

High accuracy steady states obtained from the Universal Lindblad Equation

Frederik Nathan¹ and Mark S. Rudner²

¹*Institute for Quantum Information and Matter, Caltech, Pasadena, California 91125, USA*

²*Department of Physics, University of Washington, Seattle, Washington 98195, USA*

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We show that the universal Lindblad equation (ULE) captures steady-state expectation values of observables up to rigorously bounded corrections that scale linearly with the system-bath coupling, Γ . We moreover identify a simple quasilocal transformation, whose application guarantees a *relative* deviation generically scaling to zero with Γ , even for observables such as currents whose steady-state values themselves vanish in the weak coupling limit. This result provides a solution to recently identified limitations on the accuracy of Lindblad-form master equations, which imply significant relative errors for observables whose steady-state values vanish with Γ , while most generic observables are otherwise captured faithfully. The transformation allows for high-fidelity computation of sensitive observables while retaining the stability and physicality of a Lindblad-form master equation.

Modelling the dynamics of open quantum systems is an important scientific problem, relevant across a wide range of fields. While the groundwork for the theory of open quantum systems was laid in the context of quantum optics and quantum chemistry [1–6], recent advances in the control of many-component quantum systems necessitates the development of new theoretical techniques that apply to quantum many-body systems [7–20].

Here we focus on the broadly relevant Markovian regime, which arises when the system-environment coupling is weak relative to the inverse characteristic memory time of the environment. In this context, the “Lindblad form” plays a key role in providing the most general structure of Markovian quantum evolution that preserves the Hermiticity, trace, and positivity of the system’s density matrix [21, 22]. Moreover, Lindblad-form master equations admit stable and relatively efficient numerical solutions via stochastic evolution methods [23–25].

The primary routes for obtaining Lindblad equations have historically assumed (and required) the energy levels of the system to be well-separated [5, 6]. This approach is inapplicable to generic many-body systems, however, due to their exponentially small level spacings. Recently, a number of independent works proposed new Lindblad-form master equations, free of such restrictions [8–10, 12–17]. Here we focus on the “Universal Lindblad Equation” (ULE), which was rigorously derived with bounds on approximation-induced errors in Ref. [15].

Interestingly, several groups have recently identified nontrivial tradeoffs that arise when describing open quantum systems via Lindblad equations [8, 19, 26]: when a system is connected to multiple baths which are mutually out of equilibrium, the relative (i.e., fractional) errors of resulting particle, spin, and/or heat currents may remain finite even in the limit of vanishing system-bath coupling. This relative error arises because the steady state of any Lindblad equation must deviate from the exact steady state by a correction that scales linearly with a characteristic system-bath coupling strength [26], here identified as Γ [see Eq. (1) for definition]. At the same time, the expectation values of the currents also scale linearly with Γ in the limit $\Gamma \rightarrow 0$. While the result-

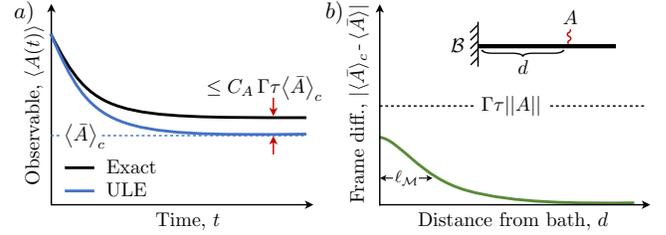


FIG. 1. Accuracy of steady state observables of the ULE. The value of a generic observable A evaluated in the steady state of the ULE deviates from its exact value by a bounded error that scales to zero with the dimensionless number that controls the validity of the ULE, $\Gamma\tau \ll 1$ [Eqs. (1), (10)]. a) Incorporating the inverse of the “Lindblad frame transformation” [Eq. (2)] in the computation of the observable yields a corrected expectation value $\langle \bar{A} \rangle_c$ [Eq. (8)] that deviates from the exact result by a bounded *relative error* that scales to zero with $\Gamma\tau$ [Eq. (9)]. b) The support of the transformation is localized in regions of size ℓ_M around points of contact with the bath, \mathcal{B} . Thus all local observables with support far from the bath are faithfully captured without the correction.

ing deviations of currents can be kept small in absolute scale [15], non-negligible values in relative scale can lead to apparent violations of the second law of thermodynamics [8, 19], or of microscopic continuity equations [26].

In this work we show how these apparent limitations can be overcome for the universal Lindblad equation. Specifically, we show how high-accuracy results can be obtained for *any* generic observable, with a bounded relative error that scales to zero as $\Gamma \rightarrow 0$ [Fig. 1a]. By reexamining the rigorous derivation in Ref. [15], we first confirm that the ULE yields steady state observables with bounded absolute errors that generically scale to zero as $\Gamma \rightarrow 0$. We then identify the source of the $O(1)$ relative errors for current-like observables to be a fixed, near-identity, linear transformation – henceforth referred to as the “Lindblad frame transformation” – that was applied to the system’s density matrix in Ref. [15] to obtain the Lindblad-form master equation. We show that the transformation is quasilocal, implying that the relative error in the weak-coupling limit is only significant for local current-like observables with support close to

points of contact with the bath [Fig. 1b]. Moreover, by applying the inverse transformation to the output of the ULE, the contribution from the transformation can be eliminated, thus yielding accurate steady-state values of *all* generic observables, including currents [27]. Our analysis is supported by numerical simulations [Fig. 2].

The Lindblad frame and the ULE.— We begin by briefly reviewing the key steps of the derivation in Ref. [15], which leads to the ULE. These steps elucidate the role of the Lindblad frame transformation and allow us to bound the accuracy of steady-state observables.

