Renormalization approach to non-Markovian open-quantum-system dynamics

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We show that time induces a dynamical renormalization of the system-environment coupling in open-quantum-system dynamics. The renormalizability condition, of the interactions being either local, or, alternatively, defined on a finite continuum support, is generally fulfilled for both discrete and continuous environments. As a consequence, we find a generalized Lieb-Robinson bound to hold for local and, surprisingly, also for nonlocal interactions. This unified picture allows us to devise a controllable approximation for arbitrary non-Markovian dynamics with an *a priori* estimate of the worst-case computational cost.

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I. INTRODUCTION

The interaction with its environment causes a quantum system to lose energy and phase—this is termed decoherence [1]. Decoherence poses a severe challenge to the application of quantum technologies since a quantum system can never completely be isolated from its environment. On the other hand, the effect of the environment is not necessarily detrimental and can likewise be used for robust implementation of quantum processes [2]. A rigorous treatment of decoherence is challenging because the system and environmental degrees of freedom become entangled due to their interaction. This entanglement is neglected when invoking the Markov approximation [1]. However, non-Markovian effects are abundant, in particular in the condensed phase. Examples of current interest include mechanical oscillators close to their ground state [3], carbon nanotubes and graphene [4], excitons of the light-harvesting complex [5], and solid-state devices based on quantum dots [6], superconducting junctions [7], or nitrogen-vacancy centers in diamond [8–10]. A correct treatment of the non-Markovian dynamics is important for application of these systems in quantum technologies which require a sufficient amount of control. Controllability is expected to be better for non-Markovian than Markovian systems due to the equivalence of non-Markovianity and information backflow from the environment to the system [11]. Currently, non-Markovian dynamics are tackled with stochastic methods provided certain assumptions can be made [12–14]. Alternatively, one can simulate the non-Markovian dynamics for finite times, starting from a microscopic model for system and environment and truncating the number of environmental degrees of freedom. This approach is particularly interesting in view of quantum devices which always operate in finite time. It has been successfully employed in the context of single spins in diamond [8], hydrogen diffusion [15] and femtosecond photochemistry at surfaces [16,17], spin dynamics in NMR [18], and the spin-boson toy model [19]. The observation that the truncation approach works for such diverse systems suggests an underlying general property of quantum dynamics: Apparently it takes time to establish correlations between system and environment. Proving such a conjecture would allow one to rigorously quantify the necessary ingredients for an accurate and efficient simulation of open quantum systems.

Here, we prove this conjecture and show that it yields a general approach to modeling decoherence. Our proof allows us to answer the question of why a comparatively small number of environmental degrees of freedom often turns out to be sufficient [8,15–19]. Moreover, we show that no specific structure of the environment and system-environment interaction is required for the truncation approach to be applicable. This allows for simulating arbitrary open-quantum-system dynamics with a prespecified accuracy, employing only a finite number of environmental modes.

Our proof is based upon a fresh look at decoherence by combining the Lieb-Robinson bound known in many-body physics [20,21] with the surrogate Hamiltonian method developed in physical chemistry [15–17]. Technically, for discrete environments, the Lieb-Robinson bound translates the inherent locality of quantum dynamics into a quantitative estimate for the information propagation speed. We show that the notion of an effective light cone can be used to set up a dynamical renormalization procedure for the generator of the "surrogate" evolution. For continuous environments, the interactions are generally nonlocal. We show that the concept of *quasifinite resolution* represents the equivalent of quasilocality for discrete environments. In both cases, time naturally induces a renormalization of the system-environment interaction.

II. DISCRETE ENVIRONMENTS: QUASILOCALITY OF QUANTUM DYNAMICS

We first consider the environment to be comprised of discrete degrees of freedom. Assuming the interactions between system and environment to be bounded and, for simplicity, bilinear, the total Hamiltonian can be defined on a generic lattice in arbitrary dimensions,

$$\hat{H} = \hat{H}_S + \sum_{i=1}^{N_S^{\text{int}}}\sum_{j=1}^{N_B^{\text{int}}} \hat{\Phi}_{ij}^{SB} + \sum_{i<j=1}^{N_B} \hat{\Phi}_{ij}^{B} \tag{1}$$

with N_S and N_B the system and environmental degrees of freedom (DOFs), $N_B \to \infty$. In Eq. (1), each DOF is defined on a finite-dimensional Hilbert space $\mathcal{H}_i$. $N_S^{\text{int}} \leqslant N_S$ ($N_B^{\text{int}} \leqslant N_B$) are those system (environmental) DOFs that interact with the environment (system). The interactions $\hat{\Phi}_{ij}$ can be expressed in terms of linear operators $\hat{O}_i \in \mathcal{B}(\mathcal{H}_i)$,

$$\hat{\Phi}_{ij} = \sum_{\mu=0}^{\dim[\mathcal{B}(\mathcal{H}_i)]-1} \sum_{\nu=0}^{\dim[\mathcal{B}(\mathcal{H}_j)]-1} J_{ij}^{\mu\nu} \hat{O}_i^{\mu} \hat{O}_j^{\nu},$$

with $|J_{ij}^{\mu\nu}| < \infty$ and assuming $[\hat{O}_i, \hat{O}_j] = 0$ for $i \neq j$. Our goal is to truncate the sums over the environmental DOFs in Eq. (1) in a well-defined manner. To this end, we need to quantify the influence of the DOFs upon each other, i.e., we need to introduce a metric. A suitable metric arises naturally by representing the Hamiltonian $\hat{H}$ as a graph G. The set of nodes of the graph is composed of all the system and environmental DOFs $N = \{N_S + N_B\}$, i.e., a possibly infinite number of elements. The edges of the graph are made up by all nonzero elements of the coupling matrix $J_{ij} = [\sum_{\mu\nu}(J_{ij}^{\mu\nu})^2]^{1/2}$, $E = \{J_{ij} \neq 0\}$. The bare structure of the graph is encoded in the adjacency matrix $A = A(G)$ whose entries A_{ij} $(A_{ij} = 0,1)$ represent the edges connecting two nodes i and j. The metric induced by $\hat{H}$ on G is defined as the shortest path connecting two nodes,

$$d(i,j) := \min\{n \in \mathbb{N}_0 : [A^n]_{ij} \neq 0\}.$$

A walk of length n from node i to j is a sequence of n adjacent nodes. Their weight is $\prod_{k=1}^{n-1} J_{i_k,i_{k+1}}$ with the weight of the zero-length walk set equal to 1. Then the overall weight of all paths of length n between i and j is $[J^n]_{ij}$, and the weight of the shortest path(s) is $[J^{d(i,j)}]_{ij}$. Equipped with the metric $d(i,j)$, we can order the environmental DOFs according to their graph distance from the system, i.e., their minimum distance from a node in $\{N_S^{\text{int}}\}$. For the sake of simplicity, we consider a single system node S; the generalization to $N_S > 1$ is straightforward. Reordering the environmental DOFs is expressed by rewriting Hamiltonian (1),

$$\hat{H} = \sum_{d=0}^{\infty} (\hat{h}_d + \hat{h}_{d,d+1}), \tag{2}$$

where $\hat{h}_d$ groups the interactions between DOFs at distance d from the system, i.e., those in the dth layer. $\hat{h}_{d,d+1}$ contains the interactions between DOFs in two successive layers, e.g., $\hat{H}_S = \hat{h}_0$ and $\hat{H}_{SB} = \hat{h}_{0,1}$.

The dynamical evolution of a generic system operator $\hat{A}_S \in \mathcal{B}(\mathcal{H}_S)$ is given by $\hat{A}_S(t) = e^{i\hat{H}t}\hat{A}_S e^{-i\hat{H}t}$. Using the Baker-Campbell-Hausdorff formula, $\hat{A}_S(t)$ can be written in terms of nested commutators,

$$\hat{A}_S(t) = \hat{A}_S + \sum_{d=1}^{\infty} \frac{(-it)^d}{d!} \hat{C}_d, \tag{3}$$

where $\hat{C}_d = [\hat{H}, \hat{C}_{d-1}]$ and $\hat{C}_0 = \hat{A}_S$. We show in Appendix A that $\hat{C}_d$ has nonvanishing commutators only with those terms in $\hat{H}$ that act on DOFs in the layers $d' \leqslant d$, including $\hat{h}_{d,d+1}$. This implies $\hat{C}_n = [\hat{H}, \hat{C}_{n-1}] \equiv [\hat{H}_n, \hat{C}_{n-1}]$ at the nth perturbative order, where

$$\hat{H}_n = \sum_{d=0}^{n-1} (\hat{h}_d + \hat{h}_{d,d+1}) \tag{4}$$

is the truncation of the full generator $\hat{H}$ to the first n layers of the graph. In other words, terms corresponding to bath DOFs at distance n from the system start contributing to the system dynamics only at the nth perturbative order. The system dynamics is thus appreciably affected by those bath modes only after a time that is sufficiently long to make the corresponding perturbative term non-negligible.

