Quantum Trajectories for Time-Local Non-Lindblad Master Equations

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For the efficient simulation of open quantum systems, we often use quantum jump trajectories given by pure states that evolve stochastically to unravel the dynamics of the underlying master equation. In the Markovian regime, when the dynamics is described by a Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) master equation, this procedure is known as Monte Carlo wave function approach. However, beyond ultraweak system-bath coupling, the dynamics of the system is not described by an equation of GKSL type, but rather by the Redfield equation, which can be brought into pseudo-Lindblad form. Here, negative dissipation strengths prohibit the conventional approach. To overcome this problem, we propose a pseudo-Lindblad quantum trajectory (PLQT) unraveling. It does not require an effective extension of the state space, like other approaches, except for the addition of a single classical bit. We test the PLQT for the eternal non-Markovian master equation for a single qubit and an interacting Fermi-Hubbard chain coupled to a thermal bath and discuss its computational effort compared to solving the full master equation.

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Introduction.—Away from thermodynamic equilibrium, the properties of an open quantum system do not simply follow from the fundamental principles of statistical mechanics, but depend on the very details of the surrounding environment. This includes both transient dynamics, as the algorithm of a quantum computer or the relaxation following a quantum quench, and nonequilibrium steady states. Therefore, it is crucial to find an effective equation of motion for the open system that accurately captures the impact of the environment. At the same time, and equally important, the theoretical description should allow for efficient numerical simulations. A powerful approach for the latter is quantum trajectory simulations, where a stochastic process for the evolution of pure states is considered, the ensemble average of which describes the open system. Compared to the evolution of the full density operator (scaling quadratically with the state-space dimension D), these simulations require less memory, since pure states scale only linearly with D. Moreover, such unravelings can also directly describe stochastic processes of measured systems [1–3].

Quantum trajectory simulations are rather straightforward in the ultraweak-coupling limit, where the system-bath coupling is weak compared to the (quasi)energy level splitting in the system. In this case, the system is described by a master equation of GKSL (Gorini-Kossakowski-Sudarshan-Lindblad) form [4,5] ($\hbar = 1$),

$$\dot{\varrho} = -i[H, \varrho] + \sum_i \gamma_i \left(L_i \varrho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \varrho\} \right), \quad (1)$$

with the coherent evolution captured by some Hamiltonian H and dissipation described by jump operators L_i with associated non-negative strengths γ_i. Here, H, γ_i, and L_i can be time dependent.

From this equation, we can immediately obtain a stochastic process for the evolution of pure states known as the Monte Carlo wave function (MCWF) approach [6–13]. In each time step δt, the state either evolves coherently according to $|\psi(t+\delta t)\rangle \propto [1 - i\delta t H_{\text{eff}}(t)]|\psi(t)\rangle$ with probability $1 - \sum_i r_i(t)\delta t$ and effective Hamiltonian

$$H_{\text{eff}}(t) = H - \frac{i}{2}\sum_i \gamma_i L_i^\dagger L_i, \quad (2)$$

or a quantum jump occurs, $|\psi(t+\delta t)\rangle \propto L_i|\psi(t)\rangle$, with probability $r_i(t)\delta t$, with jump rates $r_i(t) = \gamma_i \langle\psi(t)|L_i^\dagger L_i|\psi(t)\rangle$. The state of the system is then given (or approximated) by the ensemble average $\rho(t) = \overline{|\psi(t)\rangle\langle\psi(t)|}$ over an infinitely (or sufficiently) large number N of trajectories $|\psi_n(t)\rangle$, where $\bar{X} \equiv (1/N)\sum_{n=1}^N X_n$.

However, the assumption of ultraweak coupling is questionable in various situations, for instance, in large systems, with small finite-size gaps and tiny avoided crossings between many-body states, as well as in Floquet systems with driving frequency ω, where the average quasienergy level spacing is ω/D [14].