Our aim is to describe the evolution of a quantum system \mathcal{S} , which is coupled to an external “bath,” \mathcal{B} . The combined system has Hamiltonian $H_{\mathcal{S}\mathcal{B}} = H_{\mathcal{S}} + H_{\mathcal{B}} + H_{\text{int}}$, which we assume to be time-independent for the discussion below. Here $H_{\mathcal{S}}$ and $H_{\mathcal{B}}$ act exclusively on \mathcal{S} and \mathcal{B} , respectively, while H_{int} contains all remaining terms. These three terms comprise the system Hamiltonian, the bath Hamiltonian, and the system-bath coupling, respectively. We assume that \mathcal{B} is Gaussian (e.g., comprised of free bosonic or fermionic modes).

The non-equilibrium currents considered in Refs. [8, 19, 26] arise when the system is connected to multiple independent baths. To keep our discussion simple we initially focus on the case of a single bath, where $H_{\text{int}} = \sqrt{\gamma}XB$ with X and B Hermitian operators acting exclusively on \mathcal{S} and \mathcal{B} , respectively. Here γ is a (redundant) energy scale that parametrizes the strength of the system-bath coupling. The essential features and consequences of the Lindblad frame transformation will appear in this model; for details of the ULE when multiple system and bath operators are coupled, see Ref. [15]. Without loss of generality we take the bath to be in a state where B has expectation value zero, and also assume X to have unit spectral norm [28]. The Gaussian bath is fully characterized by its two-point correlation function $J(t) = \langle B(t)B(0) \rangle$ with $B(t) \equiv e^{iH_{\mathcal{B}}t} B e^{-iH_{\mathcal{B}}t}$.

The system \mathcal{S} is fully described by its reduced density matrix, $\rho(t) \equiv \text{Tr}_{\mathcal{B}}[\rho_{\mathcal{S}\mathcal{B}}(t)]$, where $\rho_{\mathcal{S}\mathcal{B}}(t)$ gives the state of the combined system, and $\text{Tr}_{\mathcal{B}}$ traces over all degrees of freedom in \mathcal{B} . Expanding $\partial_t \rho$ to leading order in γ yields [4, 14, 15]: $\partial_t \rho(t) = \mathcal{L}_{\text{BR}}[\rho(t)] + \xi_{\text{BR}}(t)$, where $\mathcal{L}_{\text{BR}}[\mathcal{O}] \equiv -i[H_{\mathcal{S}}, \mathcal{O}] - \gamma \int_0^\infty dt (J(t)[X, e^{-iH_{\mathcal{B}}t} X e^{iH_{\mathcal{B}}t} \mathcal{O}] + \text{h.c.})$ is the Bloch-Redfield (BR) Liouvillian and $\xi_{\text{BR}}(t)$ captures the difference between the exact value of $\partial_t \rho$ and that resulting from the Born-Markov approximation [15], $\mathcal{L}_{\text{BR}}[\rho]$.

In Ref. [15] we obtained a Lindblad-form master equation (the ULE) from the Bloch-Redfield equation above, without invoking the secular approximation (as traditionally required). The derivation reveals two timescales, Γ^{-1} and τ , that control the validity of the approximations used. These timescales are defined from the Fourier transformed bath correlation function, $J(\omega)$, through the “jump correlator” $g(t) = \int d\omega e^{-i\omega t} \sqrt{J(\omega)/2\pi}$:

$$\Gamma = 4\gamma \left[\int_{-\infty}^{\infty} dt |g(t)| \right]^2, \quad \tau = \frac{\int_{-\infty}^{\infty} dt |g(t)t|}{\int_{-\infty}^{\infty} dt |g(t)|}. \quad (1)$$

Physically, Γ bounds the rate of bath-induced evolution. In particular, the reduced density matrix in the interaction picture, $\tilde{\rho}$, satisfies $\|\partial_t \tilde{\rho}\| \leq \Gamma/2$, where $\|\cdot\|$ denotes the trace norm [15]. Here and throughout we use the tilde accent to denote (super)operators in the interaction picture [29]. The timescale τ is a characteristic timescale for the decay of correlations in the bath.

The dimensionless number $\Gamma\tau$ quantifies the “Markovianity” of the dynamics. In Ref. [15] we showed that this parameter controls the accuracy of both the Bloch-Redfield equation and the ULE. Notably, $\|\xi_{\text{BR}}(t)\| \leq 2\Gamma^2\tau$ [14, 15, 30]. Since the bath-induced contributions to \mathcal{L}_{BR} (i.e., everything except for $-i[H_{\mathcal{S}}, \cdot]$) are linear in Γ , the relative magnitude of $\xi_{\text{BR}}(t)$ vanishes when $\Gamma\tau \ll 1$.

A crucial element of the ULE derivation in Ref. [15] is a trace and Hermiticity preserving linear transformation:

$$\rho' = (1 + \mathcal{M})[\rho]. \quad (2)$$

Here \mathcal{M} is a time-independent superoperator, which in the interaction picture satisfies $\partial_t \tilde{\mathcal{M}}(t) = \tilde{\mathcal{L}}_{\text{ULE}}(t) - \tilde{\mathcal{L}}_{\text{BR}}(t)$, where $\tilde{\mathcal{L}}_{\text{BR}}(t)$ and $\tilde{\mathcal{L}}_{\text{ULE}}(t)$ are the interaction picture versions of \mathcal{L}_{BR} and the ULE Liouvillian:

$$\mathcal{L}_{\text{ULE}}[\mathcal{O}] = -i[H_{\mathcal{S}} + H_{\text{LS}}, \mathcal{O}] + L\mathcal{O}L^\dagger - \frac{1}{2}\{L^\dagger L, \mathcal{O}\}. \quad (3)$$

Here $L = \sum_{mn} \sqrt{2\pi\gamma J(E_m - E_n)} |m\rangle\langle m| X |n\rangle\langle n|$, with $H_{\mathcal{S}}|n\rangle = E_n|n\rangle$; the Lamb shift, H_{LS} , is given in Ref. [15]. Evidently, \mathcal{L}_{ULE} is in the Lindblad form. An expression for \mathcal{M} is given in Eq. (5) below. Crucially, \mathcal{M} can be chosen such that $\|\mathcal{M}\| \leq \Gamma\tau$, where we use the superoperator norm $\|\mathcal{A}\| = \sup_{\mathcal{O}} \|\mathcal{A}[\mathcal{O}]\|/\|\mathcal{O}\|$. Thus, the transformation $(1 + \mathcal{M})$ nearly coincides with the identity in the Markovian limit $\Gamma\tau \ll 1$.