In order to make this statement quantitative, we consider the error $\mathcal{R}(n) = \|\hat{A}_S(t) - \hat{A}_S^{H_n}(t)\|$ made by replacing the full evolution $\hat{A}_S(t)$ with that generated by the truncated Hamiltonian (4), $\hat{A}_S^{H_n}(t)$ with the norm understood as the operator norm. The error is bounded by the remainder of the series in Eq. (3) when truncated at order n (cf. Appendix A),

$$\mathcal{R}(n) \leqslant 2\|\hat{A}_S\| \sum_{d=n+1}^{\infty} \frac{(2t\mathcal{O})^d}{d!} \sum_{i,j\in\mathcal{I}_d} [J^d]_{ij},$$

where $\mathcal{O} = \max_{(i,j)\in N;\mu,\nu} \|\hat{O}_i^{\mu}\hat{O}_j^{\nu}\|$, and $\mathcal{I}_d = \{i \in N : d(s,i) \leqslant d\}$ represents the set of DOFs at distance at most d from the system. $\sum_{i,j\in\mathcal{I}_d}[J^d]_{ij}$ is the weight of all paths of length d involving DOFs at distance at most d from the system. If the graph is *locally finite*, i.e., if each DOF interacts with a finite number of other DOFs, then $\|J\| < \infty$ [22]. In this case, we can bound the sum, $\sum_{i,j\in\mathcal{I}_d}[J^d]_{ij} \leqslant (\bar{c}^2\|J\|)^d$, where $\bar{c}$ denotes the maximum connectivity of a node on the graph. This leads to the following Lieb-Robinson bound [20,21,23,24]:

$$\left\|\hat{A}_S(t) - \hat{A}_S^{H_n}(t)\right\| \leqslant 2\|\hat{A}_S\| e^{-(n-vt)} \tag{5}$$

with $v = 2\mathcal{O}\bar{c}^2\|J\|e$ (cf. Appendix A). As shown in Ref. [25], the Lieb-Robinson also holds for anticommuting operators. Equation (5) states the quasilocality of the quantum dynamics of an open quantum system. It implies the existence of an effective light cone for the system that spreads at most at speed v. Bath DOFs outside the effective light cone give only an exponentially vanishing contribution to the evolution of $\hat{A}_S$. The full bath is therefore needed only in the limit of infinite time.

III. CONTINUOUS ENVIRONMENTS: QUASIFINITE RESOLUTION OF QUANTUM DYNAMICS

We now consider the interaction of a central system with a continuous environment. The corresponding Hamiltonian is generically expressed by

$$\begin{aligned}\hat{H} = \hat{H}_S &+ \hat{O}_S^I \int_0^{x_{\max}} J(x)(\hat{c}_x + \hat{c}_x^\dagger)dx \\ &+ 2\int_0^{x_{\max}}\int_x^{x_{\max}} K(|x-x'|)[c_x c_{x'}^\dagger + c_x^\dagger c_{x'} \\ &+ c_x^\dagger \hat{c}_x c_{x'}^\dagger \hat{c}_{x'}]dx\,dx' + \int_0^{x_{\max}} g(x)\hat{c}_x\hat{c}_x^\dagger dx,\end{aligned} \tag{6}$$

where x denotes the relevant bath variable such as energy or position, $x_{\max} < \infty$ is a finite cutoff, and $\hat{O}_S^I$ is a generic system operator. We require the annihilation (creation) operators of bath modes $\hat{c}_x$ $(\hat{c}_x^\dagger)$ to be bounded, i.e., $\|c\| = \max_{x\in[0,x_{\max}]}\|\hat{c}_x\| < \infty$. $J(x)$ denotes the system-bath coupling, $K(|x-x'|)$ the intrabath coupling, assumed symmetric under exchange of x and x', and $g(x)$ is the bath dispersion. The Hamiltonian (6) does not obey local finiteness, since the system interacts with all bath DOFs which, in turn, all may interact among themselves. This corresponds to a graph where all bath DOFs are at distance 1 from the system, such that the results of the previous section cannot be used directly to truncate the Hamiltonian. If the bath is made up of normal modes, $K(|x-x'|)\equiv 0$, then (6) can be mapped onto a semi-infinite chain with the system at one end [26,27], thus recovering local finiteness. However, this requires the bath Hamiltonian to be quadratic and is thus not general. Here, we derive a generally applicable bound equivalent to Eq. (5) for continuous environments, employing the concept of a "surrogate Hamiltonian" [15].

We choose a sequence of n points $\{x_i\}_{i=0}^{n-1}$, in the interval $[0,x_{\max}]$, with $x_i < x_{i+1}$, thus defining a partition $P_n=\{\delta x_i\}$ of the interval with $\delta x_i = x_{i+1}-x_i$. Denoting the norm of P_n by $|P_n| = \max_{i<n}(\delta x_i)$, a sequence of partitions $\{P_n\}$ obeying the condition $|P_{n+1}| < |P_n|$ can be constructed. This defines a sequence of Hamiltonians $\{\hat{H}_{P_n}\}$ with

$$\hat{H}_{P_n} = \hat{H}_S + \hat{O}_S^I \sum_{i=0}^{n-1} \tilde{J}_i(\hat{c}_i + \hat{c}_i^\dagger) + 2\sum_{i<j=0}^{n-1} \tilde{K}_{ij}[\hat{c}_i^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_i + \hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j] + \sum_{i=0}^{n-1}\tilde{g}_i\hat{c}_i^\dagger\hat{c}_i, \tag{7}$$

where $\hat{c}_i = \hat{c}_{x_i}$, $\tilde{J}_i = J(x_i)\delta x_i$, $\tilde{K}_{ij} = K(|x_i - x_j|)\delta x_i\delta x_j$, and $\tilde{g}_i = g(x_i)\delta x_i$ are the rescaled couplings at the n sampling points. Equation (8) can be viewed as Riemann sums built on P_n approximating the corresponding integrals in Eq. (6). By construction, the sequence $\{\hat{H}_{P_n}\}$ converges with $\lim_{n\to\infty}\hat{H}_{P_n} = \hat{H}$.

When estimating the error that is made by time-evolving $\hat{A}_S$ using $\hat{H}_{P_n}$ instead of $\hat{H}$, $\mathcal{R}(P_n) = \|\hat{A}_S(t) - \hat{A}_S^{H_{P_n}}(t)\|$, we need to compare two series of the kind (3), one for $\hat{A}_S(t)$ and one for $\hat{A}_S^{H_{P_n}}(t)$. The triangle inequality can be used to split the error into two parts, $\mathcal{R}(P_n) \leqslant R_1(P_n) + R_2(P_n)$ (see Appendix B for details). The first term evaluates the error made in replacing $\exp[-i\hat{H}t]\exp[i\hat{H}_{P_n}t]$ by $\exp[-i(\hat{H}-\hat{H}_{P_n})t]$, i.e., assuming $\hat{H}$ and $\hat{H}_{P_n}$ to commute. This contribution is bounded by a second-order polynomial in $t^2\|[\hat{H},\hat{H}_{P_n}]\|$. At finite times $R_1(P_n)$ vanishes in the limit $n\to\infty$ due to the convergence of Riemann sums. The second contribution to the error, $R_2(P_n)$, represents the distance between $\hat{A}_S$ and its evolution under $\hat{H}-\hat{H}_{P_n}$. As final estimate we obtain

$$\left\|\hat{A}_S(t) - \hat{A}_S^{H_{P_n}}(t)\right\| \leqslant R_1(P_n) + \|\hat{A}_S\|(e^{2\|\hat{H}-\hat{H}_{P_n}\|t} - 1), \tag{8}$$

with $R_1(P_n)$ given by Eq. (B7). Equation (8) states quasifinite resolution of quantum dynamics: At finite times one can reproduce the system-bath dynamics within arbitrary accuracy by employing an effective generator, Eq. (8), that is constructed on a finite number of sampling points with rescaled couplings. The full continuum of environmental modes is resolved only in the limit of infinite time. The optimal sampling, maximizing the convergence time for a fixed number of modes, is determined by the specific form of the couplings in Eq. (6).

Equations (5) and (8) provide an upper bound to the error made by replacing the full generator $\hat{H}$ with an effective one $\hat{H}_n$ or $\hat{H}_{P_n}$. The bounds are general. They are therefore also very conservative. In some specific cases, tighter model-dependent bounds can be derived [28,29]. For certain classes of initial states, the scaling with time can be dramatically reduced [29,30]. Extension of the bounds Eqs. (5) and (8) to k-linear interactions is straightforward (see Appendix C). However, extension to Hamiltonians containing unbounded operators, i.e., $\mathcal{O}=\infty$, is possible only for certain classes of operators [31,32].

