

Tensor-Network Framework for Lindbladian Spectra and Steady States

Philipp Westhoff^{1,*}, Mattia Moroder^{2,3,†}, Ulrich Schollwöck^{1,‡} and Sebastian Paeckel^{1,§}

¹*Department of Physics, Arnold Sommerfeld Center for Theoretical Physics (ASC),
Munich Center for Quantum Science and Technology (MCQST),
Ludwig-Maximilians-Universität München, 80333 München, Germany*

²*School of Physics, Trinity College Dublin, College Green, Dublin 2, D02K8N4, Ireland*

³*Trinity Quantum Alliance, Unit 16, Trinity Technology and Enterprise Centre,
Pearse Street, Dublin 2, D02YN67, Ireland*



(Received 16 September 2025; revised 5 June 2026; accepted 7 August 2026; published 21 October 2026)

Quantum systems coupled to (non-) Markovian environments attract increasing attention due to their peculiar physical properties. Exciting prospects such as unconventional nonequilibrium phases beyond the Mermin-Wagner limit or dissipative state preparation demand a systematic analysis of quantum many-body phases out of equilibrium. Akin to the equilibrium case, this requires the computation of the low-lying eigenstates of Lindbladians, a problem challenging conventional approaches for simulating quantum many-body systems. Here, we undertake a first step to overcome this limitation and introduce a tensor-network-based framework to systematically compute not only steady states, but also low-lying excited states for large, driven quantum many-body systems. Our framework is based on recent advances utilizing complex-time Krylov spaces, and we leverage these ideas to create a toolbox tailored to solve the challenging non-Hermitian eigenvalue problem ubiquitous in open quantum systems. With an example of the interacting Bose-Hubbard model driven by dissipation-assisted hopping, we demonstrate the high efficiency and accuracy. From a reliable finite-size-scaling analysis of the spectral gap, we find strong evidence for nonlinear hydrodynamic behavior consistent with Kardar-Parisi-Zhang-type superdiffusive relaxation and establish the existence of exponentially accelerated, anomalous relaxation. This method unlocks the capability of spectral analysis of generic open quantum many-body systems suitable also for non-Markovian environments.

DOI: [10.1103/7kd1-kxxz](https://doi.org/10.1103/7kd1-kxxz)

Subject Areas: Computational Physics,
Condensed Matter Physics,
Quantum Physics

I. INTRODUCTION

In recent years, the rapid experimental development of quantum simulators [1,2] and digital quantum processors [3,4], the control over strong light-matter interactions [5,6], as well as the unprecedented precision in optically driving low-dimensional materials [7,8] put modern quantum physics at the brink of experimentally utilizing strong correlations in many-body systems to overcome classical limitations in terms of computational, algorithmic, and metrological capabilities. Alongside this remarkable

progress, the practical necessity to theoretically describe and analyze open quantum systems became increasingly pressing. Understanding the intriguing physics of quantum many-body systems coupled to large environments poses mathematical challenges, which reach far beyond the well-known frameworks for analyzing and classifying closed systems. Already for the simplest example of Markovian environments, analytic treatments are in general limited to noninteracting systems via third quantization [9] or the Lyapunov equation [10]. As a consequence, there is an urgent need for an efficient and flexible framework to overcome these limitations, and accessing information about Lindbladian spectra plays a crucial role in achieving this goal.

Methodological developments so far have been limited to compute the steady state, i.e., the open-system analog of the ground state in closed systems, with approaches ranging from tensor-network (TN) methods [11–20], potentially combined with Monte Carlo sampling [21–25], to neural quantum states [26–28], quantum algorithms [29–34], and phase-space methods [35]. However, besides the steady

*Contact author: p.westhoff@physik.uni-muenchen.de

†Contact author: moroderm@tcd.ie

‡Contact author: schollwoeck@lmu.de

§Contact author: sebastian.paeckel@physik.uni-muenchen.de

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

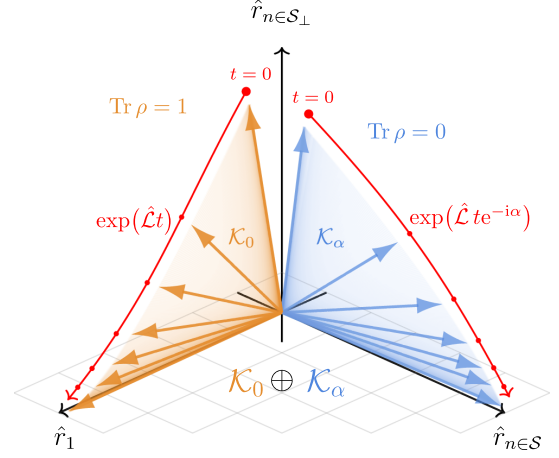
state, the capability to determine the low-lying eigenstates has become increasingly relevant. For instance, the dissipative gap, i.e., the real part of the first excited eigenvalue, dictates the experimentally relevant relaxation timescale of the system [36,37]. Many other phenomena, such as dissipative phase transitions [38,39], anomalous thermalization processes [36,40], topological effects [41–43], and metastability [44], require the explicit knowledge of the Lindbladian spectrum and eigenvectors. In Fig. 1(b), we summarize the relations between physical phenomena and the corresponding parts of the Lindbladian spectrum.

Compared to the isolated case characterized by a Hamiltonian, diagonalizing the Lindbladian $\hat{\mathcal{L}}$ presents two main additional challenges. First, $\hat{\mathcal{L}}$ is non-Hermitian, which prevents the direct application of variational algorithms such as the density-matrix renormalization group [49–51]. Here, it is important to emphasize that while there are methods to efficiently compute the steady state, or the spectral gap [52–55], these approaches typically do not efficiently generalize to the precise determination of several low-lying left or right eigenstates of the Lindbladian. Second, its dimensionality grows quadratically faster than the Hamiltonian's upon increasing the system size, which strongly limits the sizes of systems amenable to an exact diagonalization (ED) treatment.

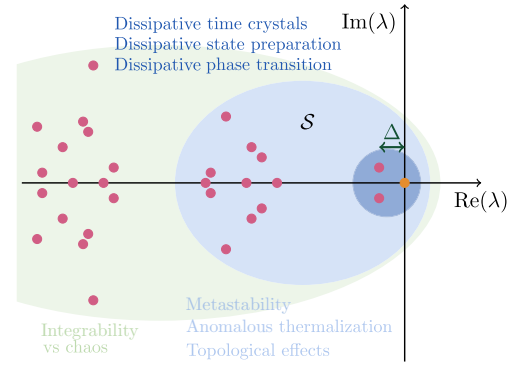
Taking a conceptual point of view, until now, the additional spectral structures inherent to Lindbladians barely have been exploited. For instance, the spectrum is restricted to the semi-infinite half space $\text{Re}(\lambda) \leq 0$, eigenvalues and eigenstates always come in complex-conjugated pairs, and excited states are always traceless. In this work, we leverage these—compared to the closed-system case—strong mathematical constraints and formulate a generally applicable framework to obtain highly precise low-rank approximations of the Lindbladian.

The arguably most relevant consequence of the spectral structure of any Lindbladian is that the vectorized exponential map $t \mapsto e^{\hat{\mathcal{L}}t}$ is always contractive as long as $t \in \mathbb{R}$; i.e., it constitutes a spectral filter with respect to the steady state of $\hat{\mathcal{L}}$. The key observation is now that allowing for complex-time contours, for instance, replacing $t \rightarrow te^{-i\alpha}$, the contribution of certain modes to the dynamics can be enhanced exponentially, which transforms the exponential map into a tunable spectral filter [illustrated in Fig. 1(a)]. Based on this insight, we generalize the idea of constructing a Krylov subspace from time-evolved states, which recently has been shown to provide an efficient faster-than-the-clock algorithm to approximate the steady state [56]. Upon exploiting the trace-preserving property of the Lindbladian, we show that within the generated complex-time Krylov subspace, the approximation quality of the low-lying excited states of $\hat{\mathcal{L}}$ [indicated by the light and dark blue shaded region in Fig. 1(b)] can be enhanced significantly when choosing proper complex-time contours [57,58] combined with traceless initial states.

(a)



(b)



(c)

Method	Target quantity	$\dim \mathcal{H}$
VQA [30, 31, 33]	Steady state	$2^{12} \approx 10^3$
NQS [26–28]	Steady state	$2^{16} \approx 10^5$
Var. MPO [12, 13, 16, 20]	Steady state	$2^{100} \approx 10^{30*}$
Quantum MC [52, 53]	Steady state	$2^{40} \approx 10^{12}$
MPS time evolution [51]	Steady state, gap	$2^{40} \approx 10^{12}$
ED [54, 55]	Full spectrum	$2^{12} \approx 10^3$
CLIK-MPS	Steady state, gap	$2^{176} \approx 10^{53}$
CLIK-MPS	Spectral region	$2^{70} \approx 10^{21}$

FIG. 1. (a) A schematic depiction of CLIK-MPS: a real-time evolution with physical initial state to capture the steady state, and a complex-time evolution with traceless initial state to approximate low-lying eigenmodes $\mathcal{S}$. (b) Physical relevance of different parts of the Lindbladian spectrum. In general, the analysis of many-body Markovian open quantum systems relies on the Lindbladian steady state (orange), the Liouvillian gap Δ (dark blue, dark green), a set of low-lying eigenvalues (light blue), or the full spectrum (green). (c) Maximal Hilbert-space dimensions and accessible Lindbladian spectral regions for various existing methods such as variational quantum algorithms (VQA) or neural quantum states (NQS) and comparison to our new framework CLIK-MPS. The * indicates that for variational matrix-product operator (MPO) methods, large system sizes of about 100 spins can be reached only for local Lindbladians that satisfy entanglement area laws [12].

The central task is now to transform these formal conclusions into an efficient numerical framework. Here, the crucial observation is that the constructed complex-time Krylov subspace also features the property of faster-than-the-clock convergence, which follows from the exponential convergence of Arnoldi schemes [58]. Consequently, the low-lying excited states approximated within the Krylov subspace—generated from time-evolved states along the complex contour—exhibit significantly better convergence than those at the final time. This ensures that already a simulation of the short-time dynamics generated by $\hat{\mathcal{L}}$ is sufficient to yield highly optimized basis states to capture the low-lying eigenmodes, a task that can be done efficiently using TN states [23,59,60].

Together with state-of-the-art tensor-network methods, these combined insights form the backbone of complex-time Lindbladian Krylov subspace matrix-product states (CLIK-MPS), a TN-based framework that allows us to specifically target a set of low-lying Lindblad eigenvalues and eigenmodes with very high accuracy. We demonstrate the efficiency of our method by studying a many-body dissipative bosonic model. As a key feature, this model exhibits a nontrivial spectral density in momentum space. Consequently, the Lindblad operators realize a minimal model for a coupling between physical single-particle states and a non-Markovian environment, i.e., a Markovian embedding [23,24]. Our simulations therefore represent a test case for determining the low-lying eigenstates of a system coupled to a non-Markovian environment, reaching striking Hilbert-space dimensions [see Fig. 1(c)] and achieving very good accuracy both for the spectrum and the eigenstates.

The article is organized as follows: In Sec. II, we introduce the CLIK-MPS framework, focusing on the role of the complex-time evolution, optimal initialization, and the efficient computation of observables in the Krylov subspace. Then, in Sec. III, we apply it to the dissipative Bose-Hubbard model, analyzing its steady state, dissipative gap, and anomalous thermalization behavior. Finally, in Sec. IV, we summarize our findings and outline promising directions for future research.

II. CLIK-MPS

In this work, we introduce a framework based on TN methods, which allows us to reliably and efficiently compute the low-lying eigenstates of a quantum system weakly coupled to a Markovian (i.e., memoryless) environment. These kinds of systems are described by a Lindblad master equation [61]

$$\begin{aligned} \frac{d\hat{\rho}(t)}{dt} &= \mathcal{L}\hat{\rho}(t) \\ &= -i[\hat{H}, \hat{\rho}(t)] + \sum_l \left(\hat{L}_l \hat{\rho}(t) \hat{L}_l^\dagger - \frac{1}{2} \{ \hat{L}_l^\dagger \hat{L}_l, \hat{\rho}(t) \} \right), \quad (1) \end{aligned}$$

where $[\cdot, \cdot]$ and $\{\cdot, \cdot\}$ indicate the commutator and the anticommutator, respectively, $\hat{\rho}$ is the system's density matrix, $\hat{H}$ is the Hamiltonian, and the influence of the environment on the system is captured by the so-called jump operators $\hat{L}_l$. Importantly, using techniques such as Markovian embeddings, this form also allows us to describe non-Markovian environments with nontrivial, structured spectral densities [23,24]. To study the spectral properties of the Lindbladian, we make use of vectorization, which consists of mapping density matrices to vectors $\hat{\rho} \rightarrow |\rho\rangle\rangle$ and the Lindbladian superoperators to operators $\mathcal{L} \rightarrow \hat{\mathcal{L}}$. Following the procedure outlined, for instance, in Ref. [10], the vectorized Lindbladian can be written as

$$\begin{aligned} \hat{\mathcal{L}} &= -i\hat{H} \otimes \hat{\mathbb{1}} + \hat{\mathbb{1}} \otimes i\hat{H}^T \\ &+ \sum_l \hat{L}_l \otimes \left(\hat{L}_l^\dagger \right)^T - \frac{1}{2} \hat{L}_l^\dagger \hat{L}_l \otimes \hat{\mathbb{1}} - \frac{1}{2} \hat{\mathbb{1}} \otimes \left(\hat{L}_l^\dagger \hat{L}_l \right)^T. \quad (2) \end{aligned}$$

For two operators $\hat{\rho}, \hat{\mu}$ given in the vectorized form $|\rho\rangle\rangle, |\mu\rangle\rangle$, the generalized scalar product is

$$\text{Tr}(\hat{\rho}^\dagger \hat{\mu}) = \langle\langle \rho | \mu \rangle\rangle. \quad (3)$$

We always represent states and operators in the MPS and matrix-product-operator (MPO) representation [49,51], but the framework is of course independent of the choice of the TN representation. Density matrices are vectorized by doubling the system size, alternating physical and auxiliary sites avoiding the introduction of long-range couplings [62] in the MPO representation of the vectorized Lindbladian Eq. (2) [12,18,19].

In this section, we detail the main components of CLIK-MPS to solve the eigenvalue problem of Eq. (2) for low-lying eigenvalues and eigenmodes. We begin with a short survey introducing the main ideas of the framework. Thereafter, we discuss some key aspects where we put special emphasis on the tilted, complex contour as well as using physical and traceless initial states to target the low-lying eigenmodes of $\hat{\mathcal{L}}$ with high precision. Finally, we demonstrate how expectation values can be evaluated efficiently and show how symmetries of the Lindbladian can be used to increase the precision of the computation of expectation values in the steady state.

