\psi(t, z^*)\rangle - L^\dagger \int_0^t ds \alpha(t-s) \frac{\delta |\psi(t, z^*)\rangle}{\delta z^*_t}.$$  

(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. NMQSD is driven by a complex valued colored Gaussian noise $z^*_t$, completely characterized by the correlations

$$M[z_t z^*_s] = \alpha(t-s), \quad M[z_t^2] = M[z_t z_s] = 0,$$

(3)

where $M[\cdot]$ 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

$$\frac{\delta}{\delta z^*_t} |\psi(z^*, t)\rangle = F(t, s) |\psi(z^*, t)\rangle.$$  

(4)

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

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

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

(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

$$P_Q[\psi, t] = M[\delta(\psi - \psi(z^*, t))]$$  

(6)

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

$$\partial_t P_Q[\psi, t] = \sum_{k=1}^d \partial_{\psi_k} c_k(\psi) P_Q[\psi, t] + \partial_{\psi^*_k} c_k^*(\psi) P_Q[\psi, t]$$

$$+ \sum_{k,l=1}^d \partial^2_{\psi_k \psi^*_l} k_{kl}(\psi) P_Q[\psi, t].$$  

(7)

where the drift and diffusion coefficients are $c_k(\psi) = \langle k | (-iH - F(t)L^\dagger L)|\psi\rangle$ and $d_{kl}(\psi) = \langle F(t) + F^*(t) \rangle \langle k | L|\psi\rangle \langle\psi| L^\dagger |l\rangle$ respectively. NMQSD thus corresponds to a second order Kramers-Moyal expansion in $P(\mathcal{H})$ [33]. If the diffusion coefficient $F(t) + F^*(t) = 2\gamma(t)$ is not negative for any time $t$ the KME2 equation is, in fact, a proper Fokker-Planck equation [34].

Non-Markovian Quantum Jumps.— Master equations of the form

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

(8)

can be unravelled with non-Markovian quantum jumps (NMQJ) [20, 22, 35]. 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

$$d\psi = -iG(t)|\psi\rangle dt + \sum_k (L_k - 1)|\psi\rangle dN_k^+(t)$$

$$+ \int d\psi'(\langle|\psi'\rangle - |\psi\rangle) dN_{\psi'(t)}^-$$(9)

where $G(t) = H_S(t) + \sum_k s_k(t)L^\dagger_k L_k - i\gamma_k(t)L^\dagger_k L_k - 1$. Increments of the Poisson processes, $dN^+_k(t)$ and $dN^-_{\psi(t)}(t)$, are mutually independent $dN^+_k(t) dN^+_l(t) = \delta_{kl} dN^+_k(t)$, $dN^+_k(t) dN^-_{\psi(t)}(t) = \delta_{kl} dN^-_{\psi(t)}(t)$ and $dN^-_{\psi(t)}(t) dN^+_l(t) = 0$. The mean values of the increments are $\mathbb{E}[dN^+_k(t)] = 2\gamma_k(t) dt$ and $\mathbb{E}[dN^-_{\psi(t)}(t)] = 2\gamma_{\psi(t)}(t) d\psi(t)$, where $\gamma_k(t) = \gamma_k(t) - \gamma_{\psi(t)}(t)$. 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 $\psi$ to a target state $\psi'$ via channel $k$ when $\gamma_k(t) < 0$. In particular, a “reverse jump” can
occur from $\psi$ to $\psi'$ 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 \cite{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. (8) is equivalent to Eq. (9) with $2m(1 \leq k \leq 2m)$ time dependent rates and time independent jump operators defined as

$$s_k(t) = \frac{s(t)}{2m|\xi_k|\varepsilon^2},\quad \gamma_k(t) = \frac{\gamma(t)}{2m|\xi_k|\varepsilon^2},$$

$$L_k = 1 + \varepsilon\xi_kL, \text{ s.t. } \varepsilon\xi_k + \xi_{k+m} = 0,$$ (10)

where $\xi_k \in \mathbb{C}$, $|\xi_k| = |\xi|$ and $\varepsilon > 0$. The deterministic part $G(t)$ of the quantum jump process in Eq. (9) transforms under $|\xi_k| \rightarrow |\xi_k| + \varepsilon\xi_kL$, s.t. $|\xi_k| + \xi_{k+m} = 0$, and $\Theta(t)$ is the ratio in the probability for these jumps which still depends on each other. The quantum memory effects are contained in the probability for these jumps which still depends on the ratio $P[L_k^{-1}|\psi\rangle\langle\psi|,t]/P[\psi,t]$. The quantum memory effects are contained in the probability for these jumps which still depends on the ratio $P[L_k^{-1}|\psi\rangle\langle\psi|,t]/P[\psi,t]$.