IV. CORRESPONDENCE BETWEEN DISCRETE AND CONTINUOUS ENVIRONMENTS

The Hamiltonian for a system interacting with a continuous environment, Eq. (6), corresponds to an infinite graph whose environmental nodes are all at distance 1 from the system. The Hamiltonians (2) and (6) thus represent the two opposite extremes of an infinite graph—with the infinite number of environmental nodes concentrated in a single layer or distributed over infinitely many layers. In both cases, the system-bath coupling can be defined as the weight $\mathcal{J}_{SB}$ of the paths needed by the system to explore all of the environment. For continuous environments, $\mathcal{J}_{SB} = \int_0^{x_{\max}} J(x)dx$, which is finite because the support of the integral is finite. For discrete environments, $\mathcal{J}_{SB} = \sum_{n=0}^{\infty}\sum_{j:d(s,j)=n}[J^n]_{sj}$, and local finiteness ensures that $\mathcal{J}_{SB}$ can be made finite by rescaling the coupling matrix, e.g., by setting $\tilde{J} = J/r$ with $r \geqslant \bar{c}\|J\|$. This amounts to penalizing longer paths and allows for bounding all quantities on the graph. The dynamics in Hilbert space remains unaffected since any rescaling of the coupling matrix is canceled out by a corresponding rescaling of time ($t\to\tilde{t}=rt$). Local finiteness and the finite cutoff $x_{\max}$ thus play the same role for the two representations of infinitely large environments, with infinitely long paths, the discrete counterpart of infinitely close modes.

V. DYNAMICAL RENORMALIZATION

This unified picture for discrete and continuous environments implies that in both cases time naturally induces a dynamical renormalization over the system-bath interaction. It is expressed by the bounds Eqs. (5) and (8), which provide a recursive update rule for the effective generators, as illustrated in Fig. 1. For discrete environments, the number of required bath modes is obtained as function of time, $n=n(t)$, by specifying the desired accuracy and inverting Eq. (5). Defining $\tilde{\mathcal{J}}(n(t)) = \sum_{d=0}^{n(t)}\sum_{j:d(s,j)=d}[\tilde{J}^d]_{sj}$, the renormalization flow is expressed as $\lim_{t\to\infty}\tilde{\mathcal{J}}(n(t)) = \tilde{\mathcal{J}}_{SB}$. For continuous environments, given a desired accuracy and simulation time, the required resolution is obtained from Eq. (8) as $|P_n| = |P_{n(t)}|$. The renormalization flow corresponds to the convergence of Riemann sums, $\mathcal{J}(P_{n(t)}) = \sum_{i\in P_{n(t)}}\tilde{J}_i$ as $\lim_{t\to\infty}\mathcal{J}(P_{n(t)}) = \mathcal{J}_{SB}$.

Due to Eqs. (5) and (8) the dynamics of any open quantum system can be simulated efficiently on a quantum computer: Once the generator is defined on a finite Hilbert space, it can be approximated by a Suzuki-Trotter decomposition [33–36]. This represents a quantum circuit, i.e., a sequence of elementary quantum gates for each time step. The cost of simulating the effective generator scales only polynomially in time and the number of effective degrees of freedom as

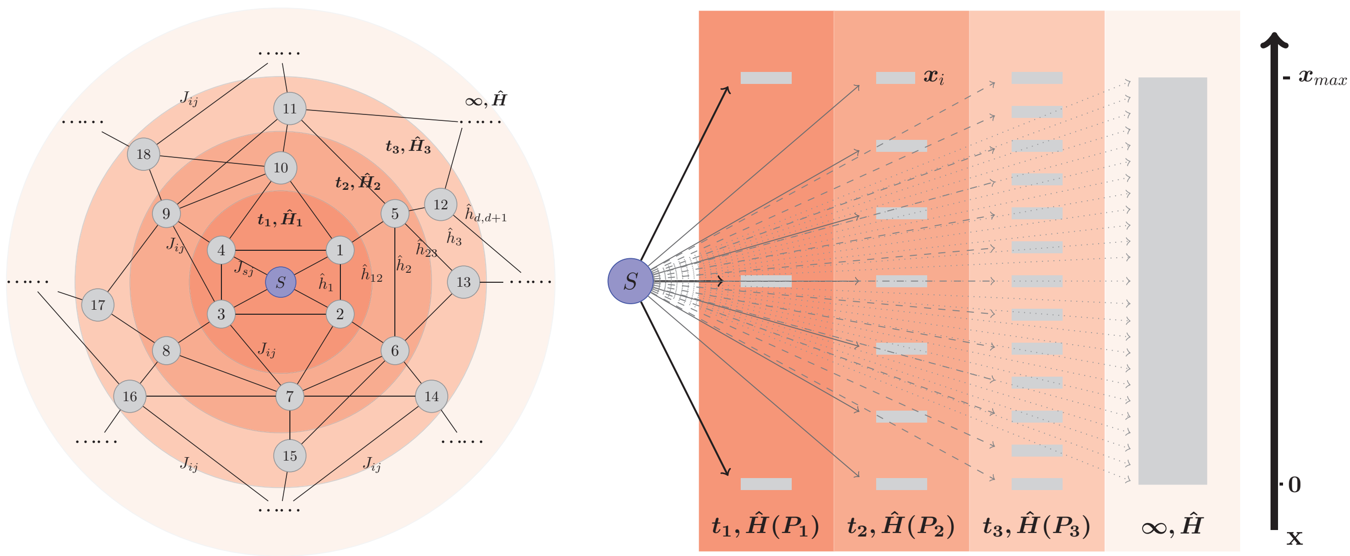

FIG. 1. (Color online) Dynamical renormalization of the system-environment coupling. Discrete environments (left): The effective generator $\hat{H}_d$ is updated by adding the interaction with all environmental degrees of freedom in the $(d+1)$st layer and the new local terms. Continuous environments (right): The effective generator $\hat{H}_{P_n}$ is updated to $\hat{H}_{P_{n+1}}$ by adding sampling points in the interval $[0, x_{\max}]$ and rescaling the couplings.

shown in Appendix D. The resources required on a classical computer are, however, exponential in the number of effective environmental degrees of freedom.

This is due to the exponential scaling of the system-plus-bath state that needs to be stored. It is in contrast to uncontrollable approximations such as the Markov approximation where the environment is completely eliminated from the reduced dynamics such that the computational resources are constant with time and depend only on the size of the system Hilbert space. The exponential scaling of the computational resources with the number of effective degrees of freedom can be reduced to a polynomial one by employing further controlled restrictions of the size of the effective Hilbert space [16–18,37–39].

VI. CONCLUSIONS

We have shown that the reduced dynamics of an arbitrary open quantum system can be obtained reliably and accurately, by employing only a finite-dimensional effective Hamiltonian. This is due to time inducing a dynamical renormalization of the system-environment interaction, i.e., the system interacts progressively with the environmental degrees of freedom rather than with all of them at once. The required renormalizability condition, locality of the interactions for discrete environments and finite support of the interactions for continuous environments, is generally fulfilled. While the Lieb-Robinson bound has been discussed in the context of dissipative dynamics before [25,40], it was not employed for the full system-bath evolution. Carrying out this very natural application of the bound, we have generalized the notion of quasilocality of quantum dynamics to nonlocal interactions. In spin dynamics, the Lieb-Robinson bound provides the theoretical foundation of truncation-based algorithms such as the time-dependent density-matrix renormalization group [24]. Similarly, our results allow assessment of the worst-case computational cost of truncation-based algorithms for non-Markovian dynamics and certify *a priori* their accuracy versus computational complexity.

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APPENDIX A: QUASILOCALITY OF QUANTUM DYNAMICS FOR DISCRETE ENVIRONMENTS

In this appendix we prove the quasilocality of quantum dynamics for a system interacting with an environment comprised of discrete degrees of freedom, such as a spin bath, obeying bosonic commutation relations. The extension to fermionic operators is found in Refs. [25,41]. The total system+environment is defined on a lattice. Hence the starting point is the Hamiltonian, Eq. (3) in the main text, written in terms of $\hat{h}_d$, grouping the interactions between DOFs at graph distance d from the system region, i.e., in the dth layer, and $\hat{h}_{d,d+1}$, comprising the interactions between DOFs in two successive layers. With these definitions, $\hat{H}_S \equiv \hat{h}_0$ and $\hat{H}_{SB} \equiv \hat{h}_{0,1}$. If the system is made up of more than a single node, the graph distance is calculated as the minimum between a bath and a system DOF.

The dynamics of a generic system operator $\hat{A}_S \in \mathcal{B}(\mathcal{H}_S)$ is described by

$$\hat{A}_S(t) = e^{i\hat{H}t}\hat{A}_S e^{-i\hat{H}t}.$$

Using the Baker-Campbell-Hausdorff formula, this can be expressed in terms of nested commutators [cf. Eq. (3) of the main paper], where the commutator $\hat{C}_n$,

$$\hat{C}_n = [\hat{H},\hat{C}_{n-1}],$$

appears at the nth order, and $\hat{C}_0 = \hat{A}_S$. Up to nth perturbative order the evolution generated by the full Hamiltonian $\hat{H}$ is the same as that generated by its truncation to n graph layers using the graph-distance-based ordering of the DOFs [cf. Eq. (4) of the main paper], i.e.,

$$C_n = [\hat{H},\hat{C}_{n-1}] = [\hat{H}_n,\hat{C}_{n-1}] = \left[\hat{H}_n,\hat{C}_{n-1}^{H_n}\right] = C_n^{H_n}.$$

The error made by evolving $\hat{A}_S$ with $\hat{H}_n$ instead of the full generator $\hat{H}$ can therefore be bounded by the operator norm of the remainder of the truncated series,

$$\begin{aligned}\mathcal{R}(n) &= \left\|\hat{A}_S(t) - \hat{A}_S^{H_n}(t)\right\| \\ &= \left\|\sum_{d=n+1}^{\infty} \frac{(-it)^d}{d!}\left(\hat{C}_d - \hat{C}_d^{H_n}\right)\right\| \\ &\leqslant 2\left\|\sum_{d=n+1}^{\infty} \frac{(-it)^d}{d!}\hat{C}_d\right\|, \end{aligned} \tag{A1}$$

where $\hat{A}_S^{H_n}(t) = \exp(i\hat{H}_n t)\hat{A}_S\exp(-i\hat{H}_n t)$. The triangular inequality yields

$$\mathcal{R}(n) \leqslant 2\sum_{n+1}^{\infty}\frac{t^d}{d!}\|\hat{C}_d\|. \tag{A2}$$

In order to estimate $\|\hat{C}_d\|$, we need to consider the following commutators between operators in $\hat{H}$:

$$\begin{aligned}&[\hat{h}_d,\hat{h}_{d'} + \hat{h}_{d',d'+1}] \\ &\quad = [\hat{h}_d,\hat{h}_{d,d+1}]\delta_{d,d'} + [\hat{h}_d,\hat{h}_{d-1,d}]\delta_{d-1,d'}, \qquad \text{(A3a)}\\ &[\hat{h}_{d,d+1},\hat{h}_{d'} + \hat{h}_{d',d'+1}] \\ &\quad = [\hat{h}_{d,d+1},\hat{h}_d]\delta_{d,d'} + [\hat{h}_{d,d+1},\hat{h}_{d+1} + \hat{h}_{d+1,d+2}]\delta_{d+1,d'} \\ &\qquad + [\hat{h}_{d,d+1},\hat{h}_{d-1,d}]\delta_{d-1,d'}. \qquad \text{(A3b)}\end{aligned}$$

"Local" operators $\hat{h}_d$, i.e., terms involving interactions between DOFs within the same layer, have nonvanishing commutators only with operators connecting the dth layer with the neighboring layers $d \pm 1$ [cf. Eq. (A3a)]. Since the $(d+1)$st layer is already accounted for in $\hat{h}_{d,d+1}$, commutators of local terms $\hat{h}_d$, Eq. (A3a), do not introduce further layers. In other words, these commutators do not increase the size of the bath Hilbert space that is "seen" by the system. Terms involving interactions between the dth and the $(d+1)$st layer, i.e., $\hat{h}_{d,d+1}$, have nonvanishing commutators at most with terms in the same, the previous, or the $(d+2)$nd layer. Therefore, commutators involving the nonlocal terms $\hat{h}_{d,d+1}$ add operators from one additional layer, i.e., they enlarge the system "view" by one graph layer at each perturbative order. Examining the generic structure of the $\hat{C}_d$'s, we find for $\hat{C}_1$,

$$\hat{C}_1 = [\hat{H},\hat{A}_S] \equiv [\hat{h}_0 + \hat{h}_{0,1},\hat{A}_S].$$

We can rewrite

$$\hat{h}_0 + \hat{h}_{0,1} = \sum_{\substack{i,j:\\ d(S,i)=0;\\ d(S,j)\leqslant 1}}\sum_{\mu,\nu} J_{ij}^{\mu\nu}\hat{O}_i^{\mu}\hat{O}_j^{\nu}$$

using Eq. (2) of the main text and the definition of $\hat{\Phi}_{ij}$'s. This highlights the fact that $\hat{h}_0 + \hat{h}_{0,1}$ groups all interactions within the system and between system and bath. It implies

$$\begin{aligned}\hat{C}_1 &= \sum_{\substack{i,j:\\ d(S,i)=0;\\ d(S,j)\leqslant 1}}\sum_{\mu,\nu} J_{ij}^{\mu\nu}\left[\hat{O}_i^{\mu}\hat{O}_j^{\nu},\hat{A}_S\right] \\ &= \sum_j\sum_{\mu,\nu} J_{Sj}^{\mu\nu}\left[\hat{O}_S^{\mu}\hat{O}_j^{\nu},\hat{A}_S\right]. \end{aligned} \tag{A4}$$

In the second line, we have used that only commutators between operators which act at least on one common DOF do not vanish, assuming, for the sake of clarity, that $\hat{A}_S$ acts on a single system DOF. Should $\hat{A}_S$ act on multiple system DOFs, a sum over these DOFs needs to be included additionally. Introducing

$$\mathcal{O} = \max_{ij\in N;\mu,\nu}\left\|\hat{O}_i^{\mu}\hat{O}_j^{\nu}\right\|,$$

the norm of $\hat{C}_1$ can be estimated,

$$\|\hat{C}_1\| \leqslant 2\|A_S\|\mathcal{O}\sum_j J_{Sj},$$

where $J_{ij} = [\sum_{\mu\nu}(J_{ij}^{\mu\nu})^2]^{1/2}$ denotes the coupling matrix on the graph. In the following, we drop the indices μ and ν, accounting for the corresponding sums in the coupling matrix J, and denote the system operator that enters the system-bath interaction by $\hat{O}_S^I$. Due to Eqs. (A3a) and (A3b), $\hat{C}_2$ is written as

$$\hat{C}_2 = [\hat{h}_0 + \hat{h}_{0,1} + \hat{h}_1 + \hat{h}_{1,2},\hat{C}_1].$$

Using Eq. (A4) and following the same argument we find

$$\begin{aligned}\hat{C}_2 &= \sum_{\substack{p,q:\\ d(S,p)\leqslant 1\\ d(S,q)\leqslant 2}}\sum_{j:d(S,j)\leqslant 1} J_{pq}J_{Sj}\left[\hat{O}_p\hat{O}_q,\left[\hat{O}_S^I\hat{O}_j,\hat{A}_S\right]\right] \\ &= \sum_{\substack{j,q:\\ d(S,j)\leqslant 1\\ d(S,q)\leqslant 2}} J_{qj}J_{Sj}\left[\hat{O}_q\hat{O}_j,\left[\hat{O}_S^I\hat{O}_j,\hat{A}_S\right]\right]. \end{aligned} \tag{A5}$$

So $\hat{C}_2$ groups the commutators along paths of length 2 that either depart from the system without returning to it ($j \neq S, p \neq S$), or pass through it one or two times ($j = S$ and/or $p = S$).

Analogously to the norm of C_1, we can estimate $\|\hat{C}_2\|$,

$$\|\hat{C}_2\| \leqslant \|A_S\|\,(2\mathcal{O})^2\sum_{i,j\in\mathcal{I}_2}[J^2]_{ji},$$

where $\mathcal{I}_2 = \{i \in N : d(S,i) \leqslant 2\}$ denotes the set of nodes at distance at most 2 from the system, and $\sum_{i,j\in\mathcal{I}_2}[J^2]_{ji}$ is the weight of all paths of length 2 that exist between DOFs in $\mathcal{I}_2$. Iterating this procedure, the general form of the $\hat{C}_d$'s is found to be

$$\begin{aligned}\hat{C}_d = &\sum_{\substack{(i_1,j_1)\in\mathcal{I}_1\\ \vdots\\ (i_d,j_d)\in\mathcal{I}_d}}\prod_{k\in[1,d]} J_{i_k,j_k} \\ &\times\left[\hat{O}_{i_d}\hat{O}_{j_d},\left[\hat{O}_{i_{d-1}}\hat{O}_{j_{d-1}},\left[\cdots\left[\hat{O}_{i_1}\hat{O}_{j_1},\hat{A}_S\right]\cdots\right]\right]\right]. \end{aligned} \tag{A6}$$

The set $\mathcal{I}_k = \{i \in N : d(s,i) \leqslant k\}$ contains the DOFs belonging to the first k layers of the graph. Thus $\mathcal{I}_k \subseteq \mathcal{I}_{k+1}$. Due to the presence of the commutators and Eqs. (A3a) and (A3b), the only nonvanishing terms in the sums over the $\mathcal{I}_k$ are those where all adjacent pairs of indices have at least one element in common, i.e., those of the general form

$$\sum_{\alpha_{d-1}\in\mathcal{I}_{d-1}} \sum_{\alpha_{d-2}\in\mathcal{I}_{d-2}} \cdots \sum_{\alpha_0\in\mathcal{I}_0} J_{i,\alpha_{d-1}} \prod_{k=0,d-2} J_{\alpha_{k+1},\alpha_k}$$

with $i \in \mathcal{I}_d$. Each of these terms represents a path of length d within the first d layers of the graph. We can therefore estimate

$$\|\hat{C}_d\| \leqslant \|\hat{A}_S\|(2\mathcal{O})^d \sum_{i,j\in\mathcal{I}_d} [J^d]_{ij}, \tag{A7}$$

where the sum accounts for all paths of length d between two DOFs that are at most at distance d from the system. Hence, we can bound the right-hand side of Eq. (A2),

$$\mathcal{R}(n) \leqslant 2\|\hat{A}_S\| \sum_{d=n+1}^{\infty} \frac{(2t\mathcal{O})^d}{d!} \sum_{i,j\in\mathcal{I}_d} [J^d]_{ij}.$$

If the graph is *locally finite*, i.e., if each DOF is connected to a finite amount of other DOFs, then

$$\|J\| \leqslant \max_{i\in N} \sum_j J_{ij} \leqslant \infty. \tag{A8}$$

Labeling the maximum connectivity of a node on the graph by $\bar{c}$, we can estimate

$$\sum_{i,j\in\mathcal{I}_d} [J^d]_{ij} \leqslant (\bar{c}^2\|J\|)^d, \tag{A9}$$

since the relevant part of the coupling matrix J^d contains at most $\bar{c}^{2d}$ elements, each of them less than or equal to $\|J\|^d$. Under the assumption of local finiteness, we thus obtain the following Lieb-Robinson bound [20,21,23,24]:

$$\begin{aligned}\mathcal{R}(n) &\leqslant 2|S|\|\hat{A}_S\| \sum_{d=n+1}^{\infty} \frac{(2t\mathcal{O}\bar{c}^2\|J\|e^{\mu})^d}{d!} e^{-\mu d} \\ &\leqslant 2|S|\|\hat{A}_S\| e^{-\mu(n-vt)},\end{aligned} \tag{A10}$$

where

$$v = 2\,\|\mathcal{O}\|\,\bar{c}^2\,\|J\|\,e^{\mu}/\mu,$$

and $|S|$ accounts for $\hat{O}_S$ acting on several system nodes. The factor $e^{\mu n}$ with $\mu > 0$ has been introduced in v to emphasize the exponential decay of the error with the number of layers taken into account. Minimizing $\mathcal{R}(n)$ as a function of μ leads to the choice $\mu = 1$ and hence Eq. (6) of the main text.

APPENDIX B: QUASIFINITE RESOLUTION OF QUANTUM DYNAMICS FOR CONTINUOUS ENVIRONMENTS

We start from the generic Hamiltonian, Eq. (7) in the main text, describing the interaction of a system with a continuous environment. The goal is to bound the error made by evolving a generic system operator $\hat{A}_S(t)$ employing the surrogate Hamiltonian $\hat{H}_{P_n}$, Eq. (8) in the main text, instead of the full generator $\hat{H}$. Using the unitary invariance of the norm, i.e., $\|\hat{U}\hat{A}\hat{U}^+\| = \|\hat{A}\|$, together with the triangle inequality, the error is expressed as

$$\begin{aligned}&\left\|\hat{A}_S(t) - \hat{A}_S^{H_{P_n}}(t)\right\| \\ &\quad= \|e^{-i\hat{H}_{P_n}t}e^{i\hat{H}t}\hat{A}_S e^{-i\hat{H}t}e^{i\hat{H}_{P_n}} - \hat{A}_S\| \\ &\quad\leqslant \|e^{-i\hat{H}_{P_n}t}e^{i\hat{H}t}\hat{A}_S e^{-i\hat{H}t}e^{i\hat{H}_{P_n}} - e^{i(\hat{H}-\hat{H}_{P_n})t}\hat{A}_S e^{-i(\hat{H}-\hat{H}_{P_n})t}\| \\ &\qquad+ \|e^{i(\hat{H}-\hat{H}_{P_n})t}\hat{A}_S e^{-i(\hat{H}-\hat{H}_{P_n})t} - \hat{A}_S\| \\ &\quad\equiv R_1(P_n) + R_2(P_n).\end{aligned} \tag{B1}$$

The strategy is now to bound each of the two terms $R_1(P_n)$ and $R_2(P_n)$.

We first consider $R_1(P_n)$ and define a function $F(\lambda)$ [35],

$$F(\lambda) = 1 - e^{i\lambda\hat{H}}e^{-i\lambda\hat{H}_{P_n}}e^{-i\lambda(\hat{H}-\hat{H}_{P_n})}, \tag{B2}$$

with $F(0) = 0$. Derivation with respect to λ yields

$$\frac{\partial F(\lambda)}{\partial\lambda} = e^{i\lambda\hat{H}}[e^{-i\lambda\hat{H}_{P_n}}, i\hat{H}]e^{-i\lambda(\hat{H}-\hat{H}_{P_n})}. \tag{B3}$$

Applying the Kubo identity [42],

$$[i\hat{H}, e^{-i\lambda\hat{H}_{P_n}}] = \int_0^{\lambda} e^{-i(\lambda-\mu)\hat{H}_{P_n}}\left[\hat{H}, \hat{H}_{P_n}\right]e^{-i\mu\hat{H}_{P_n}}\,d\mu,$$

we can rewrite Eq. (B3), obtaining

$$\begin{aligned}\frac{\partial F(\lambda)}{\partial\lambda} = &-\int_0^{\lambda} d\mu e^{i\lambda\hat{H}}e^{-i\mu\hat{H}_{P_n}} \\ &\times\left[\hat{H}, \hat{H}_{P_n}\right]e^{-i(\lambda-\mu)\hat{H}_{P_n}}e^{-i\lambda(\hat{H}-\hat{H}_{P_n})}.\end{aligned} \tag{B4}$$

Integration, using the initial condition $F(0) = 0$ and Eq. (B2), yields

$$\begin{aligned}&e^{-i(\hat{H}-\hat{H}_{P_n})t} - e^{-i\hat{H}t}e^{\hat{H}_{P_n}t} \\ &\quad= -\int_0^t d\lambda\int_0^{\lambda} d\mu e^{i\lambda\hat{H}}e^{-i\mu\hat{H}_{P_n}}\left[\hat{H}, \hat{H}_{P_n}\right] \\ &\qquad\times e^{-i(\lambda-\mu)\hat{H}_{P_n}}e^{-i\lambda(\hat{H}-\hat{H}_{P_n})}.\end{aligned} \tag{B5}$$

Estimation of the norms and of the integrals in Eq. (B5) leads to [35,36]

$$\|e^{-i(\hat{H}-\hat{H}_{P_n})t} - e^{-i\hat{H}t}e^{i\hat{H}_{P_n}t}\| \leqslant \frac{t^2}{2}\left\|\left[\hat{H}, \hat{H}_{P_n}\right]\right\|. \tag{B6}$$

Equation (B6) allows estimation of $R_1(P_n)$ as

$$\begin{aligned}R_1(P_n) &= \|e^{-i\hat{H}_{P_n}t}e^{i\hat{H}t}\hat{A}_S e^{-i\hat{H}t}e^{i\hat{H}_{P_n}t} \\ &\quad- e^{i(\hat{H}-\hat{H}_{P_n})t}\hat{A}_S e^{-i(\hat{H}-\hat{H}_{P_n})t}\| \\ &\leqslant 2\|e^{-i\hat{H}_{P_n}t}e^{i\hat{H}t}\hat{A}_S(e^{-i\hat{H}t}e^{i\hat{H}_{P_n}t} - e^{-i(\hat{H}-\hat{H}_{P_n})t})\| \\ &\quad+ \|(e^{i\hat{H}t}e^{-i\hat{H}_{P_n}t} - e^{i(\hat{H}-\hat{H}_{P_n})t}) \\ &\quad\times\hat{A}_S(e^{-i\hat{H}t}e^{i\hat{H}_{P_n}t} - e^{-i(\hat{H}-\hat{H}_{P_n})t})\| \\ &\leqslant \|\hat{A}_S\|\frac{t^2}{2}\left\|\left[\hat{H}, \hat{H}_{P_n}\right]\right\|\left(2 + \frac{t^2}{2}\left\|\left[\hat{H}, \hat{H}_{P_n}\right]\right\|\right).\end{aligned} \tag{B7}$$

We thus find that $R_1(P_n)$ is bounded by a second-order polynomial in $t^2\|[\hat{H}, \hat{H}_{P_n}]\|$ and hence depends on how well the integrals in the full generator are approximated by the sums in the surrogate one. Indeed, for finite t, $R_1(P_n)$ depends on the commutator of $\hat{H}$ and $\hat{H}_{P_n}$ which vanishes in the limit $n \to \infty$ since any operator commutes with itself. In order to give an explicit example, for the Hamiltonian (6) in the main text we can write

$$\begin{aligned}
[\hat{H},\hat{H}_{P_n}] &= [\hat{H}_S,\hat{O}_S^I]\left\{\sum_{i=0}^{n-1}\tilde{J}_i(\hat{c}_i+\hat{c}_i^\dagger)-\int_0^{x_{\max}}J(x)(\hat{c}_x+\hat{c}_x^\dagger)dx\right\}\\
&\quad+(\hat{O}_S^I)^2\left[\int_0^{x_{\max}}J(x)(\hat{c}_x+\hat{c}_x^\dagger)dx,\sum_{i=0}^{n-1}\tilde{J}_i(\hat{c}_i+\hat{c}_i^\dagger)\right]+\hat{O}_S^I\left[\int_0^{x_{\max}}J(x)(\hat{c}_x+\hat{c}_x^\dagger)dx,\sum_{i=0}^{n-1}\tilde{g}_i\hat{c}_i^\dagger\hat{c}_i\right]\\
&\quad+\left[\int_0^{x_{\max}}g(x)\hat{c}_x^\dagger\hat{c}_xdx,\sum_{i=0}^{n-1}\tilde{J}_i(\hat{c}_i+\hat{c}_i^\dagger)\right]\hat{O}_S^I+\left[\int_0^{x_{\max}}g(x)\hat{c}_x^\dagger\hat{c}_xdx,\sum_{i=0}^{n-1}\tilde{g}_i\hat{c}_i^\dagger\hat{c}_i\right]\\
&\quad+\hat{O}_S^I\left[\int_0^{x_{\max}}J(x)(\hat{c}_x+\hat{c}_x^\dagger)dx,2\sum_{i<j=0}^{n-1}\tilde{K}_{ij}(\hat{c}_i\hat{c}_j^\dagger+\hat{c}_i\hat{c}_j^\dagger+\hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j)\right]\\
&\quad+\left[2\int_0^{x_{\max}}\int_x^{x_{\max}}K(|x-x'|)(\hat{c}_x\hat{c}_{x'}^\dagger+\hat{c}_x^\dagger\hat{c}_{x'}+\hat{c}_x^\dagger\hat{c}_x\hat{c}_{x'}^\dagger\hat{c}_{x'})dxdx',\sum_{i=0}^{n-1}\tilde{J}_i(\hat{c}_i+\hat{c}_i^\dagger)\right]\hat{O}_S^I\\
&\quad+4\left[\int_0^{x_{\max}}\int_x^{x_{\max}}K(|x-x'|)(\hat{c}_x\hat{c}_{x'}^\dagger+\hat{c}_x^\dagger\hat{c}_{x'}+\hat{c}_x^\dagger\hat{c}_x\hat{c}_{x'}^\dagger\hat{c}_{x'})dxdx',\sum_{i<j=0}^{n-1}\tilde{K}_{ij}(\hat{c}_i\hat{c}_j^\dagger+\hat{c}_i^\dagger\hat{c}_j+\hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j)\right]\\
&\quad+2\left[\int_0^{x_{\max}}\int_x^{x_{\max}}K(|x-x'|)(\hat{c}_x\hat{c}_{x'}^\dagger+\hat{c}_x^\dagger\hat{c}_{x'}+\hat{c}_x^\dagger\hat{c}_x\hat{c}_{x'}^\dagger\hat{c}_{x'})dxdx',\sum_{i=0}^{n-1}\tilde{g}_i\hat{c}_i^\dagger\hat{c}_i\right]\\
&\quad+\left[\int_0^{x_{\max}}g(x)\hat{c}_x^\dagger\hat{c}_xdx,2\sum_{i<j=0}^{n-1}\tilde{K}_{ij}(\hat{c}_i\hat{c}_j^\dagger+\hat{c}_i^\dagger\hat{c}_j+\hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j)\right].
\end{aligned} \tag{B8}$$

We define

$$\hat{C}_{JJ}=(\hat{O}_S^I)^2\left[\int_0^{x_{\max}}J(x)(\hat{c}_x+\hat{c}_x^\dagger)dx,\sum_{i=0}^{n-1}\tilde{J}_i(\hat{c}_i+\hat{c}_i^\dagger)\right], \tag{B9}$$

$$\hat{C}_{gg}=\left[\int_0^{x_{\max}}g(x)\hat{c}_x^\dagger\hat{c}_xdx,\sum_{i=0}^{n-1}\tilde{g}_i\hat{c}_i^\dagger\hat{c}_i\right], \tag{B10}$$

$$\hat{C}_{Jg}+\hat{C}_{gJ}=\hat{O}_S^I\left[\int_0^{x_{\max}}J(x)(\hat{c}_x+\hat{c}_x^\dagger)dx,\sum_{i=0}^{n-1}\tilde{g}_i\hat{c}_i^\dagger\hat{c}_i\right]+\left[\int_0^{x_{\max}}g(x)\hat{c}_x^\dagger\hat{c}_xdx,\sum_{i=0}^{n-1}\tilde{J}_i(\hat{c}_i+\hat{c}_i^\dagger)\right]\hat{O}_S^I, \tag{B11}$$

$$\begin{aligned}
\hat{C}_{JK}&=\hat{O}_S^I\left[\int_0^{x_{\max}}J(x)(\hat{c}_x+\hat{c}_x^\dagger)dx,2\sum_{i<j=0}^{n-1}\tilde{K}_{ij}(\hat{c}_i\hat{c}_j^\dagger+\hat{c}_i^\dagger\hat{c}_j+\hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j)\right]\\
&\quad+2\left[\int_0^{x_{\max}}\int_x^{x_{\max}}K(|x-x'|)(\hat{c}_x\hat{c}_{x'}^\dagger+\hat{c}_x^\dagger\hat{c}_{x'}+\hat{c}_x^\dagger\hat{c}_x\hat{c}_{x'}^\dagger\hat{c}_{x'})dxdx',\sum_{i=0}^{n-1}\tilde{J}_i(\hat{c}_i+\hat{c}_i^\dagger)\right]\hat{O}_S^I,
\end{aligned} \tag{B12}$$

$$\hat{C}_K=4\left[\int_0^{x_{\max}}\int_x^{x_{\max}}K(|x-x'|)(\hat{c}_x\hat{c}_{x'}^\dagger+\hat{c}_x^\dagger\hat{c}_{x'}+\hat{c}_x^\dagger\hat{c}_x\hat{c}_{x'}^\dagger\hat{c}_{x'})dxdx',\sum_{i<j=0}^{n-1}\tilde{K}_{ij}(\hat{c}_i\hat{c}_j^\dagger+\hat{c}_i^\dagger\hat{c}_j+\hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j)\right], \tag{B13}$$

$$\begin{aligned}
\hat{C}_{gK}&=2\left[\int_0^{x_{\max}}\int_x^{x_{\max}}K(|x-x'|)(\hat{c}_x\hat{c}_{x'}^\dagger+\hat{c}_x^\dagger\hat{c}_{x'}+\hat{c}_x^\dagger\hat{c}_x\hat{c}_{x'}^\dagger\hat{c}_{x'})dxdx',\sum_{i=0}^{n-1}\tilde{g}_i\hat{c}_i^\dagger\hat{c}_i\right]\\
&\quad+2\left[\int_0^{x_{\max}}g(x)\hat{c}_x^\dagger\hat{c}_xdx,\sum_{i<j=0}^{n-1}\tilde{K}_{ij}(\hat{c}_i\hat{c}_j^\dagger+\hat{c}_i^\dagger\hat{c}_j+\hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j)\right].
\end{aligned} \tag{B14}$$

Using these definitions and the triangular inequality, the operator norm of the commutator of the full generator and the surrogate one can be rewritten,

$$\|[\hat{H},\hat{H}_{P_n}]\| \leqslant \|[\hat{H}_S,\hat{O}_S^I]\| R_J(P_n) + \|C_{JJ}\| + \|C_{gg}\| + \|\hat{C}_{Jg}+\hat{C}_{gJ}\| + \|\hat{C}_{JK}\| + \|\hat{C}_{KK}\| + \|\hat{C}_{gK}\|, \tag{B15}$$

where

$$R_J(P_n) \leqslant \sum_i \left(\left\| J(x_i)\delta x_i (c_i + c_i^\dagger) - \int_{\delta x_i} J(x)(c_x + c_x^\dagger) dx \right\| \right)$$

bounds the error made by evaluating the integral over $J(x)(c_x + c_x^\dagger)$ in terms of the Riemann sum built on the partition P_n. This error vanishes in the limit $|P_n| \to 0$, where $|P_n| = \max_{i \leqslant n} \delta x_i$. The norm of the remaining terms in Eq. (B15) can be evaluated along the same lines. First we note that if one assumes bosonic commutation rules, the terms $\hat{C}_{JJ}, \hat{C}_{gg}$, and $\hat{C}_{Jg} + \hat{C}_{gJ}$ vanish and do not contribute to $\mathcal{R}_1(P_n)$ since any commutator acting on the bath degrees of freedom has the generic form

$$[\hat{A}_x, \hat{B}_{x'}] = [\hat{A}_x, \hat{B}_x]\delta_{x,x'}. \tag{B16}$$

In case of fermionic operators the terms $\hat{C}_{gg}$ and $\hat{C}_{Jg} + \hat{C}_{gJ}$ vanish as well. Indeed the commutator between two operators, of which one is the product of an even number of fermionic operators acting on the same site, obeys Eq. (B8). The only surviving term, $\|\hat{C}_{JJ}\|$, can be bounded as

$$\|\hat{C}_{JJ}\| \leqslant 2\big(\hat{O}_S^I\big)^2 R_{JJ}(P_n) \tag{B17}$$

with

$$R_{JJ}(P_n) = \sum_i \delta x_i \int_{\delta x_i} J(x) J(x_i) (2\|\hat{c}_x \hat{c}_i\| + \|[\hat{c}_x, c_i^\dagger] - [\hat{c}_i, c_x^\dagger]\|) dx, \tag{B18}$$

which vanishes in the limit $\sum_i \delta x_i \to \int dx$ since $\hat{c}_i \to \hat{c}_x$ and $\|\hat{c}_x^2\| = 0$. From Eq. (B18), one can see that the contribution to $\mathcal{R}_1(P_n)$ coming from commutators involving local bath operators depends on how well the integrals are approximated by their Riemann sums over P_n, and hence vanish for $|P_n| \to 0$. The same happens for the remaining contributions which do not distinguish between fermionic and bosonic operators since all of them involve commutators where at least one term is the product of an even number of single-site operators. Using Eq. (B16) we thus rewrite $\hat{C}_{JK}$ in Eq. (B12),

$$\hat{C}_{JK} = 2\hat{O}_S^I \sum_{i\neq j} J(x_i)\tilde{K}_{ij}[\hat{c}_i + \hat{c}_i^\dagger, \hat{c}_i\hat{c}_j^\dagger + \hat{c}_i^\dagger\hat{c}_j + \hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j] - 2\hat{O}_S^I \int_0^{x_{\max}} \sum_{i:x_i\neq x} K(|x-x_i|)\,\tilde{J}_i[\hat{c}_i + \hat{c}_i^\dagger, \hat{c}_i\hat{c}_x^\dagger + \hat{c}_i^\dagger\hat{c}_x + \hat{c}_i^\dagger\hat{c}_i\hat{c}_x^\dagger\hat{c}_x] dx, \tag{B19}$$

such that we can estimate

$$\|C_{JK}\| \leqslant 2\left\|\hat{O}_S^I\right\| R_{JK}(P_n). \tag{B20}$$

Then

$$R_{JK}(P_n) = \sum_{j=0}^{n-1}\sum_{i\neq j}\delta x_i \left\| \int_{\delta x_j} K(|x-x_i|)\, J(x_i)[\hat{c}_i + \hat{c}_i^\dagger, \hat{c}_i\hat{c}_x^\dagger + \hat{c}_i^\dagger\hat{c}_x + \hat{c}_i^\dagger\hat{c}_i\hat{c}_x^\dagger\hat{c}_x] dx - \delta x_j K(|x_j - x_i|) J(x_i)[\hat{c}_i + \hat{c}_i^\dagger, \hat{c}_i\hat{c}_j^\dagger + \hat{c}_i^\dagger\hat{c}_j + \hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j] \right\| \tag{B21}$$

bounds the error made by evaluating the integral over x by the corresponding Riemann sum over P_n. Analogously we obtain

$$\|\hat{C}_{gK}\| \leqslant 2R_{gK}(P_n) \tag{B22}$$

with

$$R_{gK}(P_n) = \sum_{j=0}^{n-1}\sum_{i\neq j}\delta x_i \left\| \int_{\delta x_j} g(x_i) K(|x-x_i|)\,[\hat{c}_i^\dagger\hat{c}_{x'} + \hat{c}_i^\dagger\hat{c}_i\hat{c}_{x'}^\dagger\hat{c}_{x'}, \hat{c}_i^\dagger\hat{c}_i] dx - \delta x_j g(x_i) K(|x_i - x_j|)[\hat{c}_i^\dagger\hat{c}_j + \hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j, \hat{c}_i^\dagger\hat{c}_i] \right\| \tag{B23}$$

and

$$\hat{C}_K = 4\int_0^{x_{\max}} dx \sum_{\substack{i\neq j\\ i:x_i\neq x}} K(|x-x_i|) \times \tilde{K}_{ij}(\hat{d}_1 + \hat{d}_2 + \hat{d}_3 + \hat{d}_4 + \hat{d}_5), \tag{B24}$$

where

$$\hat{d}_1 = \hat{c}_x[\hat{c}_i^\dagger, \hat{c}_i]\hat{c}_j^\dagger - \hat{c}_j[\hat{c}_i^\dagger, \hat{c}_i]\hat{c}_x^\dagger, \tag{B25a}$$

$$\hat{d}_2 = \hat{c}_j^\dagger\hat{c}_j[\hat{c}_i, \hat{c}_i^\dagger\hat{c}_i]c_x^\dagger - \hat{c}_x\hat{c}_x^\dagger[\hat{c}_i, \hat{c}_i^\dagger\hat{c}_i]c_j^\dagger, \tag{B25b}$$

$$\hat{d}_3 = [\hat{c}_i, \hat{c}_i^\dagger\hat{c}_i](\hat{c}_j^\dagger\hat{c}_j c_x^\dagger - \hat{c}_x^\dagger\hat{c}_x c_j^\dagger), \tag{B25c}$$

$$\hat{d}_4 = \hat{c}_x[\hat{c}_i^\dagger, \hat{c}_i^\dagger\hat{c}_i]\hat{c}_j^\dagger\hat{c}_j - \hat{c}_j[\hat{c}_i^\dagger, \hat{c}_i^\dagger\hat{c}_i]\hat{c}_x^\dagger\hat{c}_x, \tag{B25d}$$

$$\hat{d}_5 = (\hat{c}_j^\dagger\hat{c}_j c_x^\dagger - \hat{c}_x^\dagger\hat{c}_x c_j^\dagger)[\hat{c}_i, \hat{c}_i^\dagger\hat{c}_i]. \tag{B25e}$$

Equations (B25) imply that $\hat{C}_K$ depends on the partition along x, i.e., it would vanish if $\sum_j \to \int dx$. Its norm can consequently be bounded as

$$\|\hat{C}_K\| \leqslant 2R_K(P_n), \tag{B26}$$

where

$$R_K(P_n) = 5\sum_j\sum_{i\neq j}\left|\delta x_i\delta x_j\int_{\delta x_j} K(|x-x_i|)\,K(|x_i-x_j|)\right.$$
$$\left.\times \max(\|\hat{d}_1\|,\|\hat{d}_2\|,\|\hat{d}_3\|,\|\hat{d}_4\|,\|\hat{d}_5\|)\right|dx. \quad \text{(B27)}$$