A. Survey of CLIK-MPS

Approximating the eigenvalue problem of high-dimensional non-Hermitian operators in a low-dimensional subspace is a challenging task for TN-based methods. While the lack of Hermiticity prevents a variational Rayleigh-Ritz formulation and hermitized approaches are computationally demanding [13,20], Lindbladian dynamics provides an alternative route: The steady state is obtained naturally by time evolution, with exponential convergence governed by the dissipative gap, directly seen when expanding the

dynamics of a density matrix $|\rho_0\rangle\rangle$ in the eigenbasis of the Lindbladian

$$|\rho(t)\rangle\rangle = e^{\hat{\mathcal{L}}t}|\rho_0\rangle\rangle = |\rho_{SS}\rangle\rangle + \sum_{k=2}^{D^2} e^{\lambda_k t} \langle\langle l_k | \rho_0 \rangle\rangle |r_k\rangle\rangle, \quad (4)$$

where λ_k are the eigenvalues of $\hat{\mathcal{L}}$, $|r_k\rangle\rangle$ ($\langle\langle l_k |$) the corresponding right (left) eigenvectors, and $D = \dim \mathcal{H}$ denotes the dimension of the Hilbert space of the underlying physical system. Here, each eigenmode contributes with an exponentially decaying weight dictated by $\text{Re}(\lambda_k)$, except for the steady state $|\rho_{SS}\rangle\rangle$, as $\text{Re}\lambda_k \leq 0$. Note that Eq. (4) holds only when evolving a density matrix, while the dynamics of a traceless initial state $|\rho_0\rangle\rangle$ converges to the slowest eigenmode $|r_2\rangle\rangle$ due to trace preservation. This time evolution can be computed efficiently using TN methods, yet evolution times are typically limited by the entanglement growth.

The crucial observation is that the density operators at short and intermediate times already contain valuable information about the spectrum of the Lindbladian. This motivates us to use time-evolved states to generate a Krylov basis for approximating the operator exponential of the Lindbladian. While the spectral filtering introduced by the time evolution is advantageous for extracting the steady state, it becomes a limitation when resolving excited eigenmodes. To make the Krylov space suitable also for low-lying excited eigenmodes, CLIK-MPS extends conventional real-time evolution in two ways, exploiting the spectral structure of the Lindbladian:

- (1) We consider complex-time evolution, and we show that the complex-time-evolution contours can be chosen to optimize the convergence of specific eigenmodes by reducing their decaying rate; more details in Sec. II B.
- (2) We make use of traceless initial states to explicitly target low-lying excited states of the Lindbladian; more details in Sec. II C.

In Fig. 2(b), we demonstrate the improvements of CLIK-MPS over conventional time evolution for a dissipative system of interacting bosons with $L = 5$ sites and $N = 4$ particles (see Sec. III for the model's details). The strong dependence on the chosen initial states is demonstrated by the transparent dots corresponding to the eigenvalue approximations obtained from randomly chosen initial density operators and using conventional time evolution. Note how these points are vastly scattered around the excited states obtained from exact diagonalization (green dots). In turn, the crosses are generated using CLIK-MPS. The first five eigenvalues are reproduced with excellent precision using the same maximum evolution time $T = 4$ as in the conventional time evolution. For illustrative purposes, in the inset we display the convergence of the five lowest Lindbladian eigenvalues for a significantly larger system with $L = 20$ sites and $N = 10$ interacting

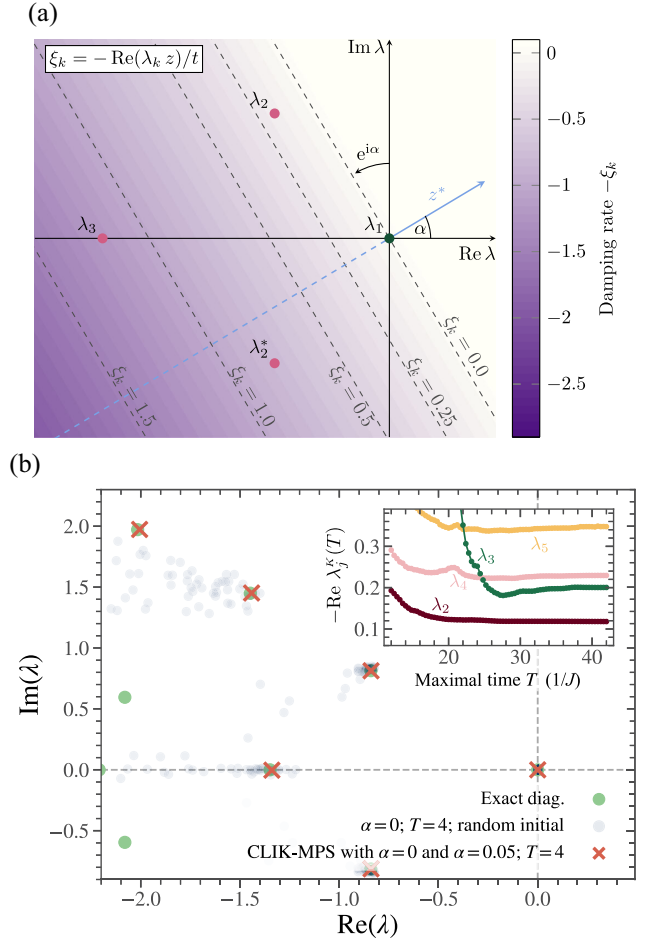


FIG. 2. (a): Linearly inclined complex-time contours $z = te^{-i\alpha}$ alter the damping rates ξ_k of Lindbladian eigenmodes [see Eq. (7)]. The color shading indicates the damping rate ξ_k for an eigenvalue located at λ_k , when evolving along the contour z . Note the tilt of the contour lines $\xi_k = \text{const}$, which are orthogonal to z^* (solid blue line) and lead to reduced damping rates of excited states with $\text{Im } \lambda > 0$. (b) Impact of the initial state on the accuracy of the spectrum of the dissipative Bose-Hubbard model specified by Eqs. (12) and (13) for $L = 5$ and $N = 4$. We compare ED ($\bullet$, green) data to the spectrum from a simple Krylov method with a single time evolution ($\bullet$, light blue), with a randomly sampled initial state. In total, 50 initial states were generated. The darkness of the blue color indicates how many points overlap at the respective position. Lastly, the results from CLIK-MPS are shown ($\times$). Inset: first four slow decaying modes approximated using CLIK-MPS for $L = 20$, $N = 10$ sites at $U/J = 0.5$ and $\kappa/J = 2$ depending on the maximal evolved time T .

bosons, using CLIK-MPS. The resulting Hilbert-space dimensions [cf. Fig. 1(c)] have long been inaccessible to existing methods, particularly for computing excited eigenmodes.

For efficiency, all operations in the Krylov space are performed directly in the inner product space spanned by the time-evolved basis states. More details on the explicit implementation can be found in Sec. II D.

It is important to note that using this approach, we effectively describe density operators with a much higher bond dimension than the one actually used during the numerics [63]. To illustrate this point, let $\chi(|\rho(t_i)\rangle\rangle) = \chi_i$ be the bond dimension of the time-evolved density operator at time step t_i and denote by N_K the number of evolved time steps, i.e., the number of (possibly linear-dependent) basis states of the Krylov space $\mathcal{K}$. If we would construct the MPS representation of the orthonormal basis states of $\mathcal{K}$ explicitly, this would involve superpositions of the N_K states $\{|\rho(t_i)\rangle\rangle\}$ such that, to a good approximation, the bond dimension of the basis states of $\mathcal{K}$ scales as

$$\chi_{\text{eff}} \sim N_K \max_i \chi_i. \quad (5)$$

Later, we will construct Krylov spaces with $N_K \sim \mathcal{O}(100)$; i.e., we approximate the Lindbladian in a Krylov space whose basis states would be represented by MPS with bond dimensions exceeding those of the time-evolved states by 2 orders of magnitude. This provides an intuitive explanation for the astonishing precision of CLIK-MPS we observed during our simulations for the steady state as well as the low-lying eigenvalues and eigenmodes of the Lindbladian.

A further interesting conclusion can be drawn by assuming that the actual parameter controlling the approximation quality is χ_{eff} . In that case, the computational costs can be reduced significantly by reducing the maximum bond dimension during the time evolution, say, by a factor of ν and in turn increasing the number of time steps by the same factor. Owing to the cubic scaling of the computational costs on the MPS bond dimension, a speedup by a factor of ν^2 can be expected. In Fig. 3, we analyze this argument quantitatively by calculating the dissipative gap of a Bose-Hubbard system (cf. Sec. III) for different system sizes. We vary the maximally allowed bond dimension χ

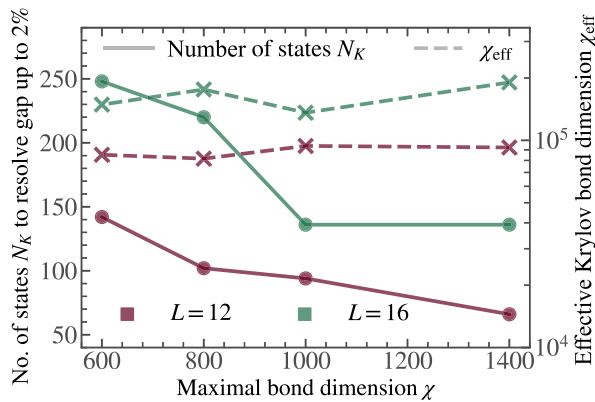


FIG. 3. The role of the effective bond dimension. Left: number of time-evolved states N_K needed to resolve the dissipative gap ($\Delta = 0.293, 0.174$ for $L = 12, 16$, respectively) up to a relative error of 2% for different system sizes. Right: the effective bond dimension χ_{eff} defined in Eq. (5). For all calculations, we chose $J = 1$, $\kappa = 2$, and $U = 0$, as well as $\delta t = 0.2$.

during time evolution, which was always saturated. Then we track the Krylov-space dimension N_K necessary to achieve a fixed accuracy of 2% in the resolution of the dissipative gap $-\text{Re}\lambda_2$. In agreement with our intuition, the number of time-evolved states N_K decreases with increasing bond dimension χ . We also find χ_{eff} [see Eq. (5)] to be approximately constant upon varying χ , indicating that it is indeed a central parameter determining the computation's accuracy. Note, however, that this observation is valid only if the bond dimension is not too small, so that projection errors completely obliterate the actual dynamics generated by the Lindbladian (a more detailed analysis is given in Appendix H).

B. Constructing the Krylov subspace

CLIK-MPS is based on time evolutions of vectorized density operators by simulating the dissipative Lindbladian dynamics, i.e., solving a Schrödinger equation with a non-Hermitian generator on a doubled Hilbert space.

The time evolution is performed using the single-site variant of the time-dependent variational principle (TDVP) [64,65]. TDVP reformulates the problem of solving the equation of motion for the density operator as a whole Eq. (1) into a local equation of motion for each site tensor of the vectorized density operator. While this already simplifies the complexity drastically, further optimizations are in order to obtain a robust time stepper. First, for our test system we choose the single-site variant of TDVP due to the large local Hilbert-space dimension of the bosons. Because in its standard formulation this does not allow for an increase of the MPS bond dimension, we additionally use the local subspace expansion (LSE) [66,67] to grow the bond dimensions after solving the local equation of motion. Second, the non-Hermitian nature of the generator rules out the standard Lanczos-based integrator. Instead, we build on previous works exploring different strategies to address this issue [68]. Since we are using a comparable small time step $\delta t = 0.01$ for all large-scale calculations, a straightforward Taylor expansion proved to be both, conceptually simple and numerically robust throughout the different parameter regimes. We discuss the numerical implementation in detail in Appendix H.

The most naive scheme to construct a Krylov space is to perform a time evolution of an initial state $|\rho_0\rangle\rangle$ where the dynamics is governed by $\hat{\mathcal{L}}$ [cf. Eq. (4)] and to store $N_K \in \mathbb{N}$ time-evolved states $|\rho(t_i)\rangle\rangle$. We denote this subspace as $\mathcal{K}_0(\rho_0) = \text{span}\{|\rho_0\rangle\rangle, \exp(\hat{\mathcal{L}}\delta t)|\rho_0\rangle\rangle, \dots, [\exp(\hat{\mathcal{L}}\delta t)]^{N_K-1}|\rho_0\rangle\rangle\}$.

However, when aiming for a high approximation quality of low-lying excited states, the exponential decay constitutes a major obstacle because it quickly suppresses the desired eigenmodes during the time evolution. We overcome this limitation by extending the time-evolution contour into the complex plane. Let us denote the path along which the time evolution is performed by $z(t) \in \mathbb{C}$, where $t = |z|$ is used to parametrize the path along the

complex plane. The goal is to adjust the exponential damping of some low-lying eigenmodes; from Eq. (4), we find that it is governed by

$$|\langle\langle l_k | \rho(z) \rangle\rangle| \sim e^{\text{Re } z \lambda_k} \equiv e^{-\xi_k t}. \quad (6)$$

Here, $\xi_k = -\text{Re}(z\lambda_k)/t$ denotes the damping rate of the k th eigenmode. Let us now consider the linearly inclined complex-time contours $z(t) = te^{-i\alpha}$ with $\alpha > 0$ as shown in Fig. 2(a). Evaluating the dynamics along this contour, the damping constants of the excited states are given by

$$\xi_k = -\text{Re}(\lambda_k) \cos \alpha - \text{Im}(\lambda_k) \sin \alpha. \quad (7)$$

We observe that the effect of the tilted contour is to increase the damping of eigenmodes with $\text{Im } \lambda_k < 0$, while reducing the damping for eigenmodes with $\text{Im } \lambda_k > 0$ and thereby enhancing their contribution to the dynamics, i.e., the Krylov space. From a geometric point of view, this can be understood by noting that the lines of the constant damping rate ξ are orthogonal to the path followed by the complex conjugated contour $z^*(t)$, as shown in Fig. 2(a). In the absence of a tilt $\alpha = 0$, these equidamping lines are parallel to the imaginary axis of the complex plane. For any finite tilt angle $\alpha > 0$, these lines are rotated counterclockwise and therefore slow down the damping of excited eigenmodes if $\text{Im } \lambda_k > 0$. Crucially, because the Lindbladian modes come in complex conjugate pairs, it suffices to accurately determine, for instance, those eigenmodes $|r_k\rangle\rangle$ with a positive imaginary part. Eigenvalues with a negative imaginary part are then readily obtained via complex conjugation $|r_k\rangle\rangle \rightarrow |r_k^*\rangle\rangle$, $\lambda_k \rightarrow \lambda_k^*$. Note, however, that α cannot be arbitrarily chosen. If $\alpha > \alpha_{\text{max}}$ for some α_{max} depending on the spectrum of $\hat{\mathcal{L}}$, bulk states with a large imaginary part get exponentially enhanced during time evolution, and the resulting Krylov space is unstable and resolves the low-lying spectrum poorly. In Appendix B, we provide detailed information on how to curtail these problems.