Beyond ultraweak coupling, master equations in pseudo-Lindblad form can be found, which look like a GKSL master equation, Eq. (1), except for the fact that the coefficients γ_i also take negative values. For instance, the Redfield equation obtained in (Floquet-)Born-Markov approximation can be brought to this form [15]. Generally, negative relaxation strengths are relevant for non-Markovian dynamics [16], stochastic Hamiltonians with non-Markovian noise [17], gauge transformed Lindbladians [18], and exact

master equations [19–21]. These negative values are incompatible with the conventional MCWF, since the probability $r_i(t)\delta t$ for a quantum jump would become negative. To overcome this problem, different quantum jump unravelings have been formulated, which, however, require significantly more computational resources [22–30]. In many approaches, the system's state space needs to be extended, so that its dimensionality at least doubles [22–26,31–33]. For oscillating strengths between positive and negative values, moreover, an alternative non-Markovian quantum jump method (NMQJ) has been proposed in which jump processes are inverted [27–29,34]. This method does not work if $\gamma_i < 0$ for all times and does not admit independent (i.e., parallel) evaluation of trajectories. For nonoscillatory strengths, the rate operator quantum jump approach can be applied [30]; however, it requires a rather costly diagonalization of a state-dependent operator in every time step of the evolution. A generalization of the non-Markovian jump method to many-body systems has been proposed in Ref. [35] and can be used to study measurement-induced phase transitions.

In this Letter, we propose pseudo-Lindblad quantum trajectories (PLQTs), which work for arbitrary γ_i, where the trajectories evolve independently and which does not require the doubling of state space. In the following, this is realized by extending the system's state space in a minimal (and for the memory requirement of simulations, practically irrelevant) fashion by a single classical bit $s \in \{-1, +1\}$, $|\psi(t)\rangle \to \{|\psi(t)\rangle, s(t)\}$.

Algorithm.—To unravel the dynamics of a pseudo-Lindblad quantum master equation by quantum trajectories $\{|\psi(t)\rangle, s(t)\}$, first choose a time step δt, which is sufficiently short for the first-order time integration, and jump rates $r_i(t) > 0$ for each jump operator L_i (to be specified below). Within one time step, a quantum jump occurs described by

$$|\psi^{(i)}(t+\delta t)\rangle = \frac{\sqrt{|\gamma_i|}L_i|\psi(t)\rangle}{\sqrt{r_i(t)}},$$
$$s^{(i)}(t+\delta t) = \frac{\gamma_i}{|\gamma_i|}s(t), \tag{3}$$

with probability $r_i(t)\delta t$ or, alternatively, with the remaining probability $1 - \sum_i r_i(t)\delta t$ the state evolves coherently, with H_{eff} [Eq. (2)] [36]

$$|\psi^{(0)}(t+\delta t)\rangle = \frac{[1 - i\delta t H_{\text{eff}}(t)]|\psi(t)\rangle}{\sqrt{1 - \delta t \sum_i r_i(t)}}, \tag{4}$$

$$s^{(0)}(t+\delta t) = s(t). \tag{5}$$

We now show that the ensemble of pure states obtained by this PLQT approach converges to the correct density operator solving Eq. (1),

$$\varrho(t) = \overline{s(t)|\psi(t)\rangle\langle\psi(t)|}. \tag{6}$$

For a pure initial state $\sigma(t) = s(t)|\psi(t)\rangle\langle\psi(t)|$, on average the update scheme is the weighted sum of the processes described above:

$$\overline{\sigma(t+\delta t)} = \sum_i r_i(t)\delta t \sigma^{(i)}(t+\delta t) + \left(1 - \sum_i r_i(t)\delta t\right)\sigma^{(0)}(t+\delta t), \tag{7}$$

with $\sigma^{(i)} = s^{(i)}|\psi^{(i)}\rangle\langle\psi^{(i)}|$ and $\sigma^{(0)} = s^{(0)}|\psi^{(0)}\rangle\langle\psi^{(0)}|$. By inserting Eqs. (3) and (4), the jump rates $r_i(t)$ cancel out, and one arrives at