Using Eqs. (B15), (B17), (B20), (B22), and (B26), the final estimate can be written

$$\begin{aligned}\|[\hat{H},\hat{H}_{P_n}]\| &\leqslant 2\big(\|[\hat{H}_S,\hat{O}_S^I]\|R_J(P_n) + (\hat{O}_S^I)^2\mathcal{R}_{JJ}(P_n)\\ &\quad + \|\hat{O}_S^I\|R_{JK}(P_n) + R_{gK}(P_n) + R_K(P_n)\big)\\ &= 2\left(\|[\hat{H}_S,\hat{O}_S^I]\|R_J(P_n) + R_B^{\text{loc}}(P_n) + R_B^{\text{int}}(P_n)\right),\end{aligned} \quad \text{(B28)}$$

where $R_B^{\text{loc}}(P_n)$ comprises all the errors due to discretization of integrals involving products of local bath operators [i.e., the function $[J(x)]^2$] and $R_B^{\text{int}}(P_n)$ comprises all the errors due to discretization of the integrals involving nonlocal bath operators [i.e., the functions $K(|x-x'|)$, $J(x)K(|x-x'|)$, and $g(x)K(|x-x'|)$]. The first term in Eq. (B28) vanishes for pure dephasing, $R_B^{\text{loc}}(P_n)$ vanishes for operators obeying bosonic canonical commutation relations, whereas $R_B(P_n)$ captures the intrabath interactions and vanishes for normal modes. Using Eqs. (B28) and (B7) one obtains

$$\begin{aligned}R_1(P_n) &\leqslant \|\hat{A}_S\|t^2\big(\|[\hat{H}_S,\hat{O}_S^I]\|R_J(P_n) + R_B^{\text{loc}}(P_n)\\ &\quad + R_B^{\text{int}}(P_n)\big)\big[2 + t^2\big(\|[\hat{H}_S,\hat{O}_S^I]\|R_J(P_n)\\ &\quad + R_B^{\text{loc}}(P_n) + R_B^{\text{int}}(P_n)\big)\big],\end{aligned} \quad \text{(B29)}$$

showing explicitly that at finite times the error $R_1(P_n)$ depends on how well the integrals are approximated by the Riemann sums.

The second contribution to the error, $R_2(P_n)$ in Eq. (B1), represents the distance between $\hat{A}_S$ and its time evolution under $\hat{H}-\hat{H}_{P_n}$. It can be estimated as

$$\begin{aligned}R_2(P_n) &= \|e^{i(\hat{H}-\hat{H}_{P_n})t}\hat{A}_S e^{-i(\hat{H}-\hat{H}_{P_n})t} - \hat{A}_S\|\\ &\leqslant \sum_{k=1}^{\infty}\frac{t^k}{k!}\|\hat{C}_k^{H-H_{P_n}}\|\end{aligned} \quad \text{(B30)}$$

with

$$\hat{C}_k^{H-H_{P_n}} = [\hat{H}-\hat{H}_{P_n},\hat{C}_{k-1}^{H-H_{P_n}}]$$

and $\hat{C}_0^{H-H_{P_n}} = \hat{A}_S$. Using the BCH formula and the triangular inequality since

$$\|\hat{C}_1^{\hat{H}-\hat{H}_{P_n}}\| = \|[\hat{H}-\hat{H}_{P_n},\hat{A}_S]\| \leqslant 2\|\hat{A}_S\|\|\hat{H}-\hat{H}_{P_n}\|,$$

we obtain for $\hat{C}_k^{\hat{H}-\hat{H}_{P_n}}$

$$\|\hat{C}_k^{H-H_{P_n}}\| \leqslant 2^k\|\hat{A}_S\|\|\hat{H}-\hat{H}_{P_n}\|^k. \quad \text{(B31)}$$

Substituting this into Eq. (B30) yields the following estimate for $R_2(P_n)$:

$$R_2(P_n) \leqslant \|\hat{A}_S\|(e^{2\|\hat{H}-\hat{H}_{P_n}\|t} - 1). \quad \text{(B32)}$$

For finite time, the error $R_2(P_n)$ vanishes in the limit $n\to\infty$.

We conclude from Eqs. (B7), (B28), and (B32) that, for a fixed finite time t, the error $R(P_n)$ can be made arbitrarily small by proper choice of the partition. It is thus sufficient to represent a continuous bath with infinitely many DOFs by a finite set of surrogate modes. Note that in our derivation no assumptions on the system-bath interaction or intrabath couplings were made.

As a final remark we note that, as long as the full Hamiltonian contains bounded operators, the bounds Eq. (A10) for discrete DOFs and Eq. (B32) for continuous DOFs depend only on the coupling structure and not on the specific algebraic form of $\hat{H}$.

APPENDIX C: EXTENSION OF THE DYNAMICAL BOUNDS TO *k*-BODY INTERACTIONS

A generic generator defined on a discrete set and containing k-body interactions is written as

$$\hat{H} = \sum_{i_1,i_2,\ldots,i_k}\hat{h}_{i_1,i_2,\ldots,i_k}, \quad \text{(C1)}$$

where $i_1,\ldots,i_k \in (0,\infty)$, and $\hat{h}_{i_1,\ldots,i_k}$ is a generic k-body interaction. This Hamiltonian defines a hypergraph, i.e., an ordered pair $G=(N,E)$ with the set of nodes N made up of all the degrees of freedom acted upon by $\hat{H}$ and E comprising the set of nonempty subsets of N, called hyperedges or links, for which $\|\hat{h}_{i_1,\ldots,i_k}\| \neq 0$. Since all interactions are k-local in Eq. (C1), all hyperedges have size k, and the hypergraph is k-uniform. A graph can therefore be regarded as a 2-uniform hypergraph. The adjacency matrix A_{ij}^h of a hypergraph G is defined as the matrix whose entries A_{ij}^h correspond to the number of hyperedges containing both degrees of freedom i and j [43]. The connectivity of a node c_i is given by the number of hyperedges involving the node, $c_i = \sum_j A_{ij}^h$. The hypergraph is therefore *locally finite* if $\max_{i\in N} c_i = \bar{c}_i < \infty$. One can then define the coupling matrix J on the hypergraph,

$$J_{ij} = \sqrt{\sum_{\mu\nu}\left(\sum_{\substack{i_1,\ldots,i_k:\\ \exists(k,k'):\, i_k=i,\, i_{k'}=j}}[J_{i_1,\ldots,i_k}^{\mu\nu}]^2\right)},$$

and consequently bound its norm by $\|J\| \leqslant \max_{i\in N}\sum J_{ij}$. This implies that Eq. (6) in the main text holds in the same form with $\mathcal{O} = \max_{i_1,\ldots,i_k}\|\hat{h}_{i_1,\ldots,i_k}\|$. Equation (9) in the main text holds formally unaltered as well, with the Riemann sums calculated for the relative k-body terms.

APPENDIX D: THE SUZUKI-TROTTER DECOMPOSITION

At finite t the effective generator of the reduced system evolution has the generic form

$$\hat{H}_{X_n} = \sum_{i,j\in X_n}\hat{h}_{ij},$$

where without loss of generality we assume two-body interactions. The set X_n is that of the relevant DOFs acted on by $\hat{H}_{X_n}$ and $\hat{h}_{ij}$ is the generic interaction between two

DOFs. At $t < \infty$ the effective propagator generated by $\hat{H}_{X_n}$ can be approximated by applying a Suzuki-Trotter expansion [33,44]

$$e^{-i\hat{H}_{X_n}t} \approx \left(\prod_{\{i,j\}\in X_n} e^{-i\hat{h}_{ij}\Delta t} \right)^{m_n}, \tag{D1}$$

where $\Delta t = t/m_n$. The generator $\hat{H}_{X_n}$ contains $K_n \leqslant |X_n|^2$ two-body terms. The error introduced by approximating $e^{-i\hat{H}_n\Delta t}$ within each Δt by a product of K_n terms is of the order $\epsilon_2 \leqslant \frac{1}{2}\mathcal{O}^2 K_n^2(\Delta t)^2$ [35,36]. A prespecified error $\epsilon_2/2$ for the whole time t is achieved by taking $m_n = \mathcal{O}^2 t^2 K_n^2/\epsilon_2$ Trotter steps, i.e., by choosing $\Delta t = \epsilon_2/(t\mathcal{O}^2 K_n^2)$. The product formula in Eq. (D1) can be generalized to generators exhibiting arbitrary time dependence [36].

For a k-body effective generator, the propagator of the form Eq. (C1) is decomposed as

$$e^{-i\hat{H}_{X_n}t} \approx \left(\prod_{\{i_1,\ldots,i_k\}\in X_n} e^{-i\hat{h}_{i_1,\ldots,i_k}t} \right)^{m_n}.$$

The error estimate in the previous section holds formally unaltered with $K_n \leqslant |X_n|^k$. One could then use the Solovay-Kitaev algorithm [45] to further decompose each k-unitary into a product of one- and two-body unitaries chosen from a suitable set. To achieve an accuracy ϵ for each k-unitary transformation, $n_{SK} = a\log_2^b(\epsilon^{-1})$ operations are required with a and b constants. If one chooses $\epsilon = \epsilon_2/(2n_d)$, the effective propagator is simulated with an accuracy ϵ_2 employing $n'_d = an_d\log_2^b(n_d/\epsilon_2)$ one- and two-body unitaries, i.e., with a computational effort that scales polynomially in time and number of effective DOFs [36].

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