Projecting the full Lindbladian onto the complex-time Krylov subspace $\mathcal{K}_\alpha(\rho_\alpha) = \text{span}\{|\rho_\alpha\rangle\rangle, \exp(\hat{\mathcal{L}}\delta z)|\rho_\alpha\rangle\rangle, \dots, [\exp(\hat{\mathcal{L}}\delta z)]^{N_K-1}|\rho_\alpha\rangle\rangle\}$ with some new initial state $|\rho_\alpha\rangle\rangle$ and the complex-time step $\delta z = e^{-i\alpha}\delta t$ results in a dramatic increase of accuracy on one quarter of the complex plane, allowing us to resolve low-lying excited states to a very high precision. In order to span an optimal Krylov space for both, the steady as well as the low-lying excited state, we thus combine a time evolution with zero complex angle with one featuring a finite angle and construct the complex-time Krylov space $\mathcal{K}_{0,\alpha} = \mathcal{K}_0(\rho_0) \oplus \mathcal{K}_\alpha(\rho_\alpha)$ in which we approximate the Lindbladian. A further advantage is that each eigenmode contributes to $\mathcal{K}_{0,\alpha}$ with two distinct exponential damping rates.

The left eigenmodes of $\hat{\mathcal{L}}$ in general are not accurately described in $\mathcal{K}_{0,\alpha}$. However, this can be resolved by

performing the time evolution generated by $\hat{\mathcal{L}}^\dagger$, which can be written in the eigenbasis of $\hat{\mathcal{L}}$ as

$$|\rho^*(z)\rangle\rangle = e^{\hat{\mathcal{L}}^\dagger z}|\rho_0\rangle\rangle = \sum_{k=1}^{D^2} e^{\lambda_k^* z} \langle\langle r_k | \rho_0 \rangle\rangle |l_k\rangle\rangle, \quad (8)$$

where ρ^* indicates that the dynamics is generated by $\hat{\mathcal{L}}^\dagger$. The resulting Krylov space $\mathcal{K}_\alpha^*(\rho_0)$ spanned by these time-evolved states now includes contributions mainly from the slowly decaying left eigenmodes. Again, we utilize two time evolutions and build the Krylov space $\mathcal{K}_{0,\alpha}^* = \mathcal{K}_0^*(\rho_0) \oplus \mathcal{K}_\alpha^*(\rho_\alpha)$. Importantly, for every Lindbladian, the left eigenspace corresponding to $\lambda_1 = 0$ features one eigenmatrix $|l_1\rangle\rangle \propto |\mathbb{1}\rangle\rangle$, and thus we can directly add it the Krylov space [69].

While being motivated by previous insights into the benefits of complex-time Krylov spaces gained by some of us [57,58], we want to emphasize that the construction schemes introduced in this work are developed to both explore and exploit the specific structure of Lindbladian spectra. In particular, we want to stress that the case of a real-time evolution in the Lindbladian case corresponds to a sole imaginary-time evolution in the Hamiltonian case. Moreover, while in the closed-system case the goal is to suppress excited states to render the time evolution tractable for tensor-network methods, this angle of attack fails as soon as one is interested in the excited states of the Lindbladian. In the latter case, the exponential decay of the low-lying eigenmodes caused by their finite negative real part constitutes a significant challenge because the weight of these very states we try to determine vanishes exponentially fast during the time evolution. For that purpose, and in stark contrast to the closed-system approaches [57,58], the complex contours are chosen to enhance the low-lying excited states of the Lindbladian.

C. Initial states

The initial states provide an important degree of freedom in the time evolutions. We exploit it through a universal property of Lindblad dynamics: trace preservation. Since the trace is conserved, a traceless initial state carries no steady-state component and, once normalized, flows toward the slowest-decaying eigenmode. Suppressing the stationary contribution in this way sharpens the resolution of the low-lying decay modes in the resulting Krylov space. We therefore initialize the real-time evolution with a physical state $|\rho_0\rangle\rangle$, which targets the steady state, and the complex-time evolution with a traceless state $|\rho_\alpha\rangle\rangle$, which targets the slowly decaying modes. The same argument also applies to models with several steady states, provided the dynamics decomposes into symmetry sectors, which can then be treated independently. Additionally, we introduce a warm-up procedure that constructs initial states with large overlap with the low-lying spectrum of the

Lindbladian. As shown in Sec. III A, its effect is subleading compared to the other ingredients of CLIK-MPS; we defer the details to Appendix C, but want to stress that especially for the complex-time evolution, this initialization tends to stabilize the time evolution.

D. Efficient subspace arithmetic

A crucial component of CLIK-MPS is to avoid explicitly representing vectorized states and operators in the generated subspaces. This can be achieved by computing the Gram matrix $\mathbf{M}_{ij} = \langle \rho_i | \rho_j \rangle$ for a given set of states $\{|\rho_i\rangle\}_i$, from which a transformation $\mathbf{X}$ into an orthonormal basis is obtained via

$$\mathbf{X} = \mathbf{U}\mathbf{S}^{-1/2}, \quad (9)$$

where the matrices $\mathbf{S}$, $\mathbf{U}$ are obtained from diagonalizing the Gram matrix $\mathbf{M} = \mathbf{U}\mathbf{S}\mathbf{U}^\dagger$. Inverting the square roots of the eigenvalues of $\mathbf{M}$ is a numerically delicate operation, in general. However, using a recursive factorization [70], the numerical precision of the computed eigenvalues can be improved to arbitrary precision such that eventually only the loss of orthogonality of the columns or rows of $\mathbf{U}$ imposes actual constraints. To ensure numerical stability, we thus discard eigenvalues and eigenstates of $\mathbf{M}$, which violate the orthogonality constraint above a given threshold $\epsilon = 10^{-14}$, i.e., perform explicit deflations.

Once we found $\mathbf{X}$, we can easily represent operators in the corresponding orthonormal eigenbasis by computing their expectation values $\mathbf{O}_{ij} = \langle \rho_i | \hat{\mathcal{O}} | \rho_j \rangle$ and evaluate $\mathbf{O}^{\text{eff}} = \mathbf{X}^\dagger \mathbf{O} \mathbf{X}$. Clearly, eigenstates of the Lindbladian are also directly obtainable by transforming expectation values $\mathbf{L}_{ij} = \langle \rho_i | \hat{\mathcal{L}} | \rho_j \rangle$ such that the representation of the Lindbladian in the Krylov subspace is given by

$$\mathbf{L}^{\text{eff}} := \mathbf{X}^\dagger \mathbf{L} \mathbf{X}. \quad (10)$$

Denoting by $\mathbf{R}$ the matrix of eigenvectors of $\mathbf{L}^{\text{eff}}$ and sorting their columns such that the k th eigenvector corresponds to the approximation of the k th eigenvalues, the Krylov-space expansion of $|r_k\rangle$ is given by

$$|r_k\rangle = \sum_{m=1}^{N_K} [\mathbf{X}\mathbf{R}]_{mk} |\rho_m\rangle. \quad (11)$$

Here, N_K denotes the number of time-evolved states, and in particular we have $\mathbf{M} \in \mathbb{C}^{N_K \times N_K}$, while D_K is the number of orthonormalized basis states, such that $\mathbf{X} \in \mathbb{C}^{N_K \times D_K}$. Finally, the dimension of the effective Lindbladian is given by $\dim \mathbf{L}^{\text{eff}} = D_K$. Again, we emphasize that Eq. (11) should never be evaluated explicitly. However, from this expansion any overlap and expectation value can be readily derived in such a way that only arithmetics with states and operators expressed in terms of the states $|\rho_i\rangle$ is needed.

Several algorithmic optimizations can be exploited to further improve the computational efficiency, using algebraic properties of states and operators in the Krylov space. In Appendixes D and E, we elaborate on the specific implementations in detail and elucidate the role of Lindbladian symmetries. Here we note that steady states must be Hermitian, yet the complex-time evolution can introduce non-Hermitian artifacts due to truncation and approximation errors of the time-evolution scheme used, as well as from the complex-time contour itself. These non-Hermitian perturbations can be easily removed by hermitizing the representation of the density operators $|\rho\rangle \rightarrow (|\rho\rangle + |\rho^\dagger\rangle)/2$ used to evaluate expectation values. Again, exploiting Eq. (11), this can be directly incorporated on the level of the Krylov-space representation, and no arithmetics in terms of tensor-network states is required.

E. High-level structure

To summarize the whole CLIK-MPS algorithm, we provide a high-level pseudocode in Algorithm 1.

Given a Lindbladian $\hat{\mathcal{L}}$, we first approximate $\alpha_{\max}$ as briefly described in Sec. II B and detailed in Algorithm 3. Now, a sensible angle for the linearly inclined contour $\alpha \ll \alpha_{\max}$ can be chosen. Two initial states are generated using the initialization procedures specified in Sec. II C and in Algorithm 6. They are a physical ($|\rho_p\rangle$) and a traceless ($|\rho_u\rangle$) one. We then start two time evolutions in parallel, a real-time evolution where we save every step δt of the physical, as well as a complex-time evolution with step δz of the traceless one. After each time step, the evolved states are appended to the Krylov space $\mathcal{K}_{0,\alpha}$. Note that the overlaps and expectations needed to express the Lindbladian inside of the Krylov space can be calculated in parallel as soon as a new time step has been performed, as detailed in Algorithm 2. For this, only a few matrix elements need to be calculated in each step, reducing the number of expectation values in each step to linear in the number of time-evolved states (this is indicated by the * in Algorithm 1). Tracking the spectrum of the Lindbladian expressed inside the Krylov space over time can be used to

Algorithm 1. CLIK-MPS algorithm.

```

1: procedure CLIK-MPS( $\hat{\mathcal{L}}$ )
2:    $\alpha_{\max} \leftarrow$  from Algorithm 3
3:    $\delta z = e^{-i\alpha} \delta t \leftarrow$  with  $\alpha \ll \alpha_{\max}$ 
4:    $|\rho_p\rangle, |\rho_u\rangle \leftarrow$  from Algorithm 6
5:   for  $n < n_{\max}$  do
6:      $|\rho_p(\delta t n)\rangle \leftarrow$  do and save time step
7:      $|\rho_u(\delta z n)\rangle \leftarrow$  do and save time step
8:     Append states to Krylov space  $\mathcal{K}_{0,\alpha}$ 
9:      $\{\lambda_i, \mathbf{r}^i\}_i \leftarrow$  do Algorithm 2 with  $\mathcal{K}_{0,\alpha}$  (*)
10:    Break if  $\mathcal{K}_{0,\alpha}$  is converged
11:   end for
12: end procedure
    
```

establish escape criteria for the time evolution. This can also be generalized to the convergence of expectations of observables in the steady state, for instance. A sensible choice of the escape criterion depends on the specific use case. Note that we did not use any automated escape criteria to generate the results provided in Sec. III to better verify the results we got.

III. RESULTS

We apply CLIK-MPS to study a driven system of interacting bosons on a one-dimensional lattice. The Hamiltonian is given by

$$\hat{H} = -J \sum_{j=1}^{L-1} (\hat{b}_{j+1}^\dagger \hat{b}_j + \text{H.c.}) + \frac{U}{2} \sum_{j=1}^L \hat{b}_j^\dagger \hat{b}_j^2, \quad (12)$$

where U and J are the on-site interaction strength and nearest-neighbor hopping amplitude, respectively, and $\hat{b}_j$ ($\hat{b}_j^\dagger$) annihilates (creates) a boson on site j . The dissipative dynamics are generated by the jump operators

$$\hat{L}_j = \sqrt{\kappa}(\hat{b}_{j+1}^\dagger + \hat{b}_j^\dagger)(\hat{b}_{j+1} - \hat{b}_j), \quad (13)$$

where κ is the dissipation strength. The resulting Lindbladian has been shown recently to exhibit a local Bose-Einstein condensate (BEC) with very slowly decaying spatial correlations [37,71,72], providing an ideal testing platform as a strongly correlated, driven system.

Physically, the system-environment couplings in this model exhibit an interesting feature: They are nonlocal in real space, yet coupled to a Markovian environment. This situation can be made more transparent by transforming the model Eq. (12), as well as the jump operators Eq. (13) to momentum space. Then, the system realizes a local coupling for the bosonic, single-particle momentum-space modes q , which now are individually coupled to a structured environment; i.e., the couplings become momentum dependent with a spectral density depending on the momentum k given by

$$|g_q(k)|^2 = 16 \cos\left(\frac{k-q}{2}\right)^2 \sin\left(\frac{k}{2}\right)^2. \quad (14)$$

Such structured spectral densities are a typical feature of non-Markovian environments and in general occur when incorporating Markovian embeddings to describe non-Markovian environments [23,24]. We thus study a problem providing a numerical challenge comparable to what can be expected for Markovian embeddings of non-Markovian setups, while still allowing us to assess the approximation quality of physical observables by comparing to analytically and numerically known results [37,71,72]. Moreover, general non-Markovian systems can readily be described

by replacing the Lindblad generator $\hat{\mathcal{L}}$ with the hierarchy of equations of motion (HEOM) generator $\hat{\mathcal{L}}_{\text{HEOM}}$ [73,74], which features the same spectral properties.

A. Comparison with ED

We begin analyzing the convergence properties of CLIK-MPS by simulating small realizations of Eqs. (12) and (13), which can be compared to ED results. To demonstrate the improvements, we compare to results obtained using a Krylov space generated from a real-time evolution of a random initial state, which was suggested very recently and, to the best of our knowledge, provides the most generic and efficient approach to study Lindbladian spectra so far [56]. In order to achieve a fair comparison to this real-time approach, which we will also refer to as the $\alpha = 0$ method in the following, we use the same maximum evolution times when comparing the $\alpha = 0$ results to the CLIK-MPS results. Additionally, to analyze the impact of the different components of CLIK-MPS, we include a Krylov space with both a real- and complex-time evolution, but without the warm-up procedure, which we will refer to as random initial CLIK-MPS, as well as a Krylov space generated from a complex-time evolution alone.

In Fig. 4(a), we show the first Krylov low-lying eigenvalues for different methods. In order to assess the performance of the methods, we plot the difference of the Krylov eigenvalues to the exact data from ED. The steady state ($\lambda_1 = 0$) is reproduced seemingly well using either the $\alpha = 0$ method (blue), a single complex-time evolution (yellow), or CLIK-MPS (orange), as well as the random initial CLIK-MPS (green). However, already for the first excited state, the results from single time evolutions have a deviation of the order of 10^{-1} , which is quite large compared to the eigenvalue $\lambda_1 = -0.84 + 0.81i$, and gets even more severe when trying to evaluate higher excited states. On the other hand, CLIK-MPS exhibits a robust and precise approximation of the first four low-lying excited states. Similarly, the random initial CLIK-MPS shows a comparable approximation quality like CLIK-MPS, indicating that the main benefit originates from combining real- and complex-time evolution and not the choice of the warm-up procedure. Note that the chosen positive angle $\alpha = 0.05$ enhances the precision of the eigenvalues with a positive imaginary part and decreases the accuracy of those with a negative imaginary part. However, the lower half-plane eigenvalues can be obtained simply by Hermitian conjugation of the eigenvalues located in the upper half plane.