$$\overline{\sigma(t+\delta t)} = \sigma(t) + \delta t\left(\sum_i \gamma_i L_i \sigma(t) L_i^\dagger - iH_{\text{eff}}(t)\sigma(t) + i\sigma(t)H_{\text{eff}}(t)^\dagger\right), \tag{8}$$

almost corresponding to the action of the master Eq. (1). The final step to arrive at Eq. (1) is to average Eq. (8) also over an ensemble of pure states at time t, so that $\overline{\sigma(t+\delta)} \to \varrho(t+\delta t)$ and $\sigma(t) \to \varrho(t)$. As will be discussed below, one consequence of the presence of negative weights $\gamma_i < 0$ is that individual wave functions $|\psi_n\rangle$ are not normalized. As a result, the ensemble-averaged trace is preserved only in the limit $N \to \infty$ of an infinite ensemble [37]. Therefore, in a finite ensemble, one obtains better convergence by explicit normalization $\varrho_N = (1/\mathcal{N})\sum_n^N s_n|\psi_n\rangle\langle\psi_n|$, with $\mathcal{N} = \sum_n^N s_n\langle\psi_n|\psi_n\rangle$ at every time t. A rigorous proof of our algorithm using the Ito formalism is outlined in the Supplemental Material [38]. In case that all γ_i are positive, the sign bits do not change, and the algorithm corresponds to the conventional MCWF approach.

Note that recently, another unraveling of non-Lindblad master equations was also proposed in Ref. [39]. It is different from our approach, but also involves an effective classical degree of freedom given by a real number of constant average, rather than our single bit, whose average is time dependent, as will be seen below.

For the PLQT approach, as for other unraveling schemes [23], the jump rates $r_i(t) > 0$ can, in principle, be chosen arbitrarily. In practice, there is, however, a trade-off. Whereas for too small rates r_i, large ensembles of trajectories are required to sample each jump process i sufficiently, we also have to require that the probability $1 - \sum_i r_i\delta t$ remains positive and large enough for the given time step δt. A typical choice is [13]

$$r_i(t) = |\gamma_i|\frac{\||L_i|\psi(t)\rangle\|^2}{\||\psi(t)\rangle\|^2}, \tag{9}$$

for which the quantum jump does not alter the norm $\||\psi\rangle\| \equiv \langle\psi|\psi\rangle^{1/2}$ of the state, i.e., $\||\psi^{(i)}(t+\delta t)\rangle\| = \||\psi(t+\delta t)\rangle\|$. Note, however, that for $\gamma_i < 0$ this choice implies that the norm increases during the coherent

time evolution with $H_{\rm eff}$, $\||\psi^{(0)}(t+\delta t)\rangle\| = [1+\delta t \sum_{\gamma_i<0} r_i(t)]\||\psi(t)\rangle\|$ [40]. This is not the case for the conventional MCWF approach, where $\gamma_i \geq 0$.

Non-Markovian dephasing for a single qubit.—As a proof of principle, we implement the PLQT algorithm for a qubit subjected to purely dissipative dynamics,

$$\dot{\varrho}(t) = \frac{1}{2}[\mathcal{L}_x + \mathcal{L}_y - \tanh(t)\mathcal{L}_z]\varrho(t), \tag{10}$$

with GKSL channels $\mathcal{L}_i\varrho = \sigma_i\varrho\sigma_i - \varrho$, where σ_i are Pauli operators, with $\sigma_i^\dagger\sigma_i = \sigma_i^2 = 1$. This equation is known as the eternal non-Markovian master equation [16,41]. The existence of a negative relaxation rate makes it inaccessible to the standard MCWF, while also the NMQJ approach fails, since $-\tanh(t) < 0$ for all t. However, for this model the PLQT approach is easily implemented and, because the jump operators are unitary, the jump rates are state independent; i.e., $\|\sigma_i|\psi(t)\rangle\|^2 = \||\psi(t)\rangle\|^2$ leads to a simplification in Eq. (9), and one has $r_x = r_y = 1/2$, $r_z(t) = \tanh(t)/2$. Also, the effective Hamiltonian $H_{\rm eff} = -(i/2)[1-\tanh(t)/2]$ entering Eq. (4) is not state dependent (since it is proportional to the identity).