To obtain the ULE, we take the time derivative on both sides of Eq. (2) in the interaction picture. Using the exact form of the Bloch-Redfield equation (above) along with the bounds $\|\partial_t \tilde{\rho}\| \leq \Gamma/2$, $\|\tilde{\mathcal{L}}_{\text{ULE}}\| \leq \Gamma/2$, and $\|\tilde{\mathcal{M}}\| \leq \Gamma\tau$, gives (after reverting to the Schrodinger picture) [15]

$$\partial_t \rho'(t) = \mathcal{L}_{\text{ULE}}[\rho'(t)] + \xi(t), \quad (4)$$

where $\|\xi(t)\| \leq 2\Gamma^2\tau$. The ULE is obtained by neglecting $\xi(t)$. Since the bath-induced contributions to \mathcal{L}_{ULE} are linear in Γ , the relative magnitude of ξ goes to zero in the limit $\Gamma\tau \ll 1$. In this sense, the ULE accurately describes the evolution of the transformed density matrix ρ' in the limit $\Gamma\tau \ll 1$. This limit also ensures $\|\rho'(t) - \rho(t)\| \ll 1$.

Evidently, the ULE captures the time-derivative of the system’s density matrix up to a correction bounded by $2\Gamma^2\tau$, in the transformed frame defined by Eq. (2). We dub this frame the *Lindblad frame*. In the limit $\Gamma\tau \ll 1$ the Lindblad frame nearly coincides with the lab frame, and the transformation can thus be ignored for many practical purposes [15]. However, since the Lindblad frame transformation induces $O(\Gamma)$ corrections to the state of the system, the transformation is relevant for computing observables such as steady-state charge

or heat currents, whose expectation values vanish when $\Gamma \rightarrow 0$. For these quantities, it is necessary to apply the inverse transformation $(1 + \mathcal{M})^{-1}$ to the state obtained with the ULE to ensure negligible relative errors. Using $\|\mathcal{M}\| \leq \Gamma\tau \ll 1$, it is straightforward to compute $(1 + \mathcal{M})^{-1}$ through a low-order Taylor expansion: $(1 + \mathcal{M})^{-1} = 1 - \mathcal{M} + \delta\mathcal{M}$, where $\|\delta\mathcal{M}\| \leq (\Gamma\tau)^2/(1 - \Gamma\tau)$.

For a time-independent Hamiltonian and $H_{\text{int}} = \sqrt{\gamma}XB$ (as used above), \mathcal{M} is given by

$$\mathcal{M}[\rho] = \gamma \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' [\tilde{X}(t), \rho \tilde{X}(t')] f(t, t') + \text{h.c.}, \quad (5)$$

with $f(t, t') \equiv \int_{-\infty}^{\infty} ds g^*(t - s)g^*(s - t')\theta(t - t')[\theta(t) - \theta(s)]$. We also provide expressions for \mathcal{M} in terms of the eigenstates of H_S , and via an iterative Taylor series expansion, in Appendix A.

The Lindblad frame transformation only significantly affects observables near points of contact with the baths, as schematically indicated in Fig. 1c. To see this, first note that the integrand defining $f(t, t')$ above is nonzero only for $t > 0, s < 0$ and vice versa. For a bath with a smooth spectral function [i.e., without long-lived memory], $g(t)$ decays to zero for large t [15], with a characteristic decay time τ_g . Hence, $f(t, t')$ also decays with a characteristic timescale of order τ_g for large $|t|$ or $|t'|$. Importantly, $\tilde{X}(t)$ only has support within a distance $v_{\text{LR}}t$ around the region where X acts, where v_{LR} denotes the Lieb-Robinson velocity in the system. Thus, the influence of \mathcal{M} on local operators with support a distance d from the bath decreases as a function of d with a characteristic length scale of order $\ell_{\mathcal{M}} = v_{\text{LR}}\tau_g$.

Steady state of the ULE. — In the long-time limit, the exact density matrix of an open quantum system typically reaches a steady state, $\bar{\rho}_{\text{exact}}$. Here we establish how accurately the ULE captures this steady state. For simplicity, we assume the Hamiltonian to be time-independent and for the system to have a unique steady state. In particular, we do not consider systems which exhibit spontaneous symmetry breaking.

We first relate $\bar{\rho}_{\text{exact}}$ to the steady state of the ULE, $\bar{\rho}_{\text{ULE}}$, defined as the state satisfying

$$\mathcal{L}_{\text{ULE}}[\bar{\rho}_{\text{ULE}}] = 0. \quad (6)$$

In the exact steady-state, the left-hand side of Eq. (4) vanishes and ρ' takes a constant value $\bar{\rho}'_{\text{exact}} = (1 + \mathcal{M})[\bar{\rho}_{\text{exact}}]$. Therefore $\xi(t)$ must also obtain a constant value $\bar{\xi} = -\mathcal{L}_{\text{ULE}}[\bar{\rho}'_{\text{exact}}]$ in the steady state. Using Eq. (6) we thus write $\bar{\rho}'_{\text{exact}} = \bar{\rho}_{\text{ULE}} - \mathcal{L}_{\text{ULE}}^{-1}[\bar{\xi}]$ [31]; see Appendix B for derivation. Inverting the Lindblad frame transformation yields

$$\bar{\rho}_{\text{exact}} = \frac{1}{1 + \mathcal{M}} [\bar{\rho}_{\text{ULE}} - \mathcal{L}_{\text{ULE}}^{-1}[\bar{\xi}]]. \quad (7)$$

Since $\mathcal{L}_{\text{ULE}}^{-1}[\bar{\xi}] \lesssim \Gamma^{-1}\|\bar{\xi}\|$ for small Γ [31], and $\|\bar{\xi}\| \leq 2\Gamma^2\tau$, we see that $\lim_{\Gamma\tau \rightarrow 0} \mathcal{L}_{\text{ULE}}^{-1}[\bar{\xi}] = 0$. This limit also gives $\mathcal{M} = 0$. In absolute scale, $\bar{\rho}_{\text{ULE}}$ thus accurately captures the true steady state, $\bar{\rho}_{\text{exact}}$, in the limit $\Gamma\tau \rightarrow 0$.