Next, we compute the deviation of the Krylov Lindbladian right and left eigenvectors $|r_j^K\rangle\rangle$, $|l_j^K\rangle\rangle$ from the ED reference data in Figs. 4(b) and 4(c), respectively. The computation of these overlaps is detailed in Appendix F. Here, the impact of the additional complex-time evolution becomes evident when comparing with the $\alpha = 0$ curves: The accuracy is improved by more than 3

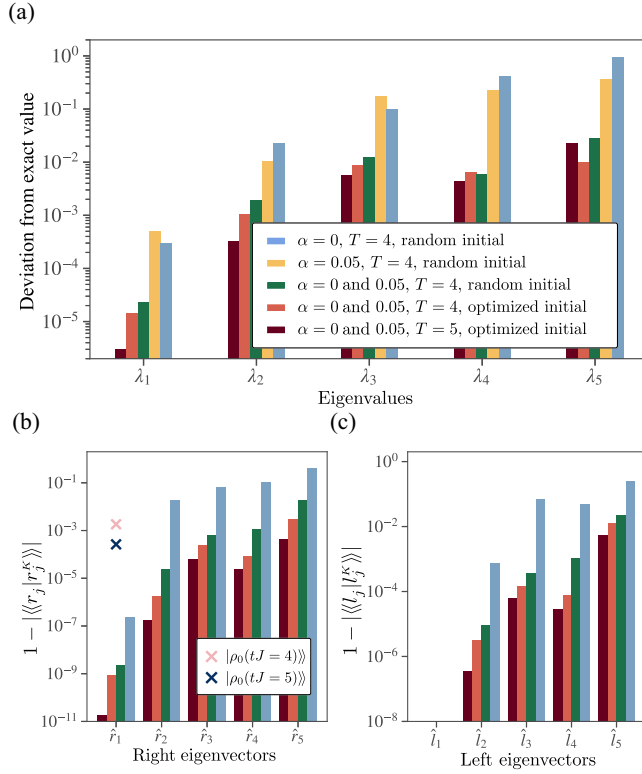


FIG. 4. Accuracy of CLIK-MPS compared against ED and real-time evolution methods [56]. In (a), we compare the lowest Lindbladian eigenvalues from different Krylov-based methods with ED reference data. We consider time evolution with $\hat{\mathcal{L}}$ for a real-time evolution method (blue) as well as a complex-time evolution (yellow) compared to CLIK-MPS with random (green) and optimized (orange) initial states. We plot the deviation of the approximated eigenvalues to the exact data. In (b), we compare the deviations of the Lindbladian right eigenmodes for real- and complex-time evolutions with $\hat{\mathcal{L}}$ for different final times. The deviations of the time-evolved state at the final evolution time from the exact steady states are also indicated ($\times$). In (c), the same analysis is shown for the left eigenmodes obtained through time evolution with $\hat{\mathcal{L}}^\dagger$. We considered $L = 5$ lattice sites, $N = 4$ particles, set $J = U = \kappa = 1$, employed a time step $dt = 0.05$ during time evolution, and used every second time-evolved state for the Krylov space. The maximal evolution time T and the complex angles α are specified in the plot. For all data relying on random initial states, we average over 50 such initializations by averaging the logarithm of the distance to the ED result. Details on the choice of initial states are given in the main text. For the data with $\hat{\mathcal{L}}$, the optimized initial states (orange and red) had expectation values -1.84 for $\alpha = 0$ and -3.32 for $\alpha = 0.05$.

orders of magnitude. The improvements are similar when considering the random initial CLIK-MPS (green). Note that here we also include a comparison against another, even simpler approach to find the steady state, namely, approximating it by a real-time evolution only (crosses). This ansatz exhibits the poorest convergence when evolving up to the same maximal evolution time as the one used

for the Krylov-space-based methods, with a loss in precision of more than 6 orders of magnitude. Moreover, increasing the duration of the time evolution systematically enhances the precision not only of the steady state $|r_1^K\rangle$, but of all right eigenvectors. For the Krylov left eigenvectors $|l_j^K\rangle$ in Fig. 4(c), note that the three slowest-decaying left eigenmodes are captured with a precision of at least 10^{-4} with the slowest-decaying one even at 10^{-6} .

B. Large-scale systems beyond ED

We now turn to an in-depth analysis of the phase diagram of Eq. (12) driven by the jump operators Eq. (13). From previous works [37,71,72], the model is known to exhibit a steady state realizing a so-called local BEC in the limit of weak interaction strength $U/J \ll 1$, or strong dissipation $\kappa/J \gg 1$. Here, local refers to the observation that in these limits, the correlation length increases rapidly such that very large system sizes are required to discriminate the exponential decay of particle correlations. In the following, we use CLIK-MPS to study the model in a large parameter regime, putting particular emphasis on this crossover where the correlation length competes with the system size. Furthermore, we show how CLIK-MPS can be used to evaluate the so-called Mpemba speedup, which provides a tool to speed up the experimental preparation time of the steady state exponentially, rendering the practical realization of Eqs. (12) and (13) a promising candidate for a platform to speed up the preparation of BECs exponentially. Note that both types of analyses require the computation not only of the steady state but also the Lindbladian gap as well as higher eigenvalues. Therefore, these investigations also illustrate the physical relevance of the ability to evaluate both the steady state, as well as the low-lying excited states with high precision. Additionally, we also benchmark the numerical cost of CLIK-MPS against a state-of-the-art pure state unraveling method [23,75] in Appendix A and Fig. 8. Finally, we also performed extensive and systematic convergence analysis for the data provided, which we discuss in depth in Appendix G, and prove an exact error bound on the steady state, as well as Krylov error bounds for the convergence of eigenvectors.

1. Correlation length and local BEC

We begin by studying the crossover behavior at repulsive interaction strengths U in the steady state at half filling $N = L/2$. We compute the correlation length ξ , which can be inferred from the two-point correlator $C(i-j) = \langle \hat{b}_i^\dagger \hat{b}_j \rangle_{\text{SS}}$ using a fitting function that captures an exponential decay in the long-distance limit

$$C(i-j) = \frac{c_1}{|i-j|^{c_2}} e^{-|i-j|/\xi} + c_3. \quad (15)$$

We fix $i = L/4$ to counteract the boundary effects and fit the tail of C . In Fig. 5, we show the extracted correlation lengths as a function of the number of lattice sites, varying the Hubbard interaction strengths, for a fixed dissipation $\kappa/J = 2$. The dependence of the correlation length on the system size L indicates the formation of a local BEC for small Hubbard repulsion strengths U . However, it is important to note that fitting the exponential decay can be misleading if the system size is too small. To illustrate this point, we indicate the case $\xi = L$ by the gray line. Any correlation length fitted above this line, i.e., $\xi > L$, should not be trusted because the system is too small to recognize the finite correlation length. On the other hand, this is exactly the region where the local BEC appears: The system behaves as a BEC on all accessible length scales.

To illustrate the superior convergence of CLIK-MPS, in the inset of Fig. 5, we compare the convergence of the leading eigenvalue of the correlator $C(i - j)$ to the values obtained using time-evolved states as a function of the maximum evolution time. This eigenvalue characterizes the condensate fraction of the bosonic particles and, hence, serves as an excellent proxy to check numerical convergence. Computing $C(i - j)$ from the right eigenstates obtained using CLIK-MPS (green symbols), we can clearly observe a rapid saturation already at times $T = 4$. In contrast, the real-time-evolution method converges

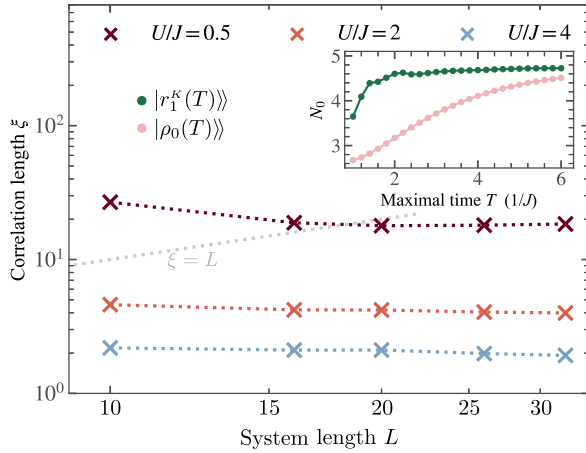


FIG. 5. Correlation lengths ξ [Eq. (15)] of the dissipative Bose-Hubbard steady state calculated within CLIK-MPS for different lengths and on-site interactions U . ξ is almost independent of the length of the chain and shrinks upon increasing U . Note that if $\xi > L$, the system is in a lattice analog of a BEC. Inset: leading eigenvalue N_0 of the correlation matrix $C(i - j)$ depending on the evolved time T . We compare the real-time-evolved state at time T (pink) to the CLIK-MPS steady-state approximation (green). We show data for a system with $L = 10$ sites at half filling, with $U = 0$, $\kappa/J = 2$. At $L = 32$, we used $T = 32$ and $\delta t = 0.4$, at $L = 26$, $T = 22$ and $\delta t = 0.4$, at $L = 20$, $T = 18$ and $\delta t = 0.2$, at $L = 16$, $T = 10$ and $\delta t = 0.1$, while at $L = 10$, we used $T = 6$, $\delta t = 0.1$. For the $L = 32$, $L = 26$, $L = 20$, and $L = 16$ sites, we used the complex angle $\alpha = 0.02$, while for $L = 10$ we employed $\alpha = 0.05$.

significantly slower (pink symbols) and considerably longer simulation times are required.

2. Dissipative gap and critical point at $U = 0$

It is well known that Eqs. (12) and (13) exhibit a critical point at $U = 0$ [37,71,72], where a true BEC is stabilized. This result can already be inferred from Fig. 5, where we observe an increasing correlation length with decreasing Hubbard interaction. Here, we investigate this crossover more systematically by studying the system size and interaction dependence of the dissipative gap $\Delta = -\text{Re}\lambda_2$. Since the limit $U/\kappa \rightarrow 0$ can be treated analytically [37], the situation is more controlled in our case, and we leave the demonstration that CLIK-MPS can be used to reliably identify dissipative phase transitions (DPTs) to future work.

In Fig. 6, we show the dissipative gap for various repulsive Hubbard interaction strengths as a function of the system size, keeping the particle density constant: $N/L = 0.5$. We consider systems of up to 40 bosonic sites with local dimension 21, resulting in Hilbert spaces of dimension $\dim \mathcal{H} \approx 2^{176}$. For the gap, it is known that $\Delta \rightarrow 0$ for $L \rightarrow \infty$ [37], and the asymptotic scaling relation is of the form [76]

$$\Delta(L) = \frac{a}{L^\alpha}. \quad (16)$$

We hence use this ansatz to infer the scaling of the gap in the infinite system limit. In Fig. 6, we show gaps evaluated for

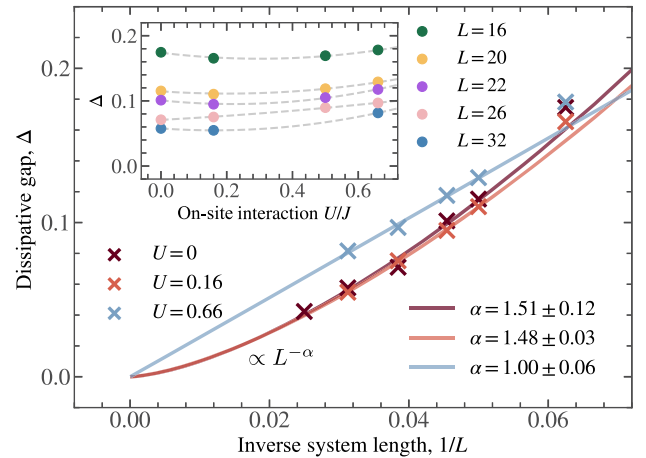


FIG. 6. Scaling of the dissipative gap at half filling. We show the dissipative gap $\Delta = -\text{Re}\lambda_2$ for three on-site interactions at $\kappa/J = 2$ depending on the inverse system size $1/L$. We perform a fit of the data according to Eq. (16), where we exclude the $L = 16$ data points. We find a power-law dependence $\Delta \propto L^{-\alpha}$ with the scaling exponent α increasing from $\alpha = 1$ toward $\alpha \approx 3/2$ when $U/J \rightarrow 0$. Inset: dissipative gap Δ for several system sizes and on-site interactions. At these small on-site interactions, the gap depends quadratically on U . For $L = 16$ and 20 , we use $\delta t = 0.2$ and $T = 18, 28$, respectively, while for $L = 22$ and 26 , we have $\delta t = 0.4$ and $T = 40$ and 50 , respectively. For $L = 32$ and $L = 40$, $\delta t = 0.6$, and T was chosen U dependent to ensure convergence (see Appendix G, for $L = 40$, $T = 120$).

various values of the Hubbard interaction and system sizes, as well as the resulting finite-size extrapolations.

Note that for the fits we had to exclude the smallest systems with $L = 16$ sites in order to reliably identify the gap closing, which is perfectly consistent with the observed correlation lengths in Fig. 5. Interestingly, we observe that for intermediate interactions ($U = 0.66$), the gap scales linearly with inverse system size $\Delta \sim L^{-1}$ corresponding to a relaxation time $\tau = 1/\Delta \sim L$. In contrast, for weak or vanishing interactions ($U = 0$ and $U = 0.16$), the gap closes more rapidly with system size, following $\Delta \sim L^{-3/2}$ within numerical accuracy. This gap corresponds to a relaxation timescaling as $\tau \sim L^{3/2}$ and indicates superdiffusive relaxation dynamics. The appearance of the exponent $3/2$ is particularly noteworthy, as it coincides with the dynamical exponent of Kardar-Parisi-Zhang (KPZ) scaling [77], revealing KPZ-type superdiffusive relaxation in a dissipative many-body system. Note that although we considered large system sizes, there is the possibility of a change of convergence speed due to an eigenvalue crossing at higher system sizes.

The observation that for a local BEC the relaxation time $\tau = 1/\Delta$ increases faster than linear with the system size seems to complicate the practical realization due to a rapidly growing timescale. However, this problem can be overcome by choosing special initial states. While it has been known for some time that the relaxation speed of driven systems can exhibit anomalous behavior for specific initial states [78], in general, identifying such states is highly nontrivial. In the next paragraph, we demonstrate how the capability to access several low-lying Lindbladian eigenstates allows us to address this issue, and we show that there is a class of experimentally simple-to-realize states for which relaxation times can be sped up exponentially.

3. Anomalous thermalization and the Mpemba effect

We now demonstrate how the capability to access spectral regions beyond the steady and first excited state allows us to determine practically relevant, physical quantities. For that purpose, we study the emergence of anomalous equilibration processes at the example of the quantum Mpemba effect (QME) [36,40,79–82] by computing the relative speedup

$$\Delta_j = \frac{\text{Re } \lambda_j}{\text{Re } \lambda_2}. \quad (17)$$

This quantity determines the magnitude of the exponential speedup in relaxation time toward the steady state for special initial states $|\rho_0\rangle$ compared to random ones, assuming that $|\rho_0\rangle$ exhibits zero overlap with the slowest-decaying mode $\langle\langle \rho_0 | l_2 \rangle\rangle = 0$. From an experimental point of view, such an exponential speedup in the preparation time constitutes an important improvement, since long preparation times are the main limiting factor for high fidelities of the desired target state [83]. In Ref. [37], it was

established using ED methods that there are easy-to-prepare states $|\rho_{\text{sym}}\rangle$, which can be constructed as product states that are invariant under mirroring about the center of the lattice and feature exponentially faster relaxation (for instance, $|1, 1, \dots, 1, 1\rangle$ and $|1, 2, \dots, 2, 1\rangle$).