On average, the sign follows the rate equation $\dot{\overline{s(t)}} = -2r_z(t)\overline{s(t)}$, which is solved by $\overline{s(t)} = 1/\cosh(t)$, as shown in Fig. 1(c) [38]. Quantum jumps are realized in the Bloch-vector representation by reflections at the y-z plane and x-z plane for σ_x and σ_y, respectively [Fig. 1(d)]. The σ_z quantum jump is a reflection at the x-y plane and, due to the negative relaxation strength, the sign flip is accounted for by an additional point reflection at the origin.

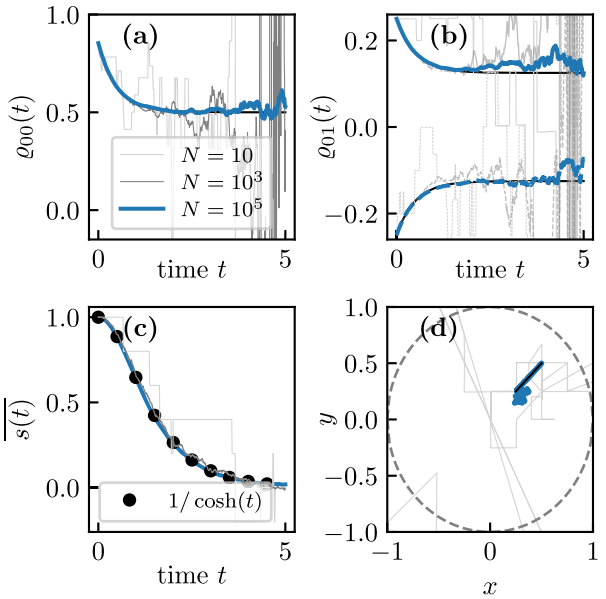

FIG. 1. Non-Markovian dynamics [Eq. (10)] for density matrix elements ϱ_{00} (a), $\mathrm{Re}\varrho_{01}$ (solid), $\mathrm{Im}\varrho_{01}$ (dashed) (b), and the Bloch vector in the x-y plane (d). Analytical solution (black) and unraveling with $N = 10^5$ PLQTs with time step $\delta t = 0.01$ in blue ($N = 10, 10^3$ in thin and intermediate gray lines) for an initial Bloch state with $\phi = \Theta = \pi/4$. (c) shows the averaged sign bit.

By simulating $N = 10^5$ trajectories in Figs. 1(a) and 1(b), we obtain accurate results for the transient dynamics until, at $t_R \sim 2$, the system reaches the steady state regime. Besides this physical relaxation time, we also find an *algorithmic* relaxation time $t_A \sim 4$, at which the number of negative and positive trajectories become equal, and the averaged sign decays to zero [Fig. 1(c)]. Beyond this algorithmic relaxation time, fluctuations are typically increased [Figs. 1(a) and 1(b)]. This effect can be understood by noting that a stochastic process of a real variable x_n with positive mean $\bar{x}$ will have bounded fluctuations $\Delta x = \overline{(x-\bar{x})^2}^{-1/2} \leq \bar{x}$ as long as $x_n > 0$, whereas Δx is not bounded, when x_n can also take negative values. Thus, ideally, t_A should be large compared to the time span of the simulation (which is t_R, if we are interested in computing the steady state). The algorithmic relaxation time is determined by the inverse sign-flip rate $r_{\rm SF} = \sum_{i,\gamma_i<0} r_i$, e.g., $t_A = r_{\rm neg}^{-1}$ for time-independent $r_{\rm SF}$. Thus, we can increase t_A simply by lowering the strengths for negative processes with weights $\gamma_i < 0$ relative to positive ones with $\gamma_i > 0$. However, this will also increase the number of trajectories needed for properly sampling those negative-weight processes. Thus, before doing this, one should first attempt to rewrite the master equation, so that the relative weight of negative processes is reduced. This can be done for pseudo-Lindblad equations derived from the Redfield equation [15], as we will recapitulate now.

Redfield dynamics.—For a microscopic model, a master equation is often derived within the Born-Markov-Redfield formalism [42,43]. We consider a system-bath Hamiltonian of the form $H_{\rm tot} = H + \sum_i S_i \otimes B_i + H_i$ with system Hamiltonian H that couples to individual baths H_i where S_i and B_i denote the system and bath coupling operators, respectively. The Redfield equation can then be written in pseudo-Lindblad form [15]

$$\dot{\varrho} = -i[H + H^{\rm LS}, \varrho] + \sum_{i,\sigma=\pm} \sigma\left(L_{i\sigma}\varrho L_{i\sigma}^\dagger - \frac{1}{2}\{L_{i\sigma}^\dagger L_{i\sigma}, \varrho\}\right), \tag{11}$$

with Lamb-shift Hamiltonian $H^{\rm LS} = (1/2i)\sum_i S_i\mathbb{S}_i + \mathrm{H.c.}$, convolution operators $\mathbb{S}_i = \int_0^\infty d\tau \langle B(\tau)B\rangle e^{iH\tau}S_i e^{-iH\tau}$, and Lindblad-like jump operators

$$L_{i\sigma} = \frac{1}{\sqrt{2}}\left[\lambda_i(t)S_i + \sigma\frac{1}{\lambda_i(t)}\mathbb{S}_i\right], \tag{12}$$

with arbitrary, time-dependent real parameters $\lambda_i(t)$. We see that due to the negative relaxation rates with $\sigma = -1$, the Redfield equation is generally not of GKSL form unless further approximations are employed in the limit of ultraweak coupling [42–44] or for high bath temperatures [15,45]. For a purely Ohmic bath, the choice [15]

$$\lambda_{i,\mathrm{glob}}(t)^2 = \sqrt{\frac{\mathrm{tr}\mathbb{S}_i^\dagger \mathbb{S}_i}{\mathrm{tr}S_i S_i}} \tag{13}$$

minimizes the norm of the negative channels in the pseudo-Lindblad equation globally, i.e., on average for all states. A further reduction of negative processes can be achieved by state-dependent optimization. Namely, according to Eq. (9), where (assuming, without loss of generality, a normalized state) the rates for negative quantum jumps with L_{i-} are given by $r_{i-}(t;\lambda_i(t)) = \frac{1}{2}(\lambda_i(t)^2\||S_i|\psi(t)\rangle\|^2 + [1/\lambda_i(t)^2]\||\mathbb{S}_i|\psi(t)\rangle\|^2 - 2\mathrm{Re}\langle\psi(t)|S_i\mathbb{S}_i|\psi(t)\rangle)$. Thus, the choice

$$\lambda_{i,\mathrm{loc}}(t)^2 = \frac{\||\mathbb{S}_i|\psi(t)\rangle\|}{\||S_i|\psi(t)\rangle\|} \tag{14}$$

minimizes the rates for negative quantum jumps in the unraveling of the Redfield equation. Since the states in the numerator and the denominator of Eq. (14) have to be evaluated for evolving the state anyway, this local optimization (which is not described in Ref. [15]) can be implemented efficiently.

We test our method using state-dependent minimization Eq. (14) for the extended Hubbard chain of spinless fermions,

$$H = -J\sum_{\ell=0}^{M-1}\left(a_\ell^\dagger a_{\ell+1} + a_{\ell+1}^\dagger a_\ell\right) + V\sum_{\ell=0}^{M-1} a_\ell^\dagger a_\ell a_{\ell+1}^\dagger a_{\ell+1}, \tag{15}$$

with fermionic operators a_ℓ, tunneling strength J, and nearest-neighbor interaction strength V. For the dissipator, we have

$$\langle n|\mathbb{S}_\ell|m\rangle = \frac{J(\Delta_{nm})}{e^{\Delta_{nm}/T}-1}\langle n|S_\ell|m\rangle, \tag{16}$$

with system operator $S_\ell = a_\ell^\dagger a_\ell$, level splitting $\Delta_{nm} = E_n - E_m$, and bath temperature T. We consider a purely Ohmic bath, with spectral density $J(E) = \gamma E$ and coupling strength γ.

In Fig. 2, we depict the decay of the interaction energy for an initial state in which pairs of adjacent sites are occupied $|\psi(0)\rangle = |011011\ldots\rangle$. Quench dynamics for such a charge density wave in a spin polarized Fermi-Hubbard model have been recently observed experimentally by Bakr and coworkers [46]. We assume strong interactions $V/J = 7$ for which the doublon pairs can only be broken when the system exchanges energy with the bath. This leads to a decay of the energy of the open system as depicted in Fig. 2(a), where the transient oscillations are well reproduced.

Numerical implementation.—Let us now discuss the numerical implementation of the PLQT approach. Since

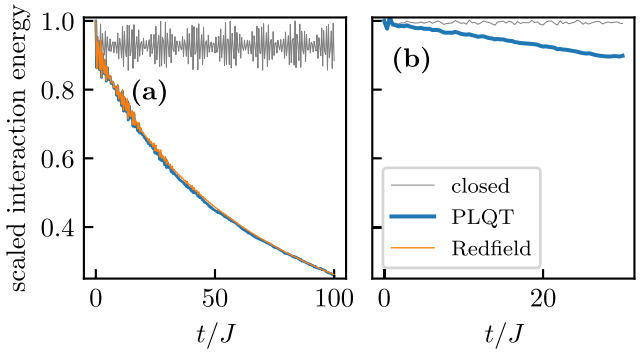

FIG. 2. Dynamics of scaled interaction energy of extended Hubbard chain of two (eight) particles on four (13) sites (a) [(b)] with $V/J = 7$. We compare the dynamics of the isolated (gray line) and open system with $\gamma/J = 0.02$ and $T/J = 1$ (blue line for PLQT, thin orange for Redfield equation). The decrease of interactions is related to bath-induced doublon-breaking processes.

the trajectories are independent, we run them in parallel. Depending on the physical quantity of interest, let us say observable A, it is often reasonable not to store the actual time-dependent state as large vectors with complex entries, but rather expectation values $\langle\psi_n(t)|A|\psi_n(t)\rangle$ together with the norm $\|\psi_n(t)\|$ and the sign $s_n(t)$. While the storage of the trajectory data boils down to a few real numbers, the time evolution requires the full state vector. The memory needed for the time integration of a quantum trajectory would grow linear with the state-space dimension D, if not only the Hamiltonian, but also the jump operators were sparse. The latter is the case, however, mainly in phenomenological master equations with local jump operators and not for the Redfield equation, so that the memory needed usually scales like D^2. The memory needed for integrating the Redfield equation scales equally like D^2 (since it is sufficient to store and apply the jump operators rather than the full superoperator). Nevertheless, we find that the memory requirement for quantum trajectories to be much lower than that for integrating the master equation. In Fig. 3, the required memory [Figs. 3(a) and 3(b)] and single-time-step run-time [Figs. 3(c) and 3(d)] is compared for solving the full Redfield master equation (blue) and a single trajectory (red). We find that the required memory is noticeably reduced for the quantum trajectory simulation, even though, as discussed above, it still scales like D^2. (The latter is not specific to our approach, but generically the case also for other forms of quantum trajectory simulations). For the run-time, the relative reduction is even stronger and shows different scaling with D. Essentially, the difference is two matrix-matrix products needed for the Redfield integration and one matrix-vector product for the PLQTs. Note that the unraveling can also be combined with matrix-product states (e.g., [47,48]). It is interesting to see how far such an approach would compare to a representation of the density operator by matrix-product operators (e.g., Refs. [49,50]).

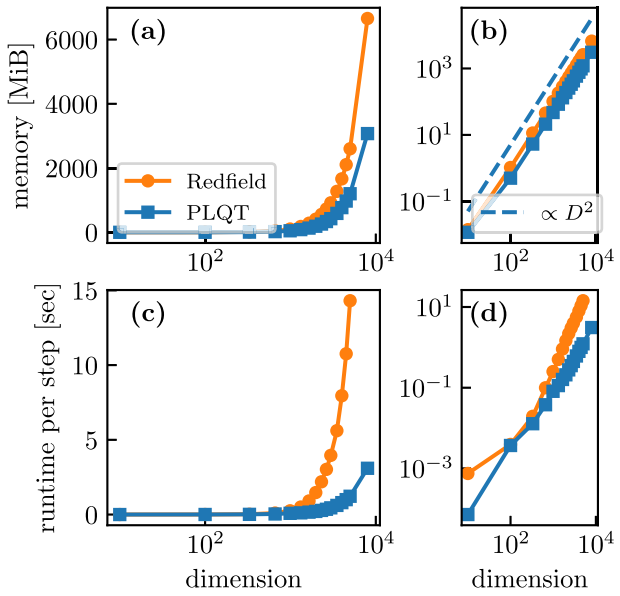

FIG. 3. Required memory [(a) linear scale, (b) logarithmic scale] versus Hilbert-space dimension in logarithmic scale and single-time-step run-time [(c) linear scale, (d) logarithmic scale] versus Hilbert-space dimension in logarithmic scale for both a single trajectory (blue) and the Redfield master equation (red). The data were obtained for an Intel Core i9-10900 processor with up to 5.2 GHz.

Finally, we would like to mention that while finalizing this manuscript, a new approach for microscopically deriving accurate local quantum master equations was proposed [51]. It is a very promising perspective to apply the PLQT to this equation, which can be broad into pseudo-Lindblad form [51]. Namely, it will give rise to equations of motion involving spars matrices for Hamiltonian and jump operators only. As a result, the overall memory requirement will scale linearly with the Hilbert-space dimension D only. Moreover, this could allow for efficient matrix-product-state approaches for individual trajectories.

Conclusion.—We have developed an efficient unraveling of master equations of pseudo-Lindblad form, which includes the Redfield equation as an important case [15]. Different from previous approaches, it requires a minimal extension of the state space by one classical sign bit only, it is applicable also for dissipation strengths that are always negative, it does not require matrix diagonalization during the time integration, and it allows for a parallel implementation, since all trajectories are independent of each other. We believe that it will be a useful tool for the simulation of open many-body systems beyond ultraweak system-bath coupling. In future work, it will be interesting to systematically investigate the impact of negative dissipation strengths γ_i on the required ensemble size and the optimal choice of the corresponding rates for efficient simulation. Moreover, our algorithm should be compared to the influence-martingale approach [39]. Finally, the combination of PLQT simulations with the recently derived local quantum master equation [51] opens a promising route for the efficient simulation of open many-body quantum systems.

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[37] The fluctuations of the trace and their dependence on N are shown in Fig. 1 of the Supplemental Material [38] for an explicit example.

[38] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.131.160401 where we provide a proof of the PLQT algorithm using the Ito formalism, discuss the impact of the choice of rates on the norm of the states, and derive an equation of motion for the averaged sign bit.

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