**LNMQJ in projective Hilbert space.**—In the projective Hilbert space LNMQJ corresponds to the following Liouville master equation \cite{22}

$$\partial_t P[\psi,t] = i \sum_k \partial_{\xi_k} \left( (k|G(t)|\psi) P[\psi,t] \right)$$

$$- \partial_{\xi_k} \left( (\psi|G^t(t)|k) P[\psi,t] \right)$$

$$+ \int d\phi \left( R[\phi|\psi]P[\phi,t] - R[\phi|\psi]P[\psi,t] \right),$$ (13)

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

$$R[\phi|\psi] = \sum_{k=1}^{2m} \frac{\gamma_k(t)}{m\varepsilon^2|\xi_k|^2} \delta(\phi - L_k\psi)$$

$$+ \frac{\gamma_2(t)}{m\varepsilon^2|\xi_k|^2} \delta(\psi - L_k\phi).$$ (14)

When comparing the drift terms in Fokker-Planck equation \cite{1} and in the Liouville master equation \cite{13}, we see that they are equal. The jump part takes the form $\int d\phi (\partial_{\xi_k} R[\phi|\psi]P[\phi,t] - R[\phi|\psi]P[\psi,t]) = \sum_{k=1}^{2m} \frac{\gamma_k(t)}{m\varepsilon^2|\xi_k|^2} F_k - \frac{\gamma_2(t)}{m\varepsilon^2|\xi_k|^2} P[\psi,t]$, where

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

After expanding $F_k[\psi]$ to second order in $\varepsilon$ and assuming $m > 2$ we find $\int d\phi (\partial_{\xi_k} R[\phi|\psi]P[\phi,t] - R[\phi|\psi]P[\psi,t]) = \sum_{k,l=0} d \partial_{\xi_k} \partial_{\xi_l} (2\gamma_k(t)|k|L|\psi\rangle\langle\psi|L^t|l\rangle P[\psi,t], while $\varepsilon \rightarrow 0$. \cite{37}. We thus have proven the validity of the part LME $\varepsilon \rightarrow 0$ 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 Supplement \cite{31}. First, Eq. (12) is expanded to first order in $\varepsilon$, resulting in

$$|d\psi| = -iG(t)|\psi\rangle dt + \sum_k \left( (L_k - \mathbb{1})|\psi_t\rangle dM^k(t) \right.$$ \n
$$+ (L_k^{-1} - \mathbb{1})|\psi_t\rangle dM^k(t),$$ (12)

with mutually independent Poisson increments $dM^k_t$ with statistics $E[dM^k(t)] = \frac{\gamma_k(t)}{m\varepsilon^2|\xi_k|^2} dt$ and $E[dM^k(t)] = P[L_k^{-1}|\psi\rangle d\xi_k] = \frac{\gamma_k(t)}{m\varepsilon^2|\xi_k|^2} dt$, 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 \cite{5} (see Sec. S. IV of the \cite{5}).

It is worth noticing 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 \cite{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 $P[L_k^{-1}|\psi\rangle\langle\psi|,t]/P[\psi,t]$. It is worth noticing 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 \cite{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 $P[L_k^{-1}|\psi\rangle\langle\psi|,t]/P[\psi,t]$.
The average evolution of NMQD equation (18) corresponds to Eq. [8] as we show in the Supplement [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 which contributes to the deterministic evolution [39].

Kernel smoothing.— A Gaussian kernel $K$ is defined

$$K[\psi] = \frac{1}{\sqrt{\pi d + 1}} e^{-||\psi||^2}, \quad \psi \in \mathbb{C}^{d+1}. \quad (20)$$

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

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

where $\sigma > 0$ is a free parameter. A rule of thumb for choosing the variance is that $\sigma = M^{\frac{1}{d+1}}$ [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

$$\frac{\partial \ln P_\sigma[\psi]}{\partial \psi^*_n} = -\frac{\sum_{\nu=1}^M e^{-||\psi_n - \psi^\nu_n\rangle^2/\sigma^2}}{\sum_{\nu=1}^M e^{-||\psi_n - \psi^\nu_n\rangle^2/\sigma^2}} - \frac{\psi_n - \langle \psi_n \rangle}{\sigma^2}, \quad (22)$$

where average $\langle \rangle$ is taken with respect to distribution

$$P_\sigma[\psi] = \frac{1}{\sqrt{\pi d + 1}} e^{-||\psi||^2/\sigma^2}, \quad \text{with} \quad Z = \sum_{\nu=1}^M e^{-||\psi_n - \psi^\nu_n||^2}. \quad (23)$$

Kernel estimation can be also used to evaluate the ratios $P_\sigma[\psi]/P_\sigma[\psi^\nu]$ and $P_\sigma[\psi]/P_\sigma[\psi^\nu]$. 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 $H_S = \frac{1}{2} \sigma_z + \frac{1}{2} \sigma_x$ 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

$$\alpha(t, s) = g \frac{\Gamma}{2} e^{-\gamma(t-s)} + \Gamma|t-s|, \quad (23)$$

where $\gamma$ is the inverse of the bath correlation time $\gamma = \Gamma^{-1}$, $\omega_c$ 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 $g$ [10] [11]. 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

$$\partial_t |\psi(t)|^2 = -i H_S |\psi(t)|^2 + z_4^* \sigma_- |\psi(t)|^2 - F(t) \sigma_+ \sigma_- |\psi(t)|^2, \quad (24)$$

with $\alpha(t, s) = \langle z(t)z(s) \rangle$ being the only non-zero correlation of the complex noise. Then the average obeys the following master equation

$$\partial_t \rho = -i\omega_c \sigma_z + \Omega \sigma_x + s(t) \sigma_+ \sigma_\rho + 2\gamma(t) \sigma_+ \rho \sigma_- - \gamma(t) \{ \sigma_+ \sigma_- \}, \quad (25)$$

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

$$d|\psi\rangle = -iG(t)|\psi\rangle dt + \sum_{k=1}^4 \epsilon_\eta_k \sigma_- |\psi\rangle dM^k_+(t)$$

$$- \sum_{k=1}^4 \epsilon_\xi_k \sigma_+ |\psi\rangle dM^k_-(t), \quad (26)$$

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 $E[dM^k_+] = \frac{\gamma(t)}{2 \epsilon_\eta_k} dt$ and $E[dM^k_-] = \frac{\gamma(t)}{2 \epsilon_\xi_k} dt$. Subsequently, the diffusive limit of LNMQJ process corresponding to the NMQD process for this system can be written as

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

$$+ \sigma_- |\psi\rangle (dZ_+ - dZ_-), \quad (27)$$

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

$$+ \sigma_- |\psi\rangle (dZ_+ - dZ_-), \quad (27)$$
where zero mean complex noises satisfy the Ito rules
\[
d Z_\pm(t) = \gamma \pm (t) dt \quad \text{and} \quad d Z_\pm(t) d Z_\mp(t) = 0.
\]

We consider the following parameters in all of the numerical examples
\[
\omega/\Gamma = 2, \quad \Omega/\Gamma = 5.5, \quad \Omega/\Gamma = 0.5, \quad \sigma = 0.25
\]
and we plot all dynamical quantities as a function of the dimensionless
time \(\Gamma t\). The decay rate \(\gamma(t)\) is temporarily negative when \(\frac{1}{2} < \Gamma t < \frac{3}{2}\) 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\(^{[12]}\). The small disagreement shows that the approximations leading to the master equation being
not fully 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\(^{[42]}\). In the bottom panel, we also show examples of single trajectories with LNMQJ
for different values of \(\epsilon\) using LNMQJ.

**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. As an
outlook, in addition of 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 diff-
dusion plays in quantum stochastic thermodynamics.

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[42] HOPS with hierarchy order 1 corresponds closely to the level of approximation we make when using- and unravelling the master quation with respect to exact dynamics. In Fig. 2 we have truncated the hierarchy after 8 levels.