In Fig. 7, we show the dependence of Δ_j on the repulsive on-site interaction strength U for various system sizes at half filling. The required eigenvalues are calculated using CLIK-MPS. While Δ_4 decays monotonically, yet slowly, for Δ_3 we observe a pronounced maximum near $UL/J \approx 6.5$ with a speedup of approximately 1.5 orders of magnitude. Note that this value increases with the system size. In order to confirm that indeed there is a QME, we also computed the overlap of $|\rho_{\text{sym}}\rangle$ with the slowest-decaying mode $|l_2\rangle$. In the inset of Fig. 7, we show this overlap (violet points) and compare it to the overlap of random initial product states $|\rho_{\text{random}}\rangle$, each averaged over 50 realizations. For the symmetric initial state, this overlap is 4–6 orders of magnitude smaller than for the random initial states. This extends the previous findings [37], in which the QME could be verified for much smaller systems only.

The fact that for finite interaction strengths the relaxation of a many-body system toward a steady state with correlation lengths beyond the lattice size can be sped up exponentially is intriguing. Apparently, for symmetric

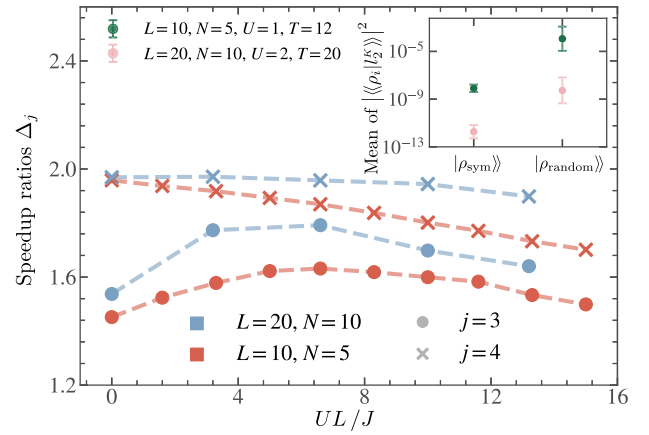


FIG. 7. The Mpemba-speedup ratios $\Delta_j = \text{Re } \lambda_j / \text{Re } \lambda_2$ [see Eq. (17)] as a function of the on-site interaction U for two lengths of the chain. Inset: mean overlaps of different product states with the obtained slowest-decaying left eigenmode $|l_2^K\rangle$. The mean was calculated with 50 randomly sampled symmetric states ($|\rho_{\text{sym}}\rangle$) and random product states ($|\rho_{\text{random}}\rangle$), respectively. For symmetric states, the overlap is 4 orders of magnitude smaller, indicating the emergence of the QME. The error bars show that this behavior is systematic. For all calculations, we use a local dimension $d = N + 1$, while we set the maximal bond dimension $\chi = 2400$ during time evolution. For data with $L = 20$ and $L = 16$, we use a Krylov time step of $\delta t = 0.2$ and complex angle $\alpha = 0.02$, while for $L = 10$, we chose $\delta t = 0.1$ and $\alpha = 0.05$. The maximal time T is set to $T = 12$ for $L = 10$, while it depends on U for $L = 20$ and was chosen such that the results are sufficiently converged (see Appendix G).

initial configurations, the Hubbard repulsion enhances incoherent scattering in the scope of the dynamics, yet incoherences are strongly suppressed once the system has thermalized. This observation highlights the important role of the complex interplay between interactions and transport properties in driven systems and how analyzing spectral regions of the Lindbladian beyond the steady state can help to disentangle their intricate relationship.

IV. CONCLUSION

We introduced CLIK-MPS, a tensor-network-based framework that not only enables the efficient computation of the steady state and the dissipative gap but also to explore the low-lying Lindbladian eigenvalues and eigenmodes with high accuracy. The framework is built on recent developments of complex-time Krylov-space methods and expands these ideas by specific complex contours and efficient construction schemes for vectorized density matrices and superoperators in high-dimensional Krylov subspaces. The resulting time-evolution schemes are combined with specific initialization methods to obtain optimized initial states, such that the subsequent dynamics yield Krylov spaces capturing the low-lying Lindbladian eigenstates for Hilbert-space dimensions, which have been far beyond reach for previous approaches. We note that recently a variant of the ESPRIT algorithm [84,85] was used to calculate Lindbladian eigenvalues [86,87], yet for significantly smaller system sizes than those analyzed here.

In order to ascertain its capabilities, we used CLIK-MPS to investigate a driven Bose-Hubbard model featuring a nontrivial, structured spectral density between the bosonic momentum-space single-particle modes, and the environment. This type of system-environment coupling is reminiscent of non-Markovian environments described via Markovian embeddings and, thereby, provides an excellent testing ground for the computational challenges occurring for non-Markovian problems. At the example of small systems amenable to ED, we benchmarked the performance of CLIK-MPS against a recently proposed Krylov-space approach [56], finding an improvement in the accuracy of nearly 4 orders of magnitude when evaluating excited Lindbladian left and right eigenmodes. Exploiting this striking accuracy and the high computational efficiency, we investigated in depth the emergence of a local BEC, which is characterized by an increasing correlation length for small, repulsive Hubbard interactions culminating to a critical point at $U/J = 0$ where a true BEC is stabilized. Examining this crossover behavior is numerically challenging due to the competition between the growing correlation length ξ and the closing of the dissipative gap Δ , which vanishes when increasing the system size. Using large-scale numerics with up to $L = 40$ lattice sites and $N = L/2$ bosons, leading to Hilbert-space dimensions of $\dim \mathcal{H} \approx 2^{176}$, we studied the closing of the dissipative gap. Our findings indicate that the scaling of the gap

transforms from a $\Delta \sim 1/L$ at intermediate Hubbard interaction strength to a $\Delta \sim 1/L^{3/2}$ behavior once the correlation length exceeds the lattice size, and the local BEC forms, yielding strong evidence for KPZ-type scaling of the relaxation dynamics at mesoscopic system sizes. As a consequence, the experimental preparation of a local BEC as suggested in Ref. [72] would suffer a superlinear increase of the relaxation time $\tau = 1/\Delta$ with the number of lattice sites, when using typical, random initial configurations for the bosons. However, using CLIK-MPS we were able to show the existence of anomalous relaxation when incorporating additional knowledge of the low-lying Lindbladian eigenmodes. Specifically, we demonstrated the realization of a QME enabling an exponentially faster relaxation toward the steady state, highlighting the practical relevance of this model as an ideal candidate for the fast, dissipative preparation of a lattice BEC using ultracold atoms.

The possible applications of CLIK-MPS are widespread and range from the numerical investigation of exceptional points [88,89], DPTs [39], dissipative time crystals [90,91], the quantum Mpemba effect [36,40], and metastability [44] in large-scale, strongly interacting open quantum systems. Moreover, combining several complex contours, the spectral regions within the bulk spectrum of the Lindbladian can also be targeted, unlocking the investigation of transport and thermalization in driven quantum many-body systems. Finally, while in this work we considered only a simple analog of a Markovian embedding, our approach can be immediately extended to the general, non-Markovian case, considering for instance the HEOM generator [74,92].

ACKNOWLEDGMENTS

We are grateful to François Damanet, Baptiste Debecker, John Martin, John Goold, and Laetitia Bettmann for enlightening discussions. P. W., U. S., and S. P. acknowledge support by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy, Grant No. 426 EXC-2111-390814868. This work was supported by Grant No. INST 86/1885-1 FUGG of the German Research Foundation (DFG). M. M. acknowledges funding from the Royal Society and Research Ireland and from the European Union's Horizon research and innovation programme under the Marie Skłodowska-Curie Grant agreement No. 101264565. This project/research is part of the Munich Quantum Valley, which is supported by the Bavarian state government with funds from the Hightech Agenda Bavaria. All tensor-network calculations were performed using the SYTEN toolkit [93,94].

DATA AVAILABILITY

The data that support the findings of this article are publicly available from Ref. [95]. The code used to analyze the data and create the figures in this article is publicly

available from Ref. [95]. The source code of CLIK-MPS used to generate the data, and parameters used to generate the simulations is publicly available from Ref. [96].

APPENDIX A: COMPARISON TO QUANTUM JUMPS

To assess the performance of CLIK-MPS, we compare it to the quantum jumps (QJ) method [75]. In the QJ, the evolution of $\hat{\rho}(t)$ is unraveled in multiple stochastic time evolutions of pure states $|\psi_k(t)\rangle$ known as quantum trajectories. The deterministic part of the dynamics is generated by the effective Hamiltonian $\hat{H}_{\text{eff}} = \hat{H} - i/2 \sum_l \hat{L}_l^\dagger \hat{L}_l$, while the stochastic part is given by the applications of jump operators $\hat{L}_l$ at random times according to a probability distribution dictated by the norm decrease of $|\psi_k(t)\rangle$ induced by the non-Hermitian $\hat{H}_{\text{eff}}$. By averaging over N_{traj} trajectories, one can reconstruct expectation value of an observable $\hat{O}$ as

$$\text{Tr}(\hat{O} \hat{\rho}(t)) \approx \frac{1}{N_{\text{traj}}} \sum_{k=1}^{N_{\text{traj}}} \langle \psi_k(t) | \hat{O} | \psi_k(t) \rangle, \quad (\text{A1})$$

where the statistical error is given by the standard deviation of the expectation value across trajectories divided by $\sqrt{N_{\text{traj}}}$ [75].

In Fig. 8, we compare CLIK-MPS to an efficient version of QJ, based on an local subspace expansion time-dependent variational principle (LSE-TDVP) time evolution [23,68]. First, in Fig. 8(a) we simulate a small system with five sites and four particles, where ED data is available. We are interested in the off-diagonal element of the one-body reduced density matrix given by $\langle \hat{b}_1^\dagger \hat{b}_5 \rangle_{\text{ss}}$. It can be seen that QJ needs about $N_{\text{traj}} = 1000$ and reaches convergence at time $t \approx 4$, while CLIK-MPS is already converged at $t \approx 2$. Then, in Figs. 8(b) and 8(c) we plot the occupation of site $j = L/4$ for the larger system sizes of $L = 20$ and $L = 32$ at half filling, respectively. To guarantee a fair comparison between CLIK-MPS and QJ, all calculations were carried out on a dual-socket Intel x86_64 cluster node with 16 cores per socket (32 physical cores; 64 hardware threads via Hyper-Threading) with 380 GB of memory and x86-64-v4 support. Each run used a single Slurm task with one CPU allocated. Since QJ is trivially parallelizable, we ran each trajectory separately. Importantly, the shown computational time for QJ is that of a single trajectory and not the total run-time. Interestingly, CLIK-MPS converges to the reference value (obtained by an accurate long time evolution with low truncation error) substantially faster than QJ in both cases. Finally, we note that the fact that the number of trajectories needed to converge QJ decreases upon increasing L is specific to the parameters we considered: For $U = 0$, the

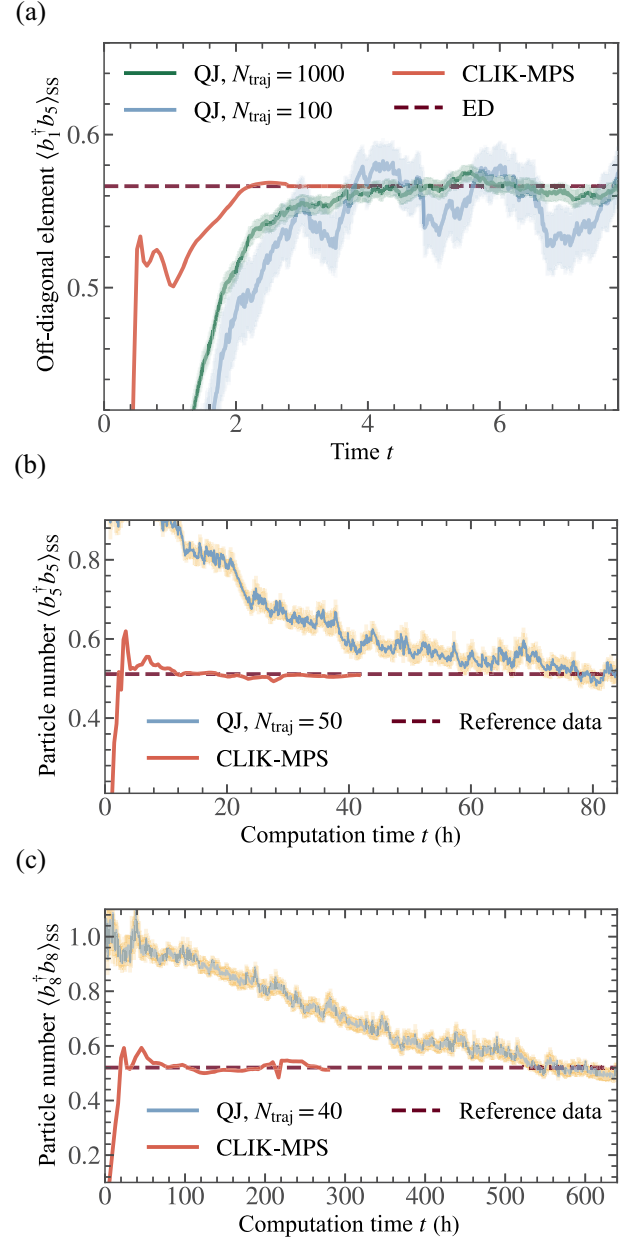


FIG. 8. Comparison of CLIK-MPS to QJ. In (a), we compare CLIK-MPS to QJ and ED data for a small system of five sites and four bosons. We used parameters $J = 1$, $U = 1$, and $\kappa = 1$, a time step of $dt = \delta t = 0.05$ for CLIK-MPS, and $dt = 0.005$ for QJ. In (b) and (c), we compare large system data ($L = 20$, $N = 10$ and $L = 32$, $N = 16$, respectively) as a function of the run-time. The statistical QJ error is shown in shaded yellow around the average value. We used parameters $J = 1$, $U = 0$, and $\kappa = 2$, a time step of $dt = 0.01$ for CLIK-MPS ($\delta t = 0.2$), and $dt = 0.005$ for QJ. For all calculations, we used local dimension $d = N + 1$. For $L = 20$, we fix a maximal bond dimension $\chi = 400$, while for $L = 32$ we increase to $\chi = 600$ for the CLIK-MPS calculations. Note that for the calculation of more complicated expectation values a larger bond dimension may be needed.

steady state is a pure state up to finite-size corrections, and each QJ trajectory converges to the same steady state, meaning that one needs to compute a single trajectory in the limit $L \rightarrow \infty$. For typical mixed steady states, the number of trajectories increases upon increasing the system size when long-range correlations cause the fluctuations of local observables across trajectories to increase with the system size [75].