We now consider how accurately the ULE captures *observables* for finite values of $\Gamma\tau$. For a given observable A , we let $\langle \bar{A} \rangle_{\text{exact}} \equiv \text{Tr}[\bar{\rho}_{\text{exact}}A]$ denote its exact steady-state value. Below, we consider the expectation value of A in the ULE steady state, $\langle \bar{A} \rangle$, and its value corrected for the transformation back to the lab frame, $\langle \bar{A} \rangle_c$:

$$\langle \bar{A} \rangle \equiv \text{Tr}[\bar{\rho}_{\text{ULE}}A], \quad \langle \bar{A} \rangle_c \equiv \text{Tr}\left(\bar{\rho}_{\text{ULE}} \frac{1}{1 + \mathcal{M}^\dagger}[A]\right). \quad (8)$$

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

We first consider how accurately $\langle \bar{A} \rangle_c$ captures $\langle \bar{A} \rangle_{\text{exact}}$. Using Eq. (7) and $\|\bar{\xi}_{\text{ULE}}\| \leq 2\Gamma^2\tau$, we obtain

$$|\langle \bar{A} \rangle_c - \langle \bar{A} \rangle_{\text{exact}}| \leq C_A \Gamma\tau |\langle \bar{A} \rangle_c|. \quad (9)$$

Here $C_A \equiv 2\Gamma\|\mathcal{L}_{\text{ULE}}^{\dagger-1}[\delta A_c]\|/|\langle \bar{A} \rangle_c|$, with $\delta A_c = (1 + \mathcal{M}^\dagger)^{-1}[A] - \langle A \rangle_c$ [32]. The dimensionless number C_A can be explicitly computed for a given observable A . Importantly, for generic A , C_A is finite and takes a constant (finite) value in the limit $\Gamma \rightarrow 0$ (see Appendix C). This in particular includes observables such as the total current, whose expectation values scale to zero with Γ [33]. A similar bound holds for the Bloch-Redfield equation [34], which follows from the error bounds identified in Refs. [14, 15].

For observables with finite expectation values in the limit $\Gamma \rightarrow 0$, the inverse Lindblad frame transformation is not required for accurate results. Specifically, the definitions of $\langle \bar{A} \rangle_c$ and $\langle \bar{A} \rangle$ imply $|\langle \bar{A} \rangle - \langle \bar{A} \rangle_c| \leq \frac{\Gamma\tau}{1 - \Gamma\tau} \|A\|_2$, where $\|\cdot\|_2$ denotes the maximal singular value norm [35]. Combining this result with Eq. (9) gives a bound

$$|\langle \bar{A} \rangle - \langle \bar{A} \rangle_{\text{exact}}| \leq C_A \Gamma\tau |\langle \bar{A} \rangle| + \frac{\Gamma\tau + C_A \Gamma^2\tau^2}{1 - \Gamma\tau} \|A\|_2. \quad (10)$$

Due to the quasilocality of \mathcal{M} , the magnitude of the contribution from the frame transformation (the second term above) further decays to zero with the distance from A to the bath, over the characteristic scale $\ell_{\mathcal{M}}$. Thus the cost of the inverse transformation can be avoided, if one can accept an absolute error that scales to zero as $\Gamma\tau$, or if the support of A is far from any bath (relative to $\ell_{\mathcal{M}}$).

Equations (9) and (10) are our main results. For observables with finite expectation values in the weak coupling limit, $\Gamma\tau \rightarrow 0$, good estimates (with relative deviations scaling to zero with $\Gamma\tau$) can be obtained by directly taking expectation values using the ULE steady state $\bar{\rho}_{\text{ULE}}$ [Eq. (6)]. For observables such as currents whose expectation values scale to zero with $\Gamma\tau$, Eq. (9) shows that high accuracy results with relative deviations that vanish for $\Gamma\tau \rightarrow 0$ can be obtained by employing the inverse Lindblad frame transformation [36]. Due to the quasilocal support of \mathcal{M} , we showed that the inverse Lindblad frame transformation can moreover be omitted for local observables deep in the bulk. We expect the same feature allows for efficient approximations of \mathcal{M} . We emphasize that the bounds in Eqs. (9)-(10) hold for

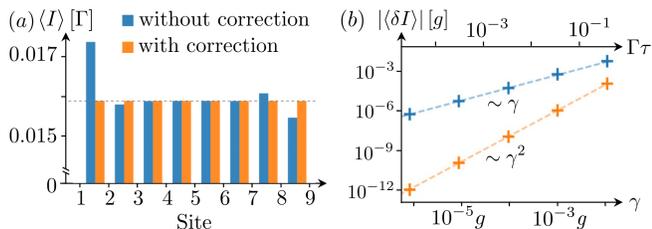


FIG. 2. Steady state observables of a 9-site spin chain connected to two baths of unequal temperatures (see text for model details). (a) Without applying the Lindblad frame correction, the bond currents vary significantly from site to site (blue bars), apparently violating current conservation. With the transformation (orange bars), the current is very nearly uniform throughout the chain. Note that the transformation has negligible effect deep in the bulk. (b) Scaling of the deviation of steady-state currents between the two bonds of a 3-site spin chain with the system bath coupling, γ (crosses). With the correction applied, we find $|\langle \delta \bar{I} \rangle_c| \sim \gamma^2$.

“worst case” scenarios; in practice we expect the corrections to be much smaller.

Demonstration.— We now study magnon transport in a spin chain to illustrate the results above. We consider a chain of L sites with Hamiltonian $H_S = \sum_{n=1}^{L-1} g(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z) + \sum_n h_n \sigma_n^z$, where σ_n^α is the $\alpha = \{x, y, z\}$ Pauli operator on spin n ; the same model was studied in Ref. [26]. We couple σ_1^x and σ_L^x to observables in two baths, \mathcal{B}_1 and \mathcal{B}_2 , respectively, setting $H_{\text{int}} = \sqrt{\gamma} \sigma_1^x B_1 + \sqrt{\gamma} \sigma_L^x B_2$. We take \mathcal{B}_1 and \mathcal{B}_2 to be Ohmic, Gaussian baths, with spectral functions $J_i(\omega) = \frac{\omega e^{-\omega^2/\Lambda^2}}{\omega_0} n_B(\beta_i \omega)$ for $i = \{1, 2\}$. Here ω_0 is a normalizing frequency scale, Λ is a high-frequency cutoff, n_B is the Bose-Einstein distribution, and $\beta_i = 1/(k_B T_i)$ is the inverse temperature of bath i , with k_B the Boltzmann constant. We simulate the model with $k_B T_1 = g$, $k_B T_2 = 6g$, $\Delta = 1.4g$, $\Lambda = 8g$, and $h_n = \frac{2}{3}(n - \frac{L+1}{2})g$ (describing a uniform field gradient).

Due to the temperature difference between the baths, magnon currents flow between them. Microscopically, the magnon current on the bond from site n to site $n+1$ is given by $I_{n+1,n} = (4ig\sigma_{n+1}^+ \sigma_n^- + \text{h.c.})$. Since the exact evolution of the combined system yields the Heisenberg equation $\partial_t \sigma_n^z = I_{n,n-1} - I_{n+1,n}$ for sites $2 \leq n \leq L-1$, the currents must be uniform in the exact steady state.

In the ULE steady state, the bond currents remain homogeneous deep in the bulk, but may be non-uniform in the vicinities of the baths. The non-uniformity arises because the equation of motion for $\sigma_n^z(t)$ under the ULE is modified by the quasilocal Lamb shift and jump operators (which act near the baths). Importantly, the bound in Eq. (9) implies that the Lindblad frame transformation restores the homogeneity of bond currents throughout the *entire* system, up to small relative deviations that vanish in the weak coupling limit. This is a nontrivial feature that does not directly follow from the form of the ULE itself. Below, we therefore use the uniformity of the bond currents as a consistency check and indicator of the accuracy of the bond currents obtained with the

ULE. 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 [34].

To support the above discussion we numerically solve the ULE to obtain the steady state for a chain of 9 sites with $\gamma = 0.0008g$. Fig. 2(a) shows the steady state bond currents computed with $[\langle \bar{I}_{n+1,n} \rangle_c]$ and without $[\langle \bar{I}_{n+1,n} \rangle]$ application of the inverse Lindblad frame transformation [37]. The uncorrected bond currents $\{\langle \bar{I}_{n+1,n} \rangle\}$ exhibit significant non-uniformities near the ends of the chain. After applying the correction, the bond currents become nearly uniform throughout the chain [with small residual fluctuations consistent with the expected $O(\Gamma^2)$ corrections, see below].

Deep in the bulk of the chain, $\langle \bar{I}_{n+1,n} \rangle$ is essentially uniform and identical to $\langle \bar{I}_{n+1,n} \rangle_c$. This observation supports our expectation that the ULE accurately captures currents in the bulk, even without applying the frame correction. In Appendix D we also confirm that the Lindblad frame correction is not needed to accurately capture the expectation values $\{\langle \bar{\sigma}_n^z \rangle\}$, which remain finite as $\gamma \rightarrow 0$.

To further illustrate the systematic improvement obtained by applying the inverse Lindblad frame transformation, in Fig. 2b we show the scaling of the difference of bond currents in a three site chain, $\delta I = I_{2,1} - I_{3,2}$, as a function of the system-bath coupling γ . As anticipated above, the uncorrected bond currents exhibit absolute deviations $|\langle \delta \bar{I} \rangle|$ that scale to zero linearly with γ ; deviations of the more accurate quantity $|\langle \delta \bar{I} \rangle_c|$ scale to zero *quadratically* with γ , as is required if the relative errors of the currents scale to zero in the limit $\gamma \rightarrow 0$.

For the 3-site spin chain we also computed the coefficient $C_{I_{2,1}}$ of the error bound in Eq. (9). For all values of γ we probed, we found $C_{I_{2,1}} \approx 760$. This constant value across several orders of magnitude of γ supports our conclusion that C_A takes a constant value in the limit $\gamma \rightarrow 0$. We emphasize that this value of $C_{I_{2,1}}$ is a rigorous (but loose) upper bound on the deviation of $\langle \delta \bar{I} \rangle_c$ from its true value; we expect the actual deviation to be much smaller.

Discussion.— We have derived rigorous bounds on the accuracy of steady state observables of the ULE. By elucidating the nature of the Lindblad frame transformation and introducing its inverse as a frame correction, we have shown how to ensure high accuracy results for *all* generic observables in the weak coupling limit. By exposing the quasilocal structure of this transformation, we furthermore showed that its influence is only significant for local observables close to points of contact with baths. We thus showed how to overcome the previously identified limitations of Lindblad-form master equations [19, 26], while preserving the stability of the Lindblad approach. Important directions for future work 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 [16].

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- [27] We note that, in the context of a different master equation, Ref. [19] showed that thermodynamically-consistent heat currents could be obtained by a redefinition of the heat current operator.
- [28] A nonzero expectation value can be absorbed into H_S after appropriate redefinition of B . If X has an unbounded spectrum, an appropriate cutoff for its eigenvalues has to be implemented.
- [29] An operator \mathcal{O} is transformed to the interaction picture using $\tilde{\mathcal{O}}(t) \equiv e^{iH_S t} \mathcal{O} e^{-iH_S t}$. A superoperator \mathcal{A} is transformed using $\tilde{\mathcal{A}}(t)[\mathcal{O}] = e^{iH_S t} \mathcal{A}[e^{-iH_S t} \mathcal{O} e^{iH_S t}] e^{-iH_S t}$. In our notation, Liouvillians, which generate time-evolution, acquire an additional term $\tilde{\mathcal{L}}(t) = e^{iH_S t} \mathcal{L}[e^{-iH_S t} \hat{\mathcal{O}} e^{iH_S t}] e^{-iH_S t} + i[H_S, \cdot]$ due to the time-dependence of the transformation.
- [30] In Ref. [15], the bound was established for the spectral norm; however the same arguments are valid for the trace norm.
- [31] Assuming the ULE has a unique steady state, \mathcal{L}_{ULE} has a single zero eigenvalue; hence $\mathcal{L}_{\text{ULE}}^{-1}$ generically has a single divergent eigenvalue, with the identity being the corresponding left eigenvector. All other eigenvalues will scale as Γ^0 or Γ^{-1} in the limit of small Γ . The inverse is thus well-defined for finite Γ , provided that it acts on traceless

operators (i.e., operators with zero overlap with the identity). Crucially, $\xi_{\text{ULE}}(t)$ is traceless, and thus $\mathcal{L}_{\text{ULE}}^{-1}[\xi_{\text{ULE}}]$ is well-defined and finite.

- [32] Note that $\mathcal{L}_{\text{ULE}}^\dagger$ has a single vanishing eigenvalue with $\tilde{\rho}'_{\text{ULE}}$ the corresponding left eigenvector (and 1 the corresponding right eigenvector). Hence $\mathcal{L}_{\text{ULE}}^{\dagger-1}$ is well-defined when acting on operators with vanishing expectation value in the steady state of the ULE (see also Ref. [31]). Alternatively, one can for example define C_A through $C_A = 2\Gamma \|\lim_{\eta \rightarrow 0} (\mathcal{L}_{\text{ULE}}^\dagger + \eta)^{-1} [\delta A_c]\| / \langle \bar{A}_c \rangle$.
- [33] One can construct operators with nonvanishing diagonal matrix elements in the energy basis, whose expectation values vanish in the limit $\Gamma \rightarrow 0$ (such that the relative deviation does not scale to zero with Γ). We expect that such observables are non-generic and require fine-tuning.
- [34] Specifically, $|\langle \bar{A} \rangle_{\text{exact}} - \langle \bar{A} \rangle_{\text{BR}}| \leq \Gamma \tau C'_A |\langle \bar{A} \rangle_{\text{BR}}|$, with $C'_A \equiv \Gamma \|(\mathcal{L}_{\text{BR}}^\dagger)^{-1} [\delta A']\| / \langle \bar{A} \rangle_{\text{BR}}$ and $\delta A' = A - \langle \bar{A} \rangle_{\text{BR}}$, where $\langle \bar{A} \rangle_{\text{BR}}$ denotes the expectation value of A in the steady state of the BR equation. For small Γ , C'_A follows similar scaling behavior to that of C_A as described in Appendix C.
- [35] This result follows from $\langle \bar{A} \rangle_{\text{ULE}} - \langle \bar{A}' \rangle_{\text{ULE}} = \text{Tr}[A(1 - (1 + \mathcal{M})^{-1})[\tilde{\rho}'_{\text{ULE}}]]$, and from using $\|\mathcal{M}\| \leq \Gamma \tau$, and $\|\tilde{\rho}'_{\text{ULE}}\| = 1$.
- [36] One can construct operators with nonvanishing diagonal matrix elements in the energy basis, whose expectation values vanish in the limit $\Gamma \rightarrow 0$ (such that the relative deviation does not scale to zero with Γ). We expect that

such observables are non-generic and require fine-tuning.

- [37] We apply the inverse Lindblad transformation through expansion to first order, setting $(1 + \mathcal{M})^{-1} \approx (1 - \mathcal{M})$.
- [38] See Supplementary Online Material for: A) expressions for the Lindblad frame transformation operator \mathcal{M} , B) derivation of Eq. (7), C) analysis of the small- Γ behavior of C_A .
- [39] This expressions follows from Eqs. (C2), (C4), and (C7) in Ref. [15], when using that $\theta(a)\theta(-b) - \theta(b)\theta(-a) = \theta(a) - \theta(b)$.
- [40] Note that Q is not uniquely defined, since adding a term diagonal in the eigenbasis of H_S to Q will not change A .

Appendix A: Expressions for \mathcal{M}

Here we provide an explicit expression for the superoperator \mathcal{M} which enters in the Lindblad frame transformation. We first show how \mathcal{M} in Eq. (5) is obtained from the corresponding expression given in Ref. [15]. Subsequently (for cases with time-independent Hamiltonians) we provide complementary expressions for \mathcal{M} in terms of the eigenbasis of the Hamiltonian (Sec. A 1) and in terms of an iterative expansion using nested commutators with the Hamiltonian (Sec. A 2). The latter expression may be used in cases where diagonalization of the Hamiltonian is not feasible.

As defined in Ref. [15], the interaction picture version of \mathcal{M} , $\tilde{\mathcal{M}}(t)$, is given by [39]:

$$\tilde{\mathcal{M}}(t)[\rho] = \int_{-\infty}^{\infty} da \int_{-\infty}^{\infty} db [\theta(a-t) - \theta(b-t)] \mathcal{G}(a, b)[\rho], \quad (\text{A1})$$

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

$$\mathcal{G}(a, b)[\rho] = -\gamma \int_{-\infty}^a dc g^*(a-b) g^*(b-c) [\tilde{X}(a), \rho \tilde{X}(c)] + \text{h.c.} \quad (\text{A2})$$

Thus we may write

$$\tilde{\mathcal{M}}(t)[\rho] = \gamma \int_{-\infty}^{\infty} da \int_{-\infty}^{\infty} dc [\tilde{X}(a), \rho \tilde{X}(c)] f(a-t, c-t) + \text{h.c.}, \quad (\text{A3})$$

with $f(t, t')$ defined below Eq. (5) in the main text:

$$f(t, t') \equiv \int_{-\infty}^{\infty} db g^*(t-b) g^*(b-t') \theta(b-t') [\theta(t) - \theta(b)]. \quad (\text{A4})$$

When H_S is time-independent, the Schrödinger picture version of $\tilde{\mathcal{M}}(t)$ can be obtained by setting $t = 0$: $\mathcal{M} = \tilde{\mathcal{M}}(0)$. Doing this above yields the result quoted in Eq. (5).

1. Expression for \mathcal{M} in energy eigenbasis

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

$$\mathcal{M}[\rho] = \sum_{m,n,k,l} [\hat{X}_{mn}, \rho \hat{X}_{kl}^\dagger] c_{mn;kl} + \text{h.c.}, \quad (\text{A5})$$

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

$$c_{mn;kl} = 2\pi\gamma \int_{-\infty}^{\infty} dq \frac{g(q)[g(q) - g(q + \omega_{mn} - \omega_{kl})]}{(\omega_{mn} - \omega_{kl})(q - \omega_{mn} - i0^+)}, \quad (\text{A6})$$

where, for $\omega_{mn} = \omega_{kl}$, the integrand should be evaluated using L'Hospital's rule.

2. Expression of \mathcal{M} in terms of commutator expansion

In cases where diagonalization of the Hamiltonian is not feasible, \mathcal{M} can be computed using an iterative series expansion akin to the one provided for the jump operator in Ref. [15]. 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 $\tilde{X}(t)$:

$$\tilde{X}(t) = \sum_n \frac{X^{(n)} t^n}{n!} + \text{h.c.}, \quad X^{(n)} = -i[H_S, X^{(n-1)}]. \quad (\text{A7})$$

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 \mathcal{M} [Eq. (5) of the main text] yields

$$\mathcal{M}[\rho] = \gamma \sum_{m,n=0}^{\infty} [X^{(m)}, \rho X^{(n)}] K_{mn} + \text{h.c.}, \quad K_{mn} \equiv \frac{1}{m!n!} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' f(t, t') t^m t'^n. \quad (\text{A8})$$

Referring back to Eq. (A1) with t set to zero (to obtain \mathcal{M} in the Schrödinger picture), and noting that $\mathcal{G}(a, b)$ decays to zero with $|a|, |b|$, we see that \mathcal{M} 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 \mathcal{M} to good accuracy for systems where exact diagonalization is not feasible.

Appendix B: Relationship between $\bar{\rho}_{\text{ULE}}$ and $\bar{\rho}'_{\text{exact}}$

Here we establish Eq. (7) of the main text. As our starting point, we write a formal solution of Eq. (4) of the main text as

$$\rho'(t) = e^{\mathcal{L}_{\text{ULE}} t} [\rho'(0)] + \int_0^t ds e^{\mathcal{L}_{\text{ULE}}(t-s)} [\xi(s)]. \quad (\text{B1})$$

We obtain the exact steady state of the system (in the Lindblad frame) by taking the $t \rightarrow \infty$ limit above: $\lim_{t \rightarrow \infty} \rho'(t) = \bar{\rho}'_{\text{exact}}$.

To compute the $t \rightarrow \infty$ limit on the right-hand side, we consider the eigendecomposition of \mathcal{L}_{ULE} . Due to its Lindblad form and our assumption of a unique steady state, the superoperator \mathcal{L}_{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 $\bar{\rho}_{\text{ULE}}$, respectively. (As in the main text, we have defined $\mathcal{L}_{\text{ULE}}[\bar{\rho}_{\text{ULE}}] = 0$.) Hence $\lim_{t \rightarrow \infty} e^{\mathcal{L}_{\text{ULE}} t} [\mathcal{O}] = \text{Tr}[\mathcal{O}] \bar{\rho}_{\text{ULE}}$. Using $\text{Tr}[\rho'] = 1$ we thus conclude $\lim_{t \rightarrow \infty} e^{\mathcal{L}_{\text{ULE}} t} [\rho'(0)] = \bar{\rho}_{\text{ULE}}$. On the other hand, Eq. (4) of the main text implies that $\text{Tr}[\xi(t)] = 0$; hence $e^{\mathcal{L}_{\text{ULE}}(t-s)}[\xi(s)]$ must decay exponentially with

$t - s$. Taking the limit $t \rightarrow \infty$ in Eq. (B1) hence gives

$$\bar{\rho}'_{\text{exact}} = \bar{\rho}_{\text{ULE}} - \mathcal{L}_{\text{ULE}}^{-1}[\bar{\xi}], \quad (\text{B2})$$

where $\mathcal{L}_{\text{ULE}}^{-1}[\bar{\xi}] \equiv -\int_0^{\infty} ds e^{\mathcal{L}_{\text{ULE}} s} \bar{\xi}$ is finite due to the fact that $\bar{\xi}$ is traceless. Further using the Lindblad frame transformation [Eq. (2) of the main text] gives Eq. (7); this was the result we wished to establish.

Appendix C: Scaling of C_A

Here we show that the dimensionless constant C_A [first appearing in Eq. (9) of the main text] is generically finite in the limit $\Gamma \rightarrow 0$. Recall the definition of C_A :

$$C_A = \frac{2\Gamma \|\mathcal{L}_{\text{ULE}}^{\dagger-1}[\delta A_c]\|}{\langle A \rangle_c}. \quad (\text{C1})$$

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

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

Next, we consider observables whose steady state values vanish in the limit $\Gamma \rightarrow 0$. Since $\lim_{\Gamma \rightarrow 0} \bar{\rho}'$ is diagonal in the eigenbasis of the Hamiltonian [15], there are two classes of operators for which $\lim_{\Gamma \rightarrow 0} \langle \bar{A} \rangle_c = 0$: the first class are operators whose diagonal matrix elements vanish in the eigenbasis of H_S . The second class of operators are those that have nonzero diagonal elements in the eigenbasis of H_S , but whose combination of diagonal elements nevertheless causes A to be orthogonal to $\bar{\rho}_{\text{ULE}}$. For the latter class of operators, C_A can be infinite. However, the vanishing steady-state value of these operators requires fine-tuning of the system and bath parameters – the operator will generically 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

$$A = -i[H_S, Q], \quad (\text{C2})$$

for some finite operator Q [40]. 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 $1 \dots n$). We now use the above property to infer the scaling behavior of C_A .

First, we rewrite Eq. (C2) as $A = \mathcal{L}_{\text{ULE}}^\dagger[Q] - \mathcal{D}_{\text{ULE}}^\dagger[Q]$, where \mathcal{D}_{ULE} denotes the bath-induced component of the ULE Liouvillian (including the Lamb shift). Writing $\frac{1}{1+\mathcal{M}^\dagger}[\hat{A}] = A + \left(\frac{1}{1+\mathcal{M}^\dagger} - 1\right)[A]$, we thus have

$$\frac{1}{1+\mathcal{M}^\dagger}A = \mathcal{L}_{\text{ULE}}^\dagger[Q] + R, \quad (\text{C3})$$

with

$$R = -\mathcal{D}_{\text{ULE}}^\dagger[Q] + \left(\frac{1}{1+\mathcal{M}^\dagger} - 1\right)[A]. \quad (\text{C4})$$

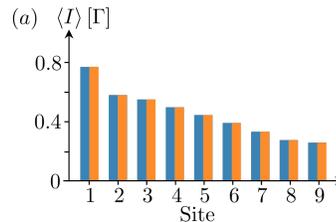


FIG. 3. Steady-state values of the on-site magnetizations in the spin-chain model considered in the main text, without ($\{\langle \bar{\sigma}_n^z \rangle\}$, blue) and with ($\{\langle \bar{\sigma}_n^z \rangle_c\}$, orange) the correction from the inverse Lindblad frame transformation applied.

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. (C3) and the definition $\langle \bar{A} \rangle_c = \text{Tr}[\bar{\rho}_{\text{ULE}}\frac{1}{1+\mathcal{M}^\dagger}A]$, we find

$$\langle \bar{A} \rangle_c = \text{Tr}[\bar{\rho}_{\text{ULE}}R]. \quad (\text{C5})$$

To infer the scaling behavior of R , we first use $\mathcal{D}_{\text{ULE}}^\dagger[Q] = \Theta(\Gamma)$ [15]. Moreover, since $\|\mathcal{M}\| \leq \Gamma\tau$, we have $((1 + \mathcal{M}^\dagger)^{-1} - 1)[A] = \Theta(\Gamma)$. Thus $R = \Theta(\Gamma)$, implying

$$\langle \bar{A} \rangle_c = \Theta(\Gamma). \quad (\text{C6})$$

This demonstrates that $\lim_{\Gamma \rightarrow 0} \langle \bar{A} \rangle_c = 0$ for operators with vanishing diagonal matrix elements in the eigenbasis of H_S , as we inferred above.

We now show that $\mathcal{L}_{\text{ULE}}^{\dagger-1}[\delta A_c] = \Theta(\Gamma^0)$ for operators that can be written in the form in Eq. (C2). Using Eq. (C3), we first note that

$$\mathcal{L}_{\text{ULE}}^{\dagger-1}[\delta A_c] = Q + \mathcal{L}_{\text{ULE}}^{\dagger-1}[R - \langle \bar{A} \rangle_c]. \quad (\text{C7})$$

To analyze the second term on the right hand side of this expression, we note two important facts. First, since $\langle \bar{A} \rangle_c = \text{Tr}[\bar{\rho}_{\text{ULE}}R]$ [see Eq. (C5)], we conclude that the argument $R - \langle \bar{A} \rangle_c$ is orthogonal to $\bar{\rho}_{\text{ULE}}$. Moreover, according to the discussion above, $R - \langle \bar{A} \rangle_c = \Theta(\Gamma)$. Therefore $\mathcal{L}_{\text{ULE}}^{\dagger-1}[R - \langle \bar{A} \rangle_c] = \Theta(\Gamma^0)$. Using $Q = \Theta(\Gamma^0)$, we find

$$\|\mathcal{L}_{\text{ULE}}^{\dagger-1}[\delta A_c]\| = \Theta(\Gamma^0). \quad (\text{C8})$$

Combining this with $\langle \bar{A} \rangle_c = \Theta(\Gamma)$ in Eq. (C1), we conclude C_A is finite in the limit $\Gamma \rightarrow 0$.

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 Lindblad frame transformation, $\langle \bar{\sigma}_n^z \rangle_c$, and $\langle \bar{\sigma}_n^z \rangle$, respectively. As for the computation of the bond current in the main text, we apply the inverse Lindblad

transformation through expansion to first order, setting $(1 + \mathcal{M})^{-1} \approx (1 - \mathcal{M})$ to compute $\langle \bar{\sigma}_n^z \rangle_c$. Evidently, the

two data sets coincide up to negligible relative corrections, as we expected due to the finite value of $\langle \bar{\sigma}_n^z \rangle$ in the weak coupling limit (see main text).