Quantifying the accuracy of steady states obtained from the Universal Lindblad Equation

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We show that steady-state expectation values predicted by the universal Lindblad equation (ULE) are accurate up to bounded corrections that scale linearly with the effective system-bath coupling, \(\Gamma\) (second order in the microscopic coupling). We also identify a near-identity, quasilocal “memory-dressing” transformation, used during the derivation of the ULE, whose inverse can be applied to achieve relative deviations of observables that generically scale to zero with \(\Gamma\), even for nonequilibrium currents whose steady-state values themselves scale to zero with \(\Gamma\). This result provides a solution to recently identified limitations on the accuracy of Lindblad equations, which highlighted a potential for significant relative errors in currents of conserved quantities. The transformation we identify allows for high-fidelity computation of currents in the weak-coupling regime, ensuring thermodynamic consistency and local conservation laws, while retaining the stability and physicality of a Lindblad-form master equation.

The theoretical description of open quantum systems is an important problem in many fields of physics. While early groundwork was laid in the context of quantum optics and physical chemistry \([1, 6]\), recent advances in the control of complex quantum systems necessitate the development of new theoretical techniques \([7, 20]\).

In this work we focus on the broadly relevant Markovian regime which emerges for weak system-bath coupling relative to the intrinsic energy scales of the baths. In this context, Lindblad equations play a key role by providing the most general form of Markovian evolution that is guaranteed to preserve the physicality of solutions \([21, 22]\). Formulating incoherent evolution in terms of randomly timed “quantum jumps,” Lindblad equations provide valuable physical insight and admit stable and relatively efficient numerical solutions via stochastic evolution of wave functions (rather than density matrices) \([23, 24]\). The latter feature allows Lindblad equations to be solved for systems of greater complexity than accessible with other approaches.

Historically, routes to deriving Lindblad equations from the evolution of a system coupled with its environment have relied on a rotating wave approximation (RWA), which assumes the spectral gaps of the system to be larger than any decoherence rate \([3, 9]\). While typically justified in the traditional contexts of quantum optics, the RWA is often not valid for complex quantum systems emerging in many fields of interest such as hybrid quantum systems \([25]\), nonequilibrium many-body systems \([26]\), and platforms for large-scale quantum simulation and information processing \([27, 28]\).

Recently, several independent works discovered routes to circumvent the RWA \([8, 13, 15, 17, 19, 29]\), opening up many of the problems above for efficient study with Lindblad equations \([8, 10, 12, 29]\). Particular applications include, e.g., bath-induced localization in driven many-body systems \([30]\), modelling of qubit readout experiments \([31, 32]\) and elucidating the conditions of validity for the Landau-Lifshitz-Gilbert equation \([33]\). In this work, we focus on the “Universal Lindblad Equation” (ULE), which was derived in Ref. \([14]\) with rigorous bounds on approximation-induced errors; the bounds are controlled by the product of a characteristic effective system-bath coupling strength \(\Gamma\) (which is second-order in the microscopic system-bath coupling matrix elements), and a bath correlation time, \(\tau\) [see Eq. \((6)\)].

In parallel with the advances above, several groups recently explored the nontrivial tradeoffs of studying...
non-equilibrium quantum systems with Lindblad equations. Even away from equilibrium, an open quantum system, e.g., as depicted in Fig. 1(a), generically converges to a unique non-equilibrium steady state, as schematically depicted for some given observable $O$ by the dashed black curve in Fig. 1(b). The authors of Ref. [34] showed that the steady state of any Lindblad equation must deviate from the exact steady state by a correction linear in the effective system-bath coupling [the green curve in Fig. 1(b) depicts the flow of $\mathcal{O}$ predicted by the ULE]. While the steady state of a Lindblad equation can approach the exact steady state in the weak-coupling limit, non-equilibrium currents such as, e.g., particle or heat currents, scale linearly with system-bath coupling. Consequently, their relative deviations generically remain finite as the coupling is taken to zero. This can lead to apparent violations of the second law of thermodynamics [8, 19] and local conservation laws [34].

To enable further progress in the field, here we quantify the fidelity of steady states resulting from the ULE, and demonstrate how the apparent inconsistencies above can be resolved. In Sec. [II] we summarize our main results. In Sec. [II] we review the problem addressed by our work: quantifying the accuracy of steady states of the ULE. In Sec. [II] we revisit the derivation and key features of the ULE relevant for the problem. In Sec. [IV] we present our solution via rigorous bounds on the deviations of observables computed with the ULE steady state compared with those obtained from the exact steady state. In Sec. [V] we demonstrate our results in numerical simulations of magnon transport in a spin chain. We conclude with a discussion in Sec. [VI]. Details of derivations and supplemental data are provided in Appendices.

I. SUMMARY OF MAIN RESULTS

We report two main results, summarized in Fig. 1(c):

1. First, we show that in the limit $\Gamma \tau \rightarrow 0$ the ULE faithfully captures the steady-state values of generic observables in absolute scale: for a generic observable, the steady-state value predicted by the ULE deviates from the true steady-state value by an amount that scales to zero with $\Gamma \tau$ [Eq. (15)].

2. Second, we demonstrate that steady-state expectation values with vanishing relative deviations in the limit $\Gamma \tau \rightarrow 0$ can be obtained by applying the inverse of a quasilocal, near-identity “memory-dressing” transformation that was employed to obtain the ULE [14] [see Eqs. (10) and (12) below]. The transformation only affects observables with support near regions connected to baths. This result enables the computation of accurate and thermodynamically-consistent nonequilibrium currents which obey local conservation laws. Our analysis is supported by numerical simulations (Fig. 2).

Before embarking on the technical discussion, we offer a few clarifying remarks about the nature of our results. As a Lindblad equation, the ULE provides a stable, positivity preserving map for the evolution of an open system’s density matrix. The ULE can therefore be used to study the trajectories and steady states of open quantum systems, by going to the long-time limit. After the positivity-preserving evolution or corresponding steady state is computed from the ULE, the inverse of the memory dressing transformation can be applied to remove some of the deviation between the steady-state solution of the ULE and the exact steady state of the system. The previously identified trade-offs or apparent limitations of Lindblad equations [34] are resolved by the fact that the inverse of the memory dressing transformation breaks the positivity of the density matrix in a small and controlled way, bounded by $\Gamma \tau$, which brings it and associated observables closer to their true values. Since the transformation is applied after the evolution, the stability of the Lindblad evolution and applicability of quantum trajectory approaches are retained.

We also emphasize that the role of the memory dressing transformation can often be neglected: it is only required for computing nonequilibrium currents or other quantities whose steady-state values vanish in absolute terms in the weak-coupling limit (i.e., not for quantities whose expectation values remain finite). Moreover, as we demonstrate below, even for observables with vanishing steady-state values in the weak-coupling limit, the memory dressing transformation is only needed if their support lies close to points of contact with baths.

II. FORMULATION OF PROBLEM

We consider a quantum system with Hamiltonian $H_S$, where one or more degrees of freedom $\{X_\alpha\}$ are coupled to degrees of freedom in the surrounding environment, or “bath,” $\{B_\alpha\}$, such as, e.g., photonic or phononic modes, or creation/annihilation operators of particles in attached reservoirs [see Fig. 1(a)]. The environment can, e.g., consist of several baths out of mutual equilibrium, where different subsets of $\{B_\alpha\}$ act on distinct baths. The combined system has Hamiltonian

$$H_{SB} = H_S + H_B + \sqrt{\gamma} \sum_{\alpha=1}^{N} X_\alpha B_\alpha,$$  \hspace{1cm} (1)  

where $H_B$ is the Hamiltonian of the bath, and we introduced $\gamma$ as a redundant energy scale parameterizing the system-bath coupling strength. We take each $X_\alpha$ to have unit spectral norm and take the environment to be in a state where each $B_\alpha$ has expectation value zero $\mathbb{E}[\{B_\alpha\}].$  

We consider the broadly relevant case where the environment is Gaussian (e.g., comprised of free bosonic or fermionic modes). A Gaussian environment is fully characterized by its two-point correlation function $J_{\alpha\beta}(t) = \mathbb{E}[X_\alpha(t) X_\beta(t)]$.  

\langle B_\alpha(t) B_\beta(0) \rangle \text{ with } B_\alpha(t) \equiv e^{iH_S t} B_\alpha e^{-iH_S t}. \text{ Our discussion considers two additional objects which equivalently encode the properties of the environment: the bath spectral function, } J_{\alpha\beta}(\omega) \equiv \int \frac{d\epsilon}{2\pi} e^{-i\omega \epsilon} J_{\alpha\beta}(\epsilon), \text{ and the "jump correlator" } g_{\alpha\beta}(t) = \int d\omega e^{-i\omega t} \sqrt{\mathcal{J}(\omega)/2\pi} |_{\alpha\beta}, \text{ with } \sqrt{\cdot} \text{ denoting the matrix square root.}

Observables of the system are determined by the reduced density matrix
\[ \rho(t) = \text{Tr}_B[\rho_{SB}(t)]. \] (2)
Here \( \rho_{SB}(t) \) denotes the exact density matrix of the combined system, whose evolution is described by \( \partial_t \rho_{SB}(t) = -i[H_S, \rho_{SB}(t)] \). For thermodynamically large environments, \( \rho(t) \) generically goes to a unique steady state in the long-time limit regardless of the initial state of the system, \( \rho_0 \) \[ \rho_{\text{exact}} \equiv \lim_{t \to \infty} \rho(t). \] (3)

Away from equilibrium, \( \bar{\rho}_{\text{exact}} \) depends on the details of the environment and the system-bath coupling. Such nonequilibrium steady states can be found by establishing approximate equations of motion for \( \rho(t) \) and seeking their steady state solutions.

In the regime where the effective system-bath coupling is small relative to the inverse correlation time of the bath, it was recently shown that the system’s evolution is well-described by the ULE \[ \partial_t \rho \approx i[\rho, H_S + H_{\text{LS}}] + \sum_{\alpha=1}^{N} \left\{ L_\alpha \rho L_\alpha^\dagger - \frac{1}{2} \{ L_\alpha^\dagger L_\alpha, \rho \} \right\}, \] (4)
with \( L_\alpha = \sum_{m\beta} \sqrt{2\pi\gamma} J(E_m - E_\beta)|\alpha\beta\rangle\langle m|X_\beta|n\rangle \) with \( H_{S}[n] = E_m[n] \). The Hermitian Lamb shift \( H_{\text{LS}} \) effectively renormalizes \( H_S \); its form is given in Ref. \[ \xi_\beta(t) \equiv \text{e}^{-\gamma t} \mathcal{L}_{\text{LS}}[\rho]. \] (5)
Our goal is to characterize the fidelity of the steady state of the ULE,
\[ \tilde{\rho}_{\text{ULE}} \equiv \lim_{t \to \infty} \text{e}^{t\mathcal{L}_{\text{ULE}}}[\rho_0]. \] (6)
Here \( \mathcal{L}_{\text{ULE}} \) denotes the ULE Liouvillian, whose action on an arbitrary density matrix \( \rho \) is given by the right-hand side of Eq. \[ \mathcal{L}_{\text{ULE}}[\rho] = \mathcal{L}_{\text{BR}}[\rho] + \xi(\rho) \text{.} \] (7)
We provide an explicit expression for \( \mathcal{V} \) in Eq. \[ \rho' = \mathcal{V}[\rho]. \] (8)
We first review the key features of the ULE \[ \mathcal{V} \] below. By design, \( \mathcal{V} \) preserves the Hermiticity and trace of \( \rho \) and satisfies \( -i[\mathcal{V}, H_S] = \mathcal{L}_{\text{ULE}}[\rho] - \mathcal{L}_{\text{BR}}[\rho] \). Evaluating \( \partial_t \rho' \) gives
\[ \partial_t \rho' = \mathcal{L}_{\text{BR}}[\rho'] + \xi(t), \] (9)
where the residual \( \xi(t) \) satisfies \( \| \xi(t) \| \leq 2\Gamma^2 \tau \). The ULE is obtained by neglecting \( \xi(t) \), which is subleading in \( \Gamma \tau \), since \( \mathcal{L}_{\text{ULE}} \) consists of terms of order \( \Gamma \) and \( \Gamma^2 \).
Ref. \[ \mathcal{L}_{\text{BR}} \] showed that \( \| \mathcal{V} - 1 \| \leq \Gamma \tau \), where \( \| \mathcal{A} \|_{SO} = \text{sup}_O\| \mathcal{A}(O) \|/\|O\| \). As a result, \( \rho \) and \( \rho' \) nearly coincide when \( \Gamma \tau \ll 1 \):
\[ \| \rho' - \rho \| \leq \Gamma \tau \]. (10)
Note that both \( \| \rho - \rho' \| \ll 1 \) and \( \xi \) are negligible in the limit \( \Gamma \tau \ll 1 \). In this sense, the ULE is accurate when \( \Gamma \tau \ll 1 \).

**B. Memory-dressing transformation**

The transformation to the memory-dressed frame, \( \mathcal{V} \), is given by \[ \delta \mathcal{V}[\rho] = \gamma \int_{-\infty}^{\infty} dt' dt \left[ \mathcal{X}_\alpha(t), \rho \mathcal{X}_\beta(t') \right] f_{\alpha\beta}(t, t') + \text{h.c.}, \] (11)
where \( \mathcal{X}_\alpha(t) = \mathcal{E}_{H_S} X_\alpha e^{-iH_S t} \). The indices \( \alpha \) and \( \beta \) are implicitly summed over, and \( f_{\alpha\beta}(t, t') \equiv \sum_s \int ds g_{\alpha\beta}^s(t - s, t') \theta(t - t') \theta(t) \theta(t - s) \). In App. \[ \text{we provide alternative expressions for } \mathcal{V} \text{ in terms of the eigenstates of } H_S, \text{ and via an iterative expansion.} \]
Whereas the standard Markov approximation made en route to the Bloch-Redfield equation \[ \text{amounts to approximating the density matrix as constant within the brief window of nonzero bath-correlations, passing to} \]
the memory-dressed frame effectively incorporates a more intricate averaging of the density matrix over the window of decaying correlations in the bath.
The memory frame transformation $V$ can be shown to induce $O(\Gamma \tau)$ corrections to $\rho$, and can thus typically be ignored in the limit $\Gamma \tau \ll 1$ \cite{14}. However, the corrections are relevant for observables whose steady-state values scale with $\Gamma$, such as nonequilibrium currents. We demonstrate below how to obtain negligible relative errors of these quantities by applying the inverse of the memory dressing transformation to the ULE steady state, i.e., by computing their expectation values with the operator $V^{-1}\{\bar{\rho}_{\text{ULE}}\}$. Using $\|V\|_{\infty} \leq \Gamma \tau$, Taylor expansion yields $V^{-1} = 1 - \delta V + \delta^{(2)} V$, where, for $\Gamma \tau < 1$, $\|\delta^{(2)} V\|_{\infty} \leq (\Gamma \tau)^2/(1 - \Gamma \tau)$. Importantly, $V$ only affects observables with support near regions connected to baths: firstly, the integrand defining $f_{n,\beta}$ below Eq. (10) is nonzero only for $t > 0$, $s < 0$ and vice versa. For a bath with a smooth spectral function (i.e., finite memory), $g(t)$ decays to zero for large $t$ \cite{13} with a characteristic decay time $\tau_\rho$. Hence, $f(t, t')$ also decays with a characteristic timescale of order $\tau_\rho$ for large $|t|$ or $|t'|$. Moreover, $\hat{X}_\alpha(t)$ only has support within a distance $v_{\text{LR}} t$ from the support of $X_\alpha$, where $v_{\text{LR}}$ denotes the system’s Lieb-Robinson velocity. Thus, $V$ only significantly affects operators with support within a distance $\ell_V \sim v_{\text{LR}} \tau_\rho$ from regions connected to baths.

IV. FIDELITY OF ULE STEADY STATE OBSERVABLES

Here we bound the differences between the exact steady-state value of a given observable, and the steady-state values resulting from the ULE with and without accounting for the memory-dressing transformation. In the following, we will use $\langle O \rangle_{\text{exact}}$ and $\langle O \rangle_{\text{ULE}}$ to denote expectation values of the observable $O$ in the exact steady-state and the ULE steady state, respectively:

$$\langle O \rangle_{\text{exact}} = \text{Tr}[\bar{\rho}_{\text{exact}} O], \quad \langle O \rangle_{\text{ULE}} = \text{Tr}[\bar{\rho}_{\text{ULE}} O].$$  

To facilitate the comparison, we first translate $\langle O \rangle_{\text{exact}}$ to the memory-dressed frame via $\langle O \rangle_{\text{exact}} = \text{Tr}[O^* \bar{\rho}_{\text{exact}}']$, where $\bar{\rho}_{\text{exact}}' = V\bar{\rho}_{\text{exact}} V^*$, and \cite{10}

$$O' \equiv V^{-1}\{O\}. \quad (12)$$

Next, by setting $\partial_t \rho' = 0$ in Eq. (8), note that

$$\bar{\rho}_{\text{exact}}' = \bar{\rho}_{\text{ULE}} + \mathcal{L}_{\text{ULE}}^{-1}\{\bar{\xi}\}, \quad (13)$$

where $\bar{\xi} = \lim_{t \to \infty} \xi(t)$; see Appendix B for derivation. Combining these results with $\|\xi\| \leq 2t\tau_\rho$, we conclude

$$\langle (O')_{\text{ULE}} - \langle O \rangle_{\text{exact}} \rangle \leq C_\Omega \Gamma \tau \| (O')_{\text{ULE}} \| \quad (14)$$

where $C_\Omega = 2t\|\mathcal{L}_{\text{ULE}}^{-1}\{O' - \langle O \rangle_{\text{ULE}}\}\|/(\| (O')_{\text{ULE}} \|)$. Crucially, as we show in Appendix D \cite{10}, $C_\Omega$ is finite for generic $O$, and remains so as $\Gamma \to 0$, including for currents whose steady-state values scale to zero with $\Gamma$ \cite{14}. Thus, the relative deviation of $\langle (O')_{\text{ULE}} \rangle = \text{Tr}[V^{-1}\{\bar{\rho}_{\text{ULE}}\} O]$ generically vanishes in the limit $\Gamma \tau \ll 1$.

The transformation to the memory-dressed frame can typically be neglected if $O$ has a finite steady-state value in the limit $\Gamma \tau \ll 1$. Specifically, using Eq. (14) along with $\| (O')_{\text{ULE}} - \langle O \rangle_{\text{ULE}} \| \leq \Gamma \tau / \| (O')_{\text{ULE}} \|$ (where $\| \cdot \|_2$ denotes the maximal singular value norm) \cite{42} gives

$$\langle (O')_{\text{ULE}} - \langle O \rangle_{\text{exact}} \rangle \leq C_\Omega \Gamma \tau \| (O')_{\text{ULE}} \| \Gamma + C_\Omega \Gamma^2 \tau^2 \| (O)_{\text{ULE}} \|_2. \quad (15)$$

The right hand side of Eq. (15) scales to zero when $\Gamma \tau \to 0$, implying that the absolute deviation of $\langle O \rangle_{\text{ULE}}$ vanishes in this limit. The magnitude of the correction from the memory-dressing transformation (second term above) moreover decays to zero with the distance from $O$ to the bath, over the characteristic scale $\ell_V$, due to the quasi-locality of $V$. Thus, in the weak-coupling limit, the correction from $V$ is only relevant if $\lim_{n \to 0} O = 0$ and $O$ has support within a distance $\ell_V$ from regions connected to baths.

Equations (14) and (15) are our main results: Eq. (15) demonstrates that steady-state expectation values of observables computed from the ULE have vanishing absolute deviations from their exact counterparts in the weak-coupling limit. Equation (14) shows that ULE steady-state observables are guaranteed to have vanishing relative deviations when the transformation to the memory-dressed frame is accounted for by using the memory-dressed observable, $\langle O \rangle_{\text{ULE}} = \text{Tr}[\bar{\rho}_{\text{ULE}} O']$, rather than the bare observable, $\langle O \rangle_{\text{ULE}} = \text{Tr}[\bar{\rho}_{\text{ULE}} O]$. We emphasize that the bounds in Eqs. (14) and (15) are loose, and define “worst case” deviations. We expect that actual deviations can often be much smaller.

V. NUMERICAL DEMONSTRATION

We demonstrate our results in simulations of magnon transport in a spin chain. We consider a spin of 9 sites with Hamiltonian $H_S = \sum_{n=1}^9 g(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z) + \sum_{n=1}^9 h_n \sigma_n^z$, where $\sigma_\alpha$ is the $\alpha = \{x, y, z\}$ Pauli operator on spin $n$; the same model was studied in Ref. \cite{34}. We couple $\sigma_1^z$ and $\sigma_9^z$ to two Gaussian baths through the terms $\sqrt{\sigma_1^z} B_1 + \sqrt{\sigma_9^z} B_2$. The baths are Ohmic, with temperatures $T_1$ and $T_2$. The bath spectral function reads $J_{\alpha \beta}(\omega) = \delta_{\alpha \beta} \omega \varepsilon - \omega^2/\lambda^2$ $n_B(\omega/k_B T_n)$, with $\delta_{\alpha \beta}$ the Kronecker delta, $\omega \varepsilon$ a normalizing frequency, $\lambda$ a high-frequency cutoff, $n_B$ the Bose-Einstein distribution, and $k_B$ the Boltzmann constant. We simulate the model with $k_B T_1 = g, k_B T_2 = g_2, \Delta = 1.4g, \Lambda = 8g$, and $h_n = g/2(n - 5)g$, describing a uniform field gradient.

The system’s spectrum, $\{E_m - E_n\}$, has mean adjacent-value spacing 4.9 $\times 10^{-3} g$, while the mean decay rate prescribed by Fermi’s golden rule is given by $2\pi \gamma \sum_{n,m=1}^D |J_1(E_m - E_n)| n(\sigma_1^z |m\rangle)^2 + |J_2(E_m - E_n)| (|n\sigma_1^z |m\rangle)^2 \approx 23\gamma$, where $D = 2^9$ is the system’s Hilbert space dimension. The commonly used Davies equation \cite{5, 43} (based on the RWA) is thus expected...
to be valid when $\gamma \ll 2.2 \cdot 10^{-6} g$. On the other hand, explicit calculation shows $\Gamma \gamma \approx 31 \gamma / g$, implying that the approximations leading to the ULE are justified when $\gamma \ll 0.06 g$.

Microscopically, the magnon current on the bond from site $n$ to site $n+1$ is given by $I_{n+1,n} = \langle 4i g \sigma_{n+1}^z \sigma_n^+ + \text{h.c.} \rangle$. Since the exact evolution of the combined system yields $\partial_t \sigma_{n}^z = I_{n,n-1} - I_{n+1,n}$ for $1 < n < 9$, $\langle I_{n,n+1} \rangle_{\text{exact}}$ must be uniform throughout the system. On the other hand, $\langle I_{n+1,n} \rangle_{\text{ULE}}$ may be non-uniform near the baths, because the quasilocal Lamb shift and jump operators of the ULE modify the equation of motion for $\sigma_n^z(t)$. Non-trivially, Eq. (14) predicts that the dressed bond currents, $\langle I_{n,n+1} \rangle_{\text{ULE}}$, are homogeneous throughout the system, up to relative deviations that scale to zero with $\gamma$. This feature thus serves as a consistency check of our analysis and indicator of the fidelity of the bond currents obtained with the ULE.

Fig. 2(a) shows the steady state values of $\langle I_{n+1,n} \rangle_{\text{ULE}}$ and $\langle I_{n+1,n} \rangle_{\text{exact}}$, obtained for $\gamma = 10^{-3} g$. Near-identical data are found for all probed values of $\gamma$ smaller than $10^{-2} g$. Evidently, the bare currents exhibit significant non-uniformities near the ends of the chain, while the dressed currents are nearly uniform. These deviations are consistent with expected subleading $O(\gamma^2)$ corrections: in Fig. 2(b), we show the $\gamma$-scaling of the standard deviations of the bare and dressed current. While the standard deviation of the bare currents scales linearly with $\gamma$, that of the dressed currents scales quadratically with $\gamma$. Deep in the bulk, the bare and dressed bond currents in Fig. 2(a) are near-identical, indicating that the memory dressing transformation only affects observables in vicinities of baths. In Appendix D we provide data confirming that the memory dressing transformation is not needed to accurately capture the expectation values of $\{\sigma_n^z\}$, which remain finite when $\gamma \to 0$.

We finally bound the deviation of the magnon current predicted by the ULE via Eq. (14). We obtain $C_{1,2} \approx 1300$ for multiple values of $\gamma$ between $10^{-5} g$ and $10^{-2} g$ (indicating that $\lim_{\gamma \to 0} C_{1,2}$ is finite), and $\Gamma \gamma \approx 31 \gamma / g$.

Hence the current predicted by the ULE is guaranteed to be accurate (have relative deviation much smaller than 1) when $\gamma \ll 2.5 \cdot 10^{-5} g$. We expect $\langle I_{1,2} \rangle_{\text{ULE}}$ to be accurate for values of $\gamma$ above this rigorous, but loose, bound: the standard deviation of the dressed bond currents is of order $1\%$ even for $\gamma \approx 10^{-2} g$ [see Fig. 2(b)], suggesting that the corrected ULE observables may remain accurate up to this value.

VI. DISCUSSION

In this work, we established upper bounds on the steady-state deviations of observables computed from the ULE. Our analysis revealed two results: (1) We demonstrated that the ULE yields accurate steady-state values of observables in the weak-coupling limit, in absolute terms, and (2) we showed that accurate steady-state values in relative terms can be achieved by applying a near-identity, quasilocal memory-dressing transformation to the observables in question [Eqs. (7)-(10)]. The transformation is only needed for current-like observables with support close to regions connected to baths.

Even for situations where the memory-dressing transformation is needed, the advantageous characteristics of the ULE remain intact. The transformation is only applied after evolving the system with the ULE until it reaches its steady state. When applied, the transformation only induces a small, bounded correction to the state or observables. As a result, the procedure remains stable and solvable with stochastic evolution methods (and is hence parallelizable and efficient). The residual deviations are comparable to those expected for the Bloch-Redfield equation (BRE), while avoiding the potential instabilities of the BRE and enabling the use of efficient computational schemes as mentioned above (see, e.g., Ref. [16], where extensive benchmarking was recently performed for a dissipative harmonic oscillator, albeit without the memory-dressing transformation.)

Our results facilitate accurate computation of nonequilibrium currents in the weak-coupling limit via Lindblad equations, ensuring thermodynamic consistency and local conservation laws. Thereby, we demonstrated how to overcome the fundamental limitations intrinsic to any Lindblad equation that were pointed out in Refs. [19][34]. Important future directions will be to obtain tighter error bounds and to extend the proven regime of validity of the ULE, e.g., by formulating conditions in terms of the spectral range of the system [15]. Other interesting directions involve extending our bounds on steady-state deviations to driven quantum systems, and exploring routes to computing nonequilibrium currents which circumvent the memory dressing transformation. More broadly, our results enable systematic studies of mixed coherent/incoherent evolution in complex quantum systems, relevant, e.g., for characterizing coherences in noisy devices for quantum information processing.

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Appendix A: Expressions for $\mathcal{V}$

Here we provide an explicit expression for the superoperator $\delta \mathcal{V}$ which enters in the memory dressing transformation. We first show how $\delta \mathcal{V}$ in Eq. (10) is obtained from the corresponding expression given in Ref. [14]. Subsequently (for cases with time-independent Hamiltonians) we provide complementary expressions for $\delta \mathcal{V}$ in terms of the eigenbasis of the Hamiltonian (Sec. A1) and in terms of an iterative expansion using nested commutators with the Hamiltonian (Sec. A2). The latter expression may be used in cases where diagonalization of the Hamiltonian is not feasible.

As defined in Ref. [14], the interaction picture version of $\delta \mathcal{V}$, $\delta \tilde{\mathcal{V}}(t)$, is given by [27]:

$$
\delta \tilde{\mathcal{V}}(t)[\rho] = \int_{-\infty}^{\infty} da \int_{-\infty}^{\infty} db \theta(a - t) - \theta(b - t)]G(a, b)[\rho],
$$

(A1)

where $G(a, b)[\rho]$ is a superoperator whose action on a generic density operator $\rho$ is given by

$$
G(a, b)[\rho] = -\gamma \int_{-\infty}^{\infty} dc g^*(a - b)g^*(b - c)[\dot{X}(a), \rho \dot{X}(c)] + \text{h.c.}.
$$

(A2)

Thus we may write

$$
\delta \tilde{\mathcal{V}}(t)[\rho] = \gamma \int_{-\infty}^{\infty} da \int_{-\infty}^{\infty} dc [\dot{X}(a), \rho \dot{X}(c)]f(a - t, c - t) + \text{h.c.},
$$

(A3)

with $f(t, t')$ defined below Eq. (10) in the main text:

$$
f(t, t') \equiv \int_{-\infty}^{\infty} db g^*(t - b)g^*(b - t')\theta(b - t')\theta(t) - \theta(b)).
$$

(A4)

When $H_S$ is time-independent, the Schrödinger picture version of $\delta \tilde{\mathcal{V}}$ can be obtained by setting $t = 0$: $\delta \mathcal{V} = \delta \tilde{\mathcal{V}}(0)$. Doing this above yields the result quoted in Eq. (10).

1. Expression for $\mathcal{V}$ in energy eigenbasis

When $H_S$ is time-independent we can conveniently express $\mathcal{V}$ in terms of the energy eigenbasis: writing $\dot{X}(t) = \sum_{mn} X_{mn} e^{-i\omega_{mn}t}$, where $\omega_{mn} = E_m - E_n$, $X_{mn} \equiv |m\rangle \langle m| |X| \langle n|$, and $H_S |n\rangle = E_n |n\rangle$, gives us

$$
\delta \mathcal{V}[\rho] = \sum_{m,n,k,l} [X_{mn}, \rho X_{kl}] c_{mn;kl} + \text{h.c.,}
$$

(A5)

with $c_{mn;kl} = 4\pi^2 f(-\omega_{mn}, \omega_{kl})$. Here $f(\omega, \omega') = \frac{1}{\pi^2} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' e^{i\omega t} e^{i\omega' t'} f(t, t')$ denotes the Fourier transform of $f(t, t')$. A straightforward evaluation of the Fourier transform yields

$$
c_{mn;kl} = 2\pi \gamma \int_{-\infty}^{\infty} dq \frac{g(q)[g(q) - g(q + \omega_{mn} - \omega_{kl})]}{(\omega_{mn} - \omega_{kl})(q - \omega_{mn} - i\delta)}
$$

(A6)

where, for $\omega_{mn} = \omega_{kl}$, the integrand should be evaluated using L’Hospital’s rule.
2. Expression of $V$ in terms of commutator expansion

In cases where diagonalization of the Hamiltonian is not feasible, $V$ can be computed using an iterative series expansion akin to the one provided for the jump operator in Ref. [14]. We review this expansion for the case of a single bath and a time-independent Hamiltonian, while noting that our results can be extended to multiple baths and time-dependent Hamiltonians. Our first step is to write an expansion for the interaction picture operator $\tilde{X}(t)$:

$$\tilde{X}(t) = \sum_{n=0}^{\infty} \frac{X^{(n)} t^n}{n!} + \text{h.c.}, \quad X^{(n)} = -i[H_S, X^{(n-1)}].$$

(A7)

Here $X^{(n)}$ is the operator obtained from $X$ after $n$ commutation operations with $-iH_S$, where we define $X^{(0)} \equiv X$. Using this expression in the definition of $V$ [Eq. (10) of the main text] yields

$$V[\rho] = \gamma \sum_{m,n=0} X^{(m)}, \rho X^{(n)}]K_{mn} + \text{h.c.}, \quad K_{mn} = \frac{1}{m! n!} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' f(t,t') t^m t^n.$$

(A8)

Referring back to Eq. (A1) with $t$ set to zero (to obtain $V$ in the Schrödinger picture), and noting that $G(a,b)$ decays to zero with $|a|$, $|b|$, we see that $V$ itself can be computed with a temporal cutoff with an error that goes to zero as the cutoff is increased. For any finite value of the cutoff, the corresponding integrals in Eq. (A8) are finite, and the sum converges. The coefficients $\{K_{mn}\}$ are inexpensive to compute and depend only on the bath jump correlator (but not on any details of the system). Thus the expression in Eq. (A1) provides a viable way to calculate $V$ to good accuracy for systems where exact diagonalization is not feasible.

Appendix B: Relationship between $\rho_{\text{ULE}}$ and $\rho_{\text{exact}}$

Here we establish that $\rho_{\text{exact}} = \rho_{\text{ULE}} - \mathcal{L}_{\text{ULE}}^{-1}[\xi]$. The result is quoted above Eq. (13) in the main text. As our starting point, we write a formal solution of Eq. (8) of the main text as

$$\rho'(t) = e^{\mathcal{L}_{\text{ULE}}[\rho'][0]} + \int_0^t ds e^{\mathcal{L}_{\text{ULE}}[t-s]}[\xi(s)].$$

(B1)

We obtain the exact steady state of the system (in the memory-dressed frame) by taking the $t \to \infty$ limit above:

$$\lim_{t \to \infty} \rho'(t) = \rho_{\text{exact}}.$$

To compute the $t \to \infty$ limit on the right-hand side, we consider the eigendecomposition of $\mathcal{L}_{\text{ULE}}$. Due to its Lindblad form and our assumption of a unique steady state, the superoperator $\mathcal{L}_{\text{ULE}}$ has a single vanishing eigenvalue, while all other eigenvalues have strictly negative real parts. The left and right eigenvectors corresponding to the vanishing eigenvalue are the identity operator and $\rho_{\text{ULE}}$, respectively. (As in the main text, we have defined $\rho_{\text{ULE}}[\rho_{\text{ULE}}] = 0$.) Hence $\lim_{t \to \infty} e^{\mathcal{L}_{\text{ULE}}[\rho']} = \lim_{t \to \infty} e^{\mathcal{L}_{\text{ULE}}[\rho_{\text{ULE}}]}. Using Tr[$\rho'$] = 1 we thus conclude $\lim_{t \to \infty} e^{\mathcal{L}_{\text{ULE}}[t-s]}[\xi(s)]$ must decay exponentially with $t-s$. Taking the limit $t \to \infty$ in Eq. (B1) hence gives

$$\rho_{\text{exact}} = \rho_{\text{ULE}} - \mathcal{L}_{\text{ULE}}^{-1}[\xi],$$

(B2)

where $\mathcal{L}_{\text{ULE}}^{-1}[\xi] \equiv -\int_0^{\infty} ds e^{\mathcal{L}_{\text{ULE}}[s]} \xi$ is finite due to the fact that $\xi$ is traceless. This is the result we wished to establish.

Appendix C: Scaling of $C_O$

Here we show that the dimensionless constant $C_O$ [first appearing in Eq. (14) of the main text] is generically finite in the limit $\Gamma \to 0$. To this end, we recall the definition of $C_O$:

$$C_O = \frac{2\Gamma \mathcal{L}_{\text{ULE}}^{-1}[\Omega - \langle \Omega \rangle_{\text{ULE}}]}{\langle \langle \rangle_{\text{ULE}}}.\quad (C1)$$

In the following, we use $\Theta(\Gamma^n)$ to indicate quantities that scale as $\Gamma^n$ in the limit of small $\Gamma$. Likewise, we use $O(\Gamma^n)$ to indicate quantities that scale as $\Gamma^n$ or slower in the same limit. Our goal is to show that $C_O = O(\Gamma^0)$ for generic operators $\Omega$.

We first consider the case $\Omega = S$ where $\langle S \rangle_{\text{ULE}}$ is nonzero in the limit $\Gamma \to 0$. Since we assume the system to have a unique steady state, $\mathcal{L}_{\text{ULE}}$ has a single vanishing eigenvalue with corresponding left eigenvector $\rho_{\text{ULE}}$; all other eigenvalues either scale as $\Theta(\Gamma)$ or $\Theta(\Gamma^0)$. Thus, for any (Γ-independent) operator $M$ that is orthogonal to $\rho_{\text{ULE}}$ (in the sense of the Hilbert-Schmidt inner product), we infer that $\mathcal{L}_{\text{ULE}}^{-1}[M] = O(\Gamma^{-1})$. Since $S' - \langle S' \rangle_{\text{ULE}}$ by definition has zero expectation value in the ULE steady state and is hence orthogonal to $\rho_{\text{ULE}}$, we have $\mathcal{L}_{\text{ULE}}^{-1}[S' - \langle S' \rangle_{\text{ULE}}] = O(\Gamma^{-1})$. Using this in Eq. (C1), we conclude that $C_S = O(\Gamma^0)$ for observables with finite expectation values in the limit $\Gamma \to 0$, i.e., with $\lim_{\Gamma \to 0} \langle S' \rangle_{\text{ULE}} \neq 0$.

Next, we consider the case $\Omega = I$, where $I$ has vanishing steady-state value in the limit $\Gamma \to 0$. Since $\lim_{\Gamma \to 0} \rho_{\text{exact}}$ is diagonal in the eigenbasis of the Hamiltonian [14], there are two classes of operators for which
We now note that and the definition we thus have the ULE Liouvillian (including the Lamb shift). Writing where \( \rho \) can for example be written in the form above with \( I \) being orthogonal to \( \bar{\rho} \). For the latter class of operators, \( C_0 \) can be infinite. However, the vanishing steady-state value of these operators requires fine-tuning of the system and bath parameters – the operator will generally acquire nonzero steady-state values under perturbations of the bath parameters (such as temperature or chemical potential) or system-bath coupling. We hence expect this case to be non-generic.

Operators whose diagonal matrix elements vanish in the eigenbasis of the Hamiltonian include many physically relevant quantities, such as the total currents of conserved quantities and, in cases of Hamiltonians with time-reversal symmetry, current densities. For this class of operators, we can write

\[
I = -i [H_S, Q],
\]

for some finite operator \( Q \). The magnon current \( I_{n+1,n} \) for the spin chain we consider in the main text can for example be written in the form above with \( Q = \sum_{k=1}^{n} \sigma_k^z \) (i.e., with \( Q \) measuring the total \( z \)-component of spin on sites \( 1 \ldots n \)). We now use the above property to infer the scaling behavior of \( C_1 \).

First, we rewrite Eq. (2) as

\[
I = \mathcal{L}_{\text{ULE}}^\dagger [Q] - \mathcal{D}_{\text{ULE}}^\dagger [Q],
\]

where \( \mathcal{D}_{\text{ULE}} \) denotes the bath-induced component of the ULE Liouvillian (including the Lamb shift). Writing

\[
\mathcal{V}^{-1} [I] = I + \left( \frac{1}{1 + \delta \mathcal{V}} - 1 \right) [I],
\]

and using \( I' = \mathcal{V}^{-1} [I] \), we thus have

\[
I' = \mathcal{L}_{\text{ULE}}^\dagger [Q] + R,
\]

with

\[
R = -\mathcal{D}_{\text{ULE}}^\dagger [Q] + \left( \frac{1}{1 + \delta \mathcal{V}} - 1 \right) [I].
\]

We now note that \( \mathcal{L}_{\text{ULE}}[\bar{\rho}_{\text{ULE}}] = 0 \), implying

\[
\text{Tr} (\bar{\rho}_{\text{ULE}} \mathcal{L}_{\text{ULE}}^\dagger [Q]) = 0.
\]

Using this relation with Eq. (3) and the definition \( \langle I' \rangle_{\text{ULE}} = \text{Tr} (\rho_{\text{ULE}} \mathcal{L}_{\text{ULE}}^\dagger [I]) \), we find

\[
\langle I' \rangle_{\text{ULE}} = \text{Tr} [\bar{\rho}_{\text{ULE}} R].
\]

To infer the scaling behavior of \( R \), we first use \( \mathcal{D}_{\text{ULE}}^\dagger [Q] = \Theta (\Gamma) \). Moreover, since \( \| \delta \mathcal{V} \| \leq \Gamma \), we have \( ((1 + \delta \mathcal{V})^{-1} - 1) [I] = \Theta (\Gamma) \). Thus \( R = \Theta (\Gamma) \), implying

\[
\langle I' \rangle_{\text{ULE}} = \Theta (\Gamma).
\]

This demonstrates that \( \lim_{\Gamma \to 0} \langle \hat{A} \rangle = 0 \) for operators with vanishing diagonal matrix elements in the eigenbasis of \( H_S \), as we inferred above.

We now show that \( \mathcal{L}_{\text{ULE}}^{-1} [I' - \langle I' \rangle_{\text{ULE}}] = \Theta (\Gamma_0) \) for operators that can be written in the form in Eq. (2). Using Eq. (3), we first note that

\[
\mathcal{L}_{\text{ULE}}^{-1} [I' - \langle I' \rangle_{\text{ULE}}] = Q + \mathcal{L}_{\text{ULE}}^{-1} [R - \langle I' \rangle_{\text{ULE}}].
\]

To analyze the second term on the right hand side of this expression, we note two important facts. First, since \( \langle I' \rangle_{\text{ULE}} = \text{Tr} [\rho_{\text{ULE}} R] \) [see Eq. (5)], \( R - \langle I' \rangle_{\text{ULE}} \) is orthogonal to \( \bar{\rho}_{\text{ULE}} \). Moreover, according to the discussion above, \( R - \langle I' \rangle_{\text{ULE}} = \Theta (\Gamma) \). Therefore \( \mathcal{L}_{\text{ULE}}^{-1} [R - \langle I' \rangle_{\text{ULE}}] = \Theta (\Gamma_0) \). Using \( Q = \Theta (\Gamma_0) \), we find

\[
\| \mathcal{L}_{\text{ULE}}^{-1} [I' - \langle I' \rangle_{\text{ULE}}] \| = \Theta (\Gamma_0).
\]

Combining this with \( \langle \hat{I} \rangle_{\text{ULE}} = \Theta (\Gamma) \) in Eq. (3), we conclude \( C_1 \) is finite in the limit \( \Gamma \to 0 \).

**Appendix D: Steady-state value of magnetization**

Here we provide data for the steady-state values of magnetization on each site, \( \{ \sigma_n^z \} \), for the 9-site spin chain model considered in the main text. In Fig. 3 we show the steady-state values of the magnetization obtained with (orange) and without (blue) applying the correction from the memory dressing transformation, \( \langle \sigma_n^z \rangle_{\text{ULE}} \), and \( \langle \sigma_n^z \rangle_{\text{ULE}} \), respectively. As for the computation of the bond current in the main text, we apply the inverse memory-dressing transformation through expansion to first order, setting \( \mathcal{V}^{-1} \approx (1 - \delta \mathcal{V}) \) to compute \( \langle \sigma_n^z \rangle_{\text{ULE}} \). The two data sets coincide up to negligible relative corrections, as we expected due to the finite value of \( \langle \sigma_n^z \rangle_{\text{ULE}} \) in the weak coupling limit (see main text).

![FIG. 3. Steady-state values of the undressed (\( \{ \langle \sigma_n^z \rangle_{\text{ULE}} \} \), blue) and dressed (\( \{ \langle \sigma_n^z \rangle_{\text{ULE}} \} \), orange) on-site magnetizations in the spin-chain model considered in the main text.](image-url)

[1] P. A. M. Dirac, The quantum theory of the emission and absorption of radiation, Proc. R. Soc. Lond. **114**, 243–265 (1927).
The Bloch-Redfield Liouvillian is given by

\[ L_{\text{BR}}[\rho] = -i[H_S, \rho] - \sum_{\alpha \beta} \gamma_{\alpha \beta} \int_0^\infty dt \left( J_{\alpha \beta}(t) \left[ X_\alpha, e^{iH_S t} X_\beta e^{-iH_S t} \rho \right] + \text{h.c.} \right) \]

This follows from the property of \( V \) above, along with \( \Vert \xi \Vert \leq t^2 \tau, \Vert \partial_t \rho - i[\rho, H_S] \Vert \leq \Gamma/2, \) and \( \Vert V^\dagger - 1 \Vert_{\text{S}} \leq \Gamma \tau \) (see below).

Here \( V^\dagger \) denotes the adjoint of \( V \) with respect to the Hilbert-Schmidt inner product, \( \langle A, B \rangle \equiv \text{Tr}[A^\dagger B] \).

One can construct operators with nonvanishing diagonal matrix elements in the energy basis, whose expectation values vanish in the limit \( \Gamma \to 0 \) (such that the relative deviation does not scale to zero with \( \Gamma \)). We expect that such observables are non-generic and require fine-tuning.

This result follows from \( \langle O \rangle_{\text{ULE}} - \langle O \rangle_{\text{BR}} = \text{Tr}[\Omega(1 - V^{-1})[\rho_{\text{ULE}}]] \), and from using \( \| \delta V \| \leq \Gamma \tau, \) and \( \| P_{\text{BR}} \| = 1 \).

We emphasize that uniformity of the bond currents alone does not imply that the value of current is accurate. For example, while the BR approach ensures uniformity of the current by construction, its accuracy is guaranteed only in the weak coupling limit [19].

We apply the inverse frame transformation through expansion to first order, setting \( V^{-1} \approx 1 - \delta V \).

Specifically, \( \| \delta \langle O \rangle_{\text{BR}} \| \leq \Gamma \tau C_{\Omega} \| \langle O \rangle_{\text{BR}} \|, \) with \( C_{\Omega} \equiv \Gamma (\| \mathcal{L}_{\text{BR}} \| - 1) \| \langle 0 - \langle O \rangle_{\text{BR}} \| / \| \langle O \rangle_{\text{BR}} \| \), where \( \langle O \rangle_{\text{BR}} \) denotes the expectation value of \( O \) in the steady state of the BR equation and \( \mathcal{L}_{\text{BR}} \) denotes the Bloch-Redfield Liouvillian. For small \( \Gamma \), \( C_{\Omega} \) similar scaling behavior to that of \( C_{\Omega} \) as described in the SOM [20].

See Supplementary Online Material for: A) explicit expressions for the frame transformation \( V \), B) explicit derivation of the result \( \tilde{\rho}_{\text{exact}} = \rho_{\text{ULE}} + \mathcal{L}_{\text{ULE}}^{-1}[\xi] \), C) Data showing the steady-state value of magnetization in the simulated spin-chain model, and D) analysis of the small-\( \Gamma \) behavior of \( C_{\Omega} \).