APPENDIX B: CONSTRUCTING THE KRYLOV SUBSPACE

The starting point of the CLIK-MPS framework is to represent the vectorized Lindbladian as an MPO [62] and an initial vectorized (potentially mixed) state as an MPS [51]. Then, a time evolution is performed to obtain a set of vectorized states $\{|\rho(t_i)\rangle\rangle_i$. All the details on the efficient implementation of time evolutions can be found in Appendix H. For this set of states, we calculate the Gram matrix $\mathbf{M}_{ij} = \langle\langle\rho(t_i)|\rho(t_j)\rangle\rangle$ and diagonalize it as $\mathbf{M} = \mathbf{U}\mathbf{S}\mathbf{U}^\dagger$. Notice that the diagonalization is potentially ill-conditioned due to the high condition number of $\mathbf{M}$, which is why we use a version of the Block singular value decomposition for the diagonalization [70]. We discard eigenvalues smaller than a threshold ϵ , which we set to $\epsilon = 10^{-14}$ for all calculations in this paper, and advise choosing ϵ higher than machine precision. A transformation into an orthonormal basis (ONB) is now given by $\mathbf{X} = \mathbf{U}\mathbf{S}^{-1/2}$ [58]. The effective Lindbladian in the Krylov subspace is then calculated directly from its matrix elements $\mathbf{L}_{ij} = \langle\langle\rho(t_i)|\hat{\mathcal{L}}|\rho(t_j)\rangle\rangle$ on the time-evolved states and transformed into the ONB as $\mathbf{L}^{\text{eff}} = \mathbf{X}^\dagger \mathbf{L} \mathbf{X}$. This avoids the numerically unstable procedure of explicitly building an orthonormal basis from $\{|\rho(t_i)\rangle\rangle_i$. Note that the matrix $\mathbf{L}^{\text{eff}}$ does not contain any auxiliary zero eigenvalues that may be introduced by the lower rank of $\mathbf{S}$ due to the specific definition of $\mathbf{X}$. Diagonalizing $\mathbf{L}^{\text{eff}}$ yields the approximate eigenvalues λ_j^K and right and left eigenvectors $\mathbf{R}_j$ and $\mathbf{L}_j$, respectively. The Krylov-subspace diagonalization procedure is summarized in Algorithm 2. These eigenvectors are now given in the Krylov ONB. To write them as direct sums of the initial time-evolved states, we just need to act with $\mathbf{X}$,

$$|r_j^K\rangle\rangle = \sum_m [\mathbf{X}\mathbf{R}]_{mj} |\rho(t_m)\rangle\rangle. \quad (\text{B1})$$

Interestingly, this equation reveals a powerful property of the method. A central parameter in MPS is the bond dimension χ [51], which determines the maximum amount of correlation the MPS can capture. While larger χ allows for more accurate representations of entangled states, the computational cost of MPS operations grows polynomially with χ , making calculations increasingly demanding. Importantly, the sum of two MPSs results in a new MPS

Algorithm 2. Krylov-subspace diagonalization.

```

1: procedure KRYLOV_LINDBLADIAN( $\{|\rho(t_i)\rangle\rangle_i, \epsilon$ )
2:    $\mathbf{L} \leftarrow$  Lindbladian matrix elements  $\langle\langle\rho(t_i)|\hat{\mathcal{L}}|\rho(t_j)\rangle\rangle$ 
3:    $\mathbf{M} \leftarrow$  Gram matrix  $\langle\langle\rho(t_i)|\rho(t_j)\rangle\rangle$ 
4:    $\mathbf{S}, \mathbf{U} \leftarrow$  diagonalized Gram matrix  $\mathbf{M}$ 
5:    $\mathbf{S}, \mathbf{U} \leftarrow$  discard eigenvalues smaller than  $\epsilon$ 
6:    $\mathbf{X} \leftarrow \mathbf{U}\mathbf{S}^{-1/2}$  ▷ trafo into ONB
7:    $\mathbf{L}^{\text{eff}} \leftarrow \mathbf{X}^\dagger \mathbf{L} \mathbf{X}$  ▷ Action on ONB
8:    $\{\lambda_i, \mathbf{l}^i, \mathbf{r}^i\}_i \leftarrow$  spectral decomp. of  $\mathbf{L}^{\text{eff}}$ 
9:   return  $\{\lambda_i, \mathbf{r}^i\}_i, \mathbf{X}$ 
10: end procedure

```

whose bond dimension in general equals the sum of the bond dimensions of the original states. Thus, if the time-evolved states $|\rho(t_i)\rangle\rangle$ have corresponding bond dimension $\chi(\rho(t_i))$, then the maximal bond dimension χ_{eff} reachable within the Krylov space is the bond dimension of a linear combination

$$\chi_{\text{eff}} = \sum_{i=1}^{N_K} \chi(\rho(t_i)) \leq N_K \max_{i \leq N_K} \chi(\rho(t_i)), \quad (\text{B2})$$

where N_K denotes the number of time-evolved states in the Krylov subspace. We term χ_{eff} the effective Krylov bond dimension, as it describes the expressibility of the Krylov subspace. In many cases, χ_{eff} is 2 orders of magnitude bigger than the ones of the time-evolved states due to the linear dependence on N_K , allowing for far stronger entangled states. Crucially, however, such states with large bond dimension never need to be constructed for calculating expectation values or other quantities (see Appendix D) in the Krylov space, rendering the computations very efficient. This suggests that highly accurate Lindbladian eigenmodes can be constructed from time-evolved states with moderate or even small bond dimensions, provided that the accumulated errors during the dynamics remain controlled.

As described in the main text, we not only build the Krylov space out of time-evolved states from one evolution, but we also perform two separate time evolutions with different initial states. Besides a real-time evolution, we perform one along a complex contour parametrized by $z = te^{-i\alpha}$ with an angle $\alpha > 0$. This choice of a linearly inclined complex contour changes the weights of the different right eigenmodes during time evolution differently, which is best seen when going into the eigendecomposition of the Lindbladian, where the time evolution then reads

$$|\rho(z)\rangle\rangle = e^{\hat{\mathcal{L}}z} |\rho_0\rangle\rangle = |\rho_{\text{SS}}\rangle\rangle + \sum_{k=2}^{D^2} e^{\lambda_k z} \langle\langle l_k | \rho_0 \rangle\rangle |r_k\rangle\rangle. \quad (\text{B3})$$

Consequently, the mode $|r_k\rangle\rangle$ is modulated by an exponential with exponent $\lambda_k z$. The corresponding exponential dampening is dictated by its real part, which is given by

$$\xi_k = -\frac{\text{Re}(\lambda_k z)}{t} = -\text{Re}(\lambda_k) \cos(\alpha) - \text{Im}(\lambda_k) \sin(\alpha). \quad (\text{B4})$$

To get more insights into which spectral regions decay more slowly than for a real-time evolution, we can characterize each λ_k by $\lambda_k = |\lambda_k|e^{i\phi_k}$, yielding

$$\xi_k = -\text{Re}(\lambda_k) \frac{\cos(\alpha - \phi_k)}{\cos(\phi_k)}. \quad (\text{B5})$$

Fixing a value of α , eigenvalues whose decay is the same as for $\alpha = 0$ satisfy $\cos(\alpha - \phi_k) = \cos(\phi_k)$, which shows that eigenvalues having $\phi_k < \alpha/2 + \pi$ are enhanced [i.e., feature a lower damping rate $\xi_k < -\text{Re}(\lambda_k)$], while $\phi_k > \alpha/2 + \pi$ are suppressed. Consequently, for positive α , eigenvalues with $\text{Im}(\lambda_k) \geq 0$ are enhanced. This means that the time-evolved states with positive angle α feature higher weight on the upper half plane than real-time-evolved states ($\alpha = 0$), where the damping of a mode is dictated by $\text{Re}(\lambda_k)$, which is also the projection of the eigenvalue onto the real axis. Equation (B4) implies that this picture is slightly changed for the complex contours, and the projection axis has to be rotated by the angle α , as shown schematically in Fig. 2(a).

Note that Eq. (B5) also reveals that the choice of α is not totally free. For instance, if the angle is chosen such that $\alpha > \phi_k - (\pi/2)$ for some eigenvalue $\lambda_k = |\lambda_k|e^{i\phi_k}$, the damping rate ξ_k of the corresponding eigenvalue is negative, and the contribution is exponentially enhanced during time evolution. In this case, all eigenvalues λ_k with $\phi_k < (\pi/2) + \alpha$ get enhanced, which typically also includes bulk states, destabilizing the time evolution. Additionally, the Krylov space may contain large contributions from bulk states, decreasing the capabilities to resolve the low-lying eigenvalues accurately. It is therefore imperative to guarantee that $\alpha \ll \alpha_{\max} = \min_k \phi_k - (\pi/2)$.

We can do so by observing that the time evolution of a traceless initial state $|\rho\rangle\rangle$ shows the behavior

$$\langle\langle \rho(t) | \rho(t) \rangle\rangle \rightarrow \begin{cases} 0 & \text{if } \alpha \leq \alpha_{\max}, \\ \infty & \text{if } \alpha > \alpha_{\max}, \end{cases} \quad (\text{B6})$$

where the divergence is exponential. Consequently, by initializing a few time evolutions with different angles α and tracking the norm during a short time evolution, a good approximation to the maximal angle $\alpha_{\max}$ can be found. Afterward, a much lower angle $\alpha \ll \alpha_{\max}$ is chosen for the time evolution.

A corresponding algorithm summarizing these ideas is given in Algorithm 3. After initializing a (random) traceless state, a short time evolution is carried out for different

Algorithm 3. Approximate $\alpha_{\max}$.

```

1: procedure GET $\alpha_{\max}$ (t)
2:    $|\rho\rangle\rangle \leftarrow$  initialize (random) traceless state
3:   for  $\alpha$  in grid do
4:      $|\rho(e^{-i\alpha}t)\rangle\rangle \leftarrow$  calculate complex-time evolution
5:     if Norm is diverging then
6:        $\alpha_{\max} < \alpha$ 
7:     end if
8:   end for
9:   return  $\alpha_{\max}$ 
10: end procedure

```

values of the complex angle α . Depending on the evolution of the norm of the state, the angle $\alpha_{\max}$ can be estimated by checking Eq. (B6).

Note that the left eigenmode of the steady state to any Lindbladian is given by $|l_1\rangle\rangle = |1\rangle\rangle$. This also includes nonunique steady states, where the identity has to be understood on one specific subspace of the degeneracy, generating strong symmetry. Consequently, initial states (living in a single subspace) that are traceless (and thus unphysical) have vanishing weight on the steady-state sector,

$$0 = \text{Tr}(\hat{\rho}_{\text{initial}}) = \langle\langle 1 | \rho_{\text{initial}} \rangle\rangle = \langle\langle l_1 | \rho_{\text{initial}} \rangle\rangle. \quad (\text{B7})$$

This property is preserved by the time evolution, and thus (up to truncation errors) the set of time-evolved states will be orthogonal to the steady state. If we normalize during time evolution, these states even converge to the slowest-decaying mode instead of the steady state. Note that in the case of the dissipative Bose-Hubbard model, where the particle number conservation enforces a strong $U(1)$ symmetry, we simulate the dynamics in a specific symmetry sector (i.e., at a given particle number). A schematic summary of the main components of CLIK-MPS can be found in Fig. 9.

Note that to generate a Krylov subspace that accurately captures the left Lindbladian eigenmatrices, one needs to perform the time evolution with $\mathcal{L}^\dagger$ [see Eq. (8) in the main text]. Then, one can apply Algorithm 2, with the sole difference being that we include the steady state of $\mathcal{L}^\dagger$, which is the vectorized identity $|1\rangle\rangle$ restricted to a given strong symmetry sector. If there are no conserved quantities, we add the vectorized identity on the whole space. For example, in the case of the Bose-Hubbard model considered in the main text, we add the identity restricted to the total particle number sector we fixed through the initial state [37,65]. This way, we do not introduce contributions from other subsectors into the Krylov space. Since the right eigenmodes of $\hat{\mathcal{L}}^\dagger$ are actually the left eigenmodes of $\hat{\mathcal{L}}$, the left eigenmodes are also constructed using Eq. (B1).

Complex-time Lindbladian Krylov-subspace MPS
(CLIK-MPS):

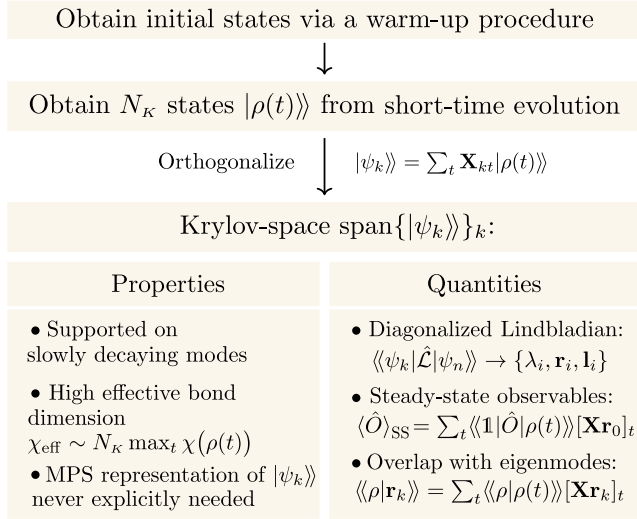


FIG. 9. Schematic depiction of the CLIK-MPS routine.

APPENDIX C: WARM-UP: OPTIMAL INITIALIZATION

Aside from the maximum evolution time and complex angle, the initial state is the most critical input to the algorithm. For the method to perform reliably, it must be chosen carefully and according to a systematic strategy. In this section, we aim to provide physically motivated algorithms to generate good initial states, which are readily generalized to other systems. The framework presented in this article spans over two different time-evolution schemes: the propagation of physical states $|\sigma_n^p\rangle$ and traceless states $|\sigma_n^u\rangle$, with either $\hat{\mathcal{L}}$ or $\hat{\mathcal{L}}^\dagger$. The efficient initialization of these requires two different optimization protocols, which we discuss below.

First, let us discuss the warm-up of $|\sigma_n^p\rangle$. At late times $t \gg 1/\text{Re}(\lambda_2)$, the time evolution of an initial state with finite trace will lead to a state close to the steady state. Since we want to capture the steady state and the slowest-decaying modes with this time evolution efficiently, an initial state with a large overlap with modes corresponding to eigenvalues with small modules of their real parts would be favorable. This is implemented by minimizing the real part of the expectation value and variance of the Lindbladian on a subspace spanned by stochastically chosen states. The resulting routine is summarized in Algorithm 4. The random subspace is initialized by a product state $|\psi_0\rangle = |n_1, n_2, \dots, n_L\rangle$ on the physical lattice, which is appended to a list S . In the case of the dissipative Bose-Hubbard model considered here, we found that states having most particles located on the ends of the chain are admissible, since they have a low expectation value. We emphasize that the effectiveness of a particular initial state strongly depends on the specific structure of the

Algorithm 4. Compute optimal initial state $|\sigma_n^p\rangle$.

```

1: procedure INITIAL_1( $|\psi_0\rangle, n_{\text{samples}}$ )
2:    $S \leftarrow [|\psi_0\rangle]$  ▷ Initialize with the input state
3:   for  $n = 1$  to  $n_{\text{samples}} - 1$  do
4:      $|\psi\rangle \leftarrow$  randomly drawn from  $S$ 
5:      $k \leftarrow$  random occupied site in  $|\psi\rangle$ 
6:      $i \leftarrow$  random number from  $\pm 1$ 
7:      $|\tilde{\psi}\rangle \leftarrow \hat{b}_{k+i}^\dagger \hat{b}_k |\psi\rangle$ 
8:     if  $|\tilde{\psi}\rangle \notin S$  then
9:       Append  $|\tilde{\psi}\rangle$  to  $S$ 
10:    else
11:      Go back to line 4
12:    end if
13:  end for
14:   $R \leftarrow [|\psi\rangle \otimes |\phi\rangle \text{ for } |\psi\rangle, |\phi\rangle \text{ in } S]$ 
15:   $\mathbf{L}^{\text{eff}} \leftarrow \langle\langle \rho_i | \hat{\mathcal{L}} | \rho_j \rangle\rangle \text{ for } |\rho_i\rangle, |\rho_j\rangle \text{ in } R$ 
16:   $\lambda_0, \mathbf{r}^0 \leftarrow$  lowest eigenvalue and right eigenvector of  $\mathbf{L}^{\text{eff}}$ 
17:   $|\rho_{\text{initial}}\rangle \leftarrow$  build  $\sum_i \mathbf{r}_i^0 |\rho_i\rangle$  for  $|\rho_i\rangle$  in  $R$ 
18:  if  $|\langle \mathbb{1} | \rho_{\text{initial}} \rangle| < \epsilon_{\text{trace}}$  then
19:    Go back to line 3
20:  end if
21:  return  $|\rho_{\text{initial}}\rangle, S$ 
22: end procedure

```

Lindbladian. Now, $n_{\text{samples}} - 1$ different states are generated stochastically as follows: In each iteration, a state $|\psi\rangle$ is randomly selected from S , along with an index k labeling an occupied site, and a neighboring site $i \in k \pm 1$ (note that if k lies at the boundary, only one neighboring site exists). A new state $|\tilde{\psi}\rangle$ is built by removing a particle on site k and inserting one at $k + i$ in $|\psi\rangle$. The state is added to S if it is not already included, generating a set of n_{samples} states that are connected through successive nearest-neighbor hoppings. This is favorable, since the Lindbladian is local, and thus finite transition rates between different states will occur. Note that for Lindbladians that do not preserve the total particle number, it might be beneficial to also include stochastic single-particle loss and injection in addition to hopping. Once again, we stress that the procedure for sampling basis states is motivated by the specific dissipative Bose-Hubbard Lindbladian that we considered here; for other systems, slight changes might improve the procedure. A set of vectorized states can then be built by taking the tensor product between states in S . This yields the set $R = S \otimes S$ containing all $|\rho\rangle = |\psi\rangle \otimes |\phi\rangle$ with $|\psi\rangle$ and $|\phi\rangle$ in S . The set R features n_{samples}^2 different orthonormal states on the vectorized lattice. The effective Lindbladian action $\mathbf{L}^{\text{eff}}$ on R is given by $\mathbf{L}_{ij}^{\text{eff}} = \langle\langle \rho_i | \hat{\mathcal{L}} | \rho_j \rangle\rangle$, where $|\rho_i\rangle, |\rho_j\rangle \in R$. We diagonalize $\mathbf{L}^{\text{eff}}$, pick the lowest-lying right eigenvector $\mathbf{r}^0$ as our initial state, and construct its MPS-representation by $|\rho_{\text{initial}}\rangle = \sum_i \mathbf{r}_i^0 |\rho_i\rangle$.

To ensure it is a traceful state, we calculate its trace norm $\langle\langle \mathbb{1} | \rho_{\text{initial}} \rangle\rangle$ and discard the state and repeat the procedure if it happens to be smaller than some threshold ϵ_{trace} .

With some minor adjustments, this algorithm can also be used to find optimal initializations for $|\sigma_n^u\rangle$, i.e., traceless states with low expectation value and variance with the Lindbladian [see also Eq. (B7)]. This constraint is elegantly incorporated by choosing only traceless basis states for the subspace R , making every spanned state in the subspace immediately traceless. The corresponding pseudocode is given in Algorithm 5. As mentioned, the basic idea stays the same, but the subspace in which the optimal state is searched for (spanned by the randomly chosen states) should contain only traceless states. Vectorized states of the form $|\psi\rangle \otimes |\phi\rangle$ with $|\psi\rangle, |\phi\rangle \in S$ if $|\psi\rangle \neq |\phi\rangle$ are already traceless and can be appended to R . However, $|\psi\rangle \otimes |\psi\rangle$ has trace one, so we may instead take $|\psi\rangle \otimes |\psi\rangle - |\phi\rangle \otimes |\phi\rangle$ into R . Notice that the procedure leads to $n_{\text{samples}}^2 - 1$ states in R living on the vectorized lattice. Different from Algorithm 4, these states are not orthonormal, and we need to build an ONB from them. This can be done by employing Algorithm 2 initialized with the set of states R and some threshold for the retained eigenvalues ϵ . Notice that due to the simple structure of the states in R , the Gram matrix may also be constructed explicitly without calculating any overlaps. Algorithm 2 returns the eigenvalues and corresponding right eigenvectors $\{\lambda_i, \mathbf{r}^i\}_i$ of the effective Lindbladian in the Krylov space, and the transformation into the Krylov ONB. The right eigenvector $\mathbf{r}^0$ to the highest eigenvalue is now the state with the lowest real part of the Lindbladian expectation in the subspace, and thus the optimal initial state. Back in the MPS representation, this state is constructed as $|\rho_{\text{initial}}\rangle\rangle = \sum_i [\mathbf{X}\mathbf{r}^0]_i |\rho_i\rangle\rangle$.

Although Algorithms 4 and 5 return a good initial state in the stochastically chosen subspaces, there is no guarantee that there might not be a better subspace in the first place. This problem can be resolved by introducing an iterative extension to the methods shown in Algorithm 6. Instead of directly building the whole subspace in one step, we now iteratively find the full subspace by successively adding a few random states and optimizing this smaller subspace in each step. Specifically, given a state list S containing n states, we stochastically generate a new state list S' by

Algorithm 5. Compute optimal initial state $|\sigma_n^u\rangle$.

```

1: procedure INITIAL_2( $|\psi_0\rangle, n_{\text{samples}}$ )
2:    $S \leftarrow$  do lines 2–13 from Algorithm 4
3:    $R \leftarrow [|\psi\rangle \otimes |\phi\rangle \text{ for } |\psi\rangle, |\phi\rangle \text{ in } S \text{ if } |\psi\rangle \neq |\phi\rangle]$ 
4:    $D \leftarrow [|\psi\rangle \otimes |\psi\rangle \text{ for } |\psi\rangle \text{ in } S]$ 
5:   for  $n = 1$  to  $n_{\text{sites}} - 1$  do
6:     Append  $|\delta_n\rangle\rangle - |\delta_{n+1}\rangle\rangle$  to  $R$  for  $|\delta_n\rangle\rangle, |\delta_{n+1}\rangle\rangle$  in  $D$ 
7:   end for
8:    $\{\lambda_i, \mathbf{r}^i\}_i, \mathbf{X} \leftarrow$  do Algorithm 2 with states  $R$ 
9:    $\lambda_0, \mathbf{r}^0 \leftarrow$  highest eigenvalue and right eigenvector
10:   $|\rho_{\text{initial}}\rangle\rangle \leftarrow$  build  $\sum_i [\mathbf{X}\mathbf{r}^0]_i |\rho_i\rangle\rangle$  for  $|\rho_i\rangle\rangle$  in  $R$ 
11:  return  $|\rho_{\text{initial}}\rangle\rangle$ 
12: end procedure
    
```

adding two states through hopping to S and evaluating the lowest eigenvalue. The same process was repeated a couple of times, and afterward, we chose the one set S' which gave rise to the lowest eigenvalue. This leaves us with a set S of size $n + 2$, and the process may be repeated. This method lowers the expectation value systematically in every iteration, and it can be ended either if a desired Krylov-space dimension is attained, or a threshold bond dimension or Lindbladian expectation value is reached. The former is implemented via the choice of n_{samples} , which bounds the Krylov-space dimension by n_{samples}^2 , while the latter is implemented as an escape criterion.

In Fig. 10, such an iterative procedure is shown for the dissipative Bose-Hubbard model with ten sites and five particles. The warm-up was performed until $n_{\text{states}} = 16$ for both a traceless and a physical initial state. In every iteration, the expectation value is lowered, which shows the benefit of iteratively applying Algorithms 4 and 5. The corresponding bond dimensions (see inset) increase with n_{states} to about $\chi = 20$ (physical) and $\chi = 60$ (traceless). Since in every iteration only two basis vectors are added, not all matrix elements have to be calculated, since some can be reused from the earlier iteration.

For the time evolution with $\hat{\mathcal{L}}^\dagger$, the search for an optimal initial state is not as easily physically motivated. Unfortunately, we do not know the structure of the left eigenvector corresponding to the steady state, and thus orthogonalizing against it is not doable. Minimizing the expectation value of $\hat{\mathcal{L}}^\dagger$ is nevertheless useful, and we thus just use the same algorithms as for the time evolution with $\hat{\mathcal{L}}$. The sole adjustment is that the effective Lindbladian $\mathbf{L}^{\text{eff}}$ has to be replaced by the adjoint effective Lindbladian,

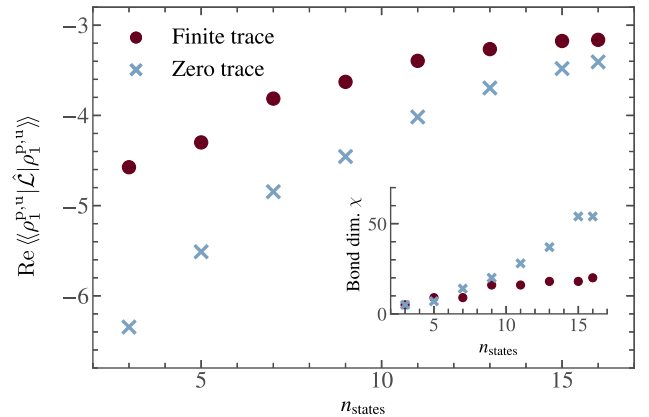


FIG. 10. Initial states optimized via the warm-up procedure. We perform a search up to $n_{\text{states}} = 16$ and compute $\langle\langle\rho_1^{p,u}|\hat{\mathcal{L}}|\rho_1^{p,u}\rangle\rangle$ for the optimal basis in every iteration, both for finding a physical initial state (red dots) and a traceless initial state (blue crosses). Inset: the corresponding maximal bond dimension of the respective states $|\rho_1^{p,u}\rangle\rangle$. All calculations were performed for a dissipative Bose-Hubbard model Eqs. (12) and (13) with $L = 10$ sites and $N = 5$ particles, setting $J = U = \kappa = 1$.

Algorithm 6. Iteratively compute optimal initial states.

```

1: procedure ITERATE_INITIAL( $|\psi_0\rangle, n_{\text{samples}}$ )
2:   for  $n = 1$  to  $n_{\text{samples}}/2$  do
3:     fork  $k = 1$  to  $3n_{\text{sites}}$  do
4:        $|\rho(k)\rangle, S(k) \leftarrow$  Do Algorithm 4 or 5 with  $(S, 2)$ 
5:     end for
6:      $k_{\text{max}} \leftarrow \text{argmax}_k \text{Re}\langle -3mu\langle \rho(k) | \hat{\mathcal{L}} | \rho(k) \rangle \rangle$ 
7:      $|\rho_{\text{initial}}\rangle, S \leftarrow |\rho(k_{\text{max}})\rangle, S(k_{\text{max}})$ 
8:     if  $\chi(\rho_{\text{initial}}) > \chi_{\text{max}}$  then
9:       Break
10:    end if
11:  end for
12:  return  $|\rho_{\text{initial}}\rangle$ 
13: end procedure

```

$\langle \rho_i | \hat{\mathcal{L}}^\dagger | \rho_j \rangle$. Thus, for time evolutions with zero complex angle $\alpha = 0$, we use Algorithm 4, whereas for finite angles, Algorithm 5 is employed (both within the iterative extension described in Algorithm 6).

APPENDIX D: COMPUTING EXPECTATION VALUES AND OVERLAPS

In most applications, also throughout this paper, the explicit MPS representation of the steady state and slowly decaying modes is not of primary interest; rather, one typically focuses on specific expectation values or overlaps with them. In CLIK-MPS it is actually possible to avoid constructing the MPS representation of the approximate eigenvectors. It suffices to compute overlaps and expectation values with the original time-evolved states.

Assume we are interested in the expectation of operator $\hat{A}$ (for instance, some particle-particle correlator $\hat{A}_{ij} = \hat{b}_i^\dagger \hat{b}_j$ in the main text). As shown in Eq. (B1), the unnormalized steady state can be represented easily in the original basis. Thus, if we define the action of $\hat{A}$ on the Krylov basis as $\mathbf{A}_n^{\text{eff}} = \langle \mathbb{1} | \hat{A} | \rho(t_n) \rangle$ and the normalization $\mathbf{N}_n = \langle \mathbb{1} | \rho(t_n) \rangle$, it is straightforward to calculate expectation values

$$\text{Tr}(\hat{A} \hat{\rho}_{\text{ss}}) = \frac{[\mathbf{A}^{\text{eff}} \mathbf{X} \mathbf{R}]_1}{[\mathbf{N} \mathbf{X} \mathbf{R}]_1}. \quad (\text{D1})$$

Note that the vectorized identity is in general well described by an MPS with low bond dimension; in all calculations performed in the scope of this article, it did not exceed $\chi \sim 10^3$.

Since the time evolution with a nonzero complex angle is not Hermiticity preserving, the steady state $|\hat{r}_1^K\rangle$ might have some non-Hermitian artifacts due to the finite α contributions, which are also present in Appendix (D1). This issue can be resolved by instead considering the Hermitian part of the density matrix given by $|\hat{r}_{1,\text{Herm}}^K\rangle = -\frac{1}{2}(|\hat{r}_1^K\rangle + |\hat{r}_1^{K\dagger}\rangle)$, where $|\hat{r}_1^{K\dagger}\rangle$ denotes the vectorization of $[\hat{r}_1^K]^\dagger$. Expectation values of $\hat{A}$ with this Hermitian steady

state can be calculated easily within the Krylov space. Besides $\mathbf{A}^{\text{eff}}$, we define $\mathbf{A}_n^{\text{eff},*} = \langle \mathbb{1} | \hat{A}^\dagger | \rho(t_n) \rangle$, and find

$$\text{Tr}(\hat{A} \hat{\rho}_{\text{ss}}) = \frac{1}{2[\mathbf{N} \mathbf{X} \mathbf{R}]_1} ([\mathbf{A}^{\text{eff}} \mathbf{X} \mathbf{R}]_1 + [\mathbf{A}^{\text{eff},*} \mathbf{X} \mathbf{R}]_1^*). \quad (\text{D2})$$

This equation eliminates non-Hermitian artifacts, and we use it throughout the main text when calculating the two-point correlator.

Similarly, overlaps of arbitrary states with the Krylov eigenvectors can be calculated. If we are interested in the overlap of some vectorized density matrix $|\rho\rangle$ with the Krylov eigenmode $|\hat{r}_j^K\rangle$, it suffices to calculate the overlap vector $\mathbf{O}_n = \langle \rho | \rho(t_n) \rangle$ to obtain

$$\langle \rho | \hat{r}_j^K \rangle = [\mathbf{O} \mathbf{X} \mathbf{R}]_j. \quad (\text{D3})$$

Crucially, we did not need to construct the explicit MPS representations of any eigenvector in the Krylov space, which drastically reduces computational complexity.

Note that it is enough to describe overlaps with right eigenvectors, as left eigenvectors of $\hat{\mathcal{L}}$ are calculated in CLIK-MPS by considering time evolution with $\hat{\mathcal{L}}^\dagger$, whose right eigenvectors are the left eigenvectors of $\hat{\mathcal{L}}$. Our framework gives access to highly accurate eigenvalues and eigenstates on the upper half plane. Because of the Lindbladian being Hermitian preserving, the spectrum is symmetric around the real axis, and eigenvalues on the lower half plane can be trivially obtained by complex conjugation. Eigenvectors on the lower half plane can also be found by Hermitian conjugation of the ones on the upper plane. Overlaps with them are nevertheless easy to calculate within CLIK-MPS; we need only the useful identity

$$\langle \hat{r}_i^\dagger | \rho \rangle = \langle \hat{r}_i | \rho \rangle^*, \quad (\text{D4})$$

which is easily proven in the density-matrix picture using the properties of the trace and $\hat{\rho}$ being Hermitian. Thus, the overlap with $|\hat{r}_i^\dagger\rangle$ is easily computed within CLIK-MPS.

An application of the observable calculation in the steady state of the Krylov space can be seen in Fig. 11. As in the main text, we are interested in the correlation function $\langle \hat{b}_i^\dagger \hat{b}_j \rangle_{\text{ss}} = \text{Tr}(\hat{b}_i^\dagger \hat{b}_j \hat{\rho}_{\text{ss}})$. For the steady state, we use the approximate steady state obtained via CLIK-MPS and label it with the maximal Krylov time T , giving $|\rho_{\text{ss}}^K(T)\rangle$. We fix the first index at $i_0 = L/4$ to avoid influence from the boundaries. The observables can be easily obtained using Eq. (D2). We find that the correlation function decays exponentially, as expected within the mean-field theory [72]. The corresponding correlation length ξ can be fitted from the tail of the correlation function using an exponential fitting function, where we again dismiss the boundary sites. Convergence of the correlation length can be monitored by building the Krylov subspace spanning

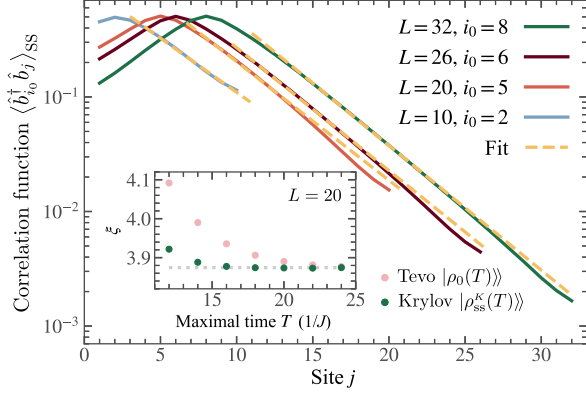


FIG. 11. Steady state from large system calculations. Correlation function for ten (blue), 20 (orange), 26 (red), and 32 (green) sites depending on the second site index j at fixed first index $i_0 = L/4$ at $U = 2J$. We fit the tail of the correlation function exponentially (yellow) and recover the correlation length ξ of the many-body mixed state. The Krylov spaces used time-evolved states until 6, 18, 22, and 32 with a sampling spacing of 0.1, 0.2, 0.4, and 0.4 for the different system sizes, respectively. Inset: correlation length ξ depending on the maximal time T for 20 sites. We compare the CLIK-MPS steady state $|\rho_{ss}^K(T)\rangle\rangle$ with the last time-evolved state $|\rho_0(T)\rangle\rangle$. For all data shown here, we chose $J = 1$, $\kappa = 2J$, a local dimension $d = N + 1$, and for $L \leq 20$ we set the maximal bond dimension $\chi = 2400$, while for $L > 20$ we had $\chi = 1400$.

over states up to a shorter maximal time T and comparing ξ . A detailed discussion of the convergence analysis can be found in Appendix G. For all correlation lengths shown in the main text in Fig. 5, the same calculations were performed.

APPENDIX E: EXPLOITING SYMMETRIES

Exploiting symmetries is a key strategy for improving the efficiency of observable calculations. Assume the Lindbladian at hand possesses a discrete symmetry, which comes with a generator $\hat{Q}$ and a unitary $\hat{U}$ connected via

$$\hat{U} = \exp(-2\pi i \hat{Q}). \quad (\text{E1})$$

In most practical cases, including the example of $\mathbb{Z}_{N_S}$ symmetries, the vectorized unitary $\hat{U}$ is constructed from another unitary $\hat{U}$ acting on the physical and auxiliary space $\hat{U} = \hat{U} \otimes \hat{U}^*$. The generator $\hat{Q}$ of $\hat{U}$ is thus given by $\hat{Q} = \hat{Q} \otimes \hat{1} - \hat{1} \otimes \hat{Q}$. In the case of $\mathbb{Z}_{N_S}$ symmetries, $\hat{Q}$ has spectrum j/N_S for $0 \leq j < N_S$. Notice that this directly fixes the spectrum of $\hat{Q}$.

If the Lindbladian now exhibits this symmetry, i.e., $[\hat{L}, \hat{U}] = 0$, it decomposes into N_S blocks, each characterized by a fixed transformation behavior and labeled by the eigenvalues q of $\hat{Q}$. All Lindbladian eigenvectors $|l_j\rangle\rangle, |r_j\rangle\rangle$ are thus also eigenvectors of $\hat{U}$ and live in a fixed

symmetry sector q . Consequently, we would like to not use the approximate Krylov eigenvector as steady state but instead its projection into the subspace it belongs to due to the symmetry. We label this symmetry sector by q_0 . In mathematical terms, this translates to

$$|\rho_{ss}^{K,q_0}\rangle\rangle = \hat{P}_{q_0} |\rho_{ss}^K\rangle\rangle, \quad (\text{E2})$$

where $\hat{P}_{q_0}$ is the projector onto the q_0 sector. Crucially, this projector can be written as a polynomial in $\hat{U}$,

$$\hat{P}_{q_0} = \frac{1}{N_S} \sum_{n=0}^{N_S-1} e^{2\pi i q_0 n} \hat{U}^n. \quad (\text{E3})$$

The key question that remains is identifying the q_0 sector in which the steady state resides. Interestingly, one can show that the steady state is always in the $q_0 = 0$ sector. Since the steady state $|\rho_{ss}\rangle\rangle$ has a finite trace, it contains a component lying in the 0 sector due to

$$\begin{aligned} \langle\langle \mathbb{1} | \hat{P}_{q_0} | \rho_{ss} \rangle\rangle &= \frac{1}{N_S} \sum_{n=0}^{N_S-1} e^{2\pi i q_0 n} \langle\langle \mathbb{1} | \hat{U}^n | \rho_{ss} \rangle\rangle \\ &= \frac{\langle\langle \mathbb{1} | \rho_{ss} \rangle\rangle}{N_S} \sum_{n=0}^{N_S-1} e^{2\pi i q_0 n} \\ &= \langle\langle \mathbb{1} | \rho_{ss} \rangle\rangle \delta_{q_0=0}. \end{aligned} \quad (\text{E4})$$

Because of the fact that $\hat{U}|\mathbb{1}\rangle\rangle = |\mathbb{1}\rangle\rangle$, which is seen by going back into the matrix picture, $\hat{U}|\mathbb{1}\rangle\rangle \rightarrow \hat{U}^\dagger \mathbb{1} \hat{U} = \mathbb{1}$. The only possible sector eligible for the steady state is thus the $q_0 = 0$ sector. Now, we can safely insert the symmetrized approximate steady state $\hat{P}_{q_0=0} |\rho_{ss}^K\rangle\rangle$ into the observable

$$\begin{aligned} \text{Tr}(\hat{A} \hat{\rho}_{ss}) &= \langle\langle \mathbb{1} | \hat{A} \hat{P}_{q_0=0} | \rho_{ss}^K \rangle\rangle \\ &= \frac{1}{N_S} \sum_{n=0}^{N_S-1} \langle\langle \mathbb{1} | \hat{U}^n (\hat{U}^\dagger)^n \hat{A} \hat{U}^n | \rho_{ss}^K \rangle\rangle. \end{aligned} \quad (\text{E5})$$

The expression is brought into its final form by defining the overlaps $\mathbf{A}_{n,k}^{\text{eff}} = \langle\langle \mathbb{1} | (\hat{U}^\dagger)^n \hat{A} \hat{U}^n | \psi_k \rangle\rangle$, which yields

$$\text{Tr}(\hat{A} \hat{\rho}_{ss}) = \frac{1}{N_S [\mathbf{N} \mathbf{X} \mathbf{R}]_1} \sum_{n=0}^{N_S-1} [\mathbf{A}^{\text{eff}} \mathbf{X} \mathbf{R}]_{n1}. \quad (\text{E6})$$

Computationally, this is equivalent to calculating Appendix (D1) N_S times. The crucial advantage we gain by avoiding applying the projector directly onto $|\rho_{ss}^K\rangle\rangle$, is that in most use cases the operator $\hat{A}$ is much simpler than the states in the Krylov space, and $(\hat{U}^\dagger)^n \hat{A} \hat{U}^n$ can be calculated exactly. Notice that Eq. (E6) can be combined with the cancellation of non-Hermitian artifacts similarly to

Eq. (D2). If we also define $\mathbf{A}_{n,k}^{\text{eff},*} = \langle\langle 1 | (\hat{U}^\dagger)^n \hat{A}^\dagger \hat{U}^n | \psi_k \rangle\rangle$, we end up with the final expression

$$\text{Tr}(\hat{A}\hat{\rho}_{\text{SS}}) = \frac{\sum_{n=0}^{N_S-1} ([\mathbf{A}^{\text{eff}} \mathbf{X} \mathbf{R}]_{n1} + [\mathbf{A}^{\text{eff},*} \mathbf{X} \mathbf{R}]_{n1}^*)}{2N_S[\mathbf{N} \mathbf{X} \mathbf{R}]_1}. \quad (\text{E7})$$

In the specific case of the dissipative Bose-Hubbard model considered in the main text, there is an additional $\mathbb{Z}_2$ symmetry given by an inversion of the lattice around the middle site(s). The corresponding unitary $\hat{U}_{\text{inv}}$ has the action $\hat{U}_{\text{inv}}^\dagger \hat{b}_j \hat{U}_{\text{inv}} = \hat{b}_{L+1-j}$, and its vectorized version is given by $\hat{\mathcal{U}}_{\text{inv}} = \hat{U}_{\text{inv}} \otimes \hat{U}_{\text{inv}}^*$. We are mainly interested in the two point correlators $\langle \hat{b}_j^\dagger \hat{b}_k \rangle_{\text{SS}}$, which means we chose $\hat{A}_{j,k} = \hat{b}_j^\dagger \hat{b}_k$ and consequently, $\hat{\mathcal{U}}_{\text{inv}}^\dagger \hat{A}_{j,k} \hat{\mathcal{U}}_{\text{inv}} = \hat{b}_{L+1-j}^\dagger \hat{b}_{L+1-k} = \hat{A}_{L+1-j, L+1-k}$. Thus, the resulting computations based on Eq. (E6) have the same numerical complexity as Appendix (D1).

The main bottleneck in generalizing the expressions (E6) and (E7) to continuous symmetries is the explicit expression of the projector $\hat{P}$ in terms of the unitary $\hat{\mathcal{U}}$. Indeed, in the case of a $U(1)$ symmetry, the generator has countably infinite eigenvalues, the unitary depends continuously on a parameter a , and Eq. (E3) takes on the very familiar form of a Fourier series

$$\hat{P}_n = \frac{1}{2\pi} \int_0^1 da e^{2\pi i a n} \hat{\mathcal{U}}(a). \quad (\text{E8})$$

Now, performing the same steps as before yields

$$\begin{aligned} \text{Tr}(\hat{A}\hat{\rho}_{\text{SS}}) &= \langle\langle 1 | \hat{\mathfrak{A}} | \rho_{\text{SS}}^K \rangle\rangle, \\ \hat{\mathfrak{A}} &= \frac{1}{2\pi} \int_0^1 da \hat{U}^\dagger(a) \hat{A} \hat{U}(a). \end{aligned} \quad (\text{E9})$$

This result is similar to Eq. (E6) and in spirit, only the sum is changed for an integral. This approach is readily generalized to other continuous symmetries in the same fashion.

Also, the derivation of Eqs. (E6), (E7), and (E9) solely relies on the fact that $\hat{\mathcal{U}}|1\rangle = |1\rangle$ and in particular the explicit form of the generator of time evolution is irrelevant, which is particularly useful for the generalization of the framework to non-Markovian settings.

APPENDIX F: COMPARING TO ED EIGENVECTORS

After the diagonalization in the Krylov subspace, we get access to a matrix $\mathbf{R}$ encoding all right eigenvectors, and Eq. (B1) tells us how to write the eigenvectors in the basis of the original time-evolved states. To assess the quality of the approximation, we can compare to ED diagonalization of the Lindbladian written as a matrix in some ONB $\{|e_j\rangle\rangle_j$. This yields the exact right eigenvectors $\mathbf{R}_j^E$ written

in the ONB. To bring the two different bases together, we represent the time-evolved states used in CLIK-MPS in the ONB used for ED by $\mathbf{E}_{mj} = \langle\langle e_m | \rho(t_j) \rangle\rangle$, making it possible to compute the overlap

$$\langle\langle r_j | r_j^K \rangle\rangle = [\mathbf{R}^{E\dagger} \mathbf{E} \mathbf{X} \mathbf{R}]_{jj}, \quad (\text{F1})$$

where $|r_j\rangle\rangle$ is the j th exact right eigenvector of the Lindbladian. Appendix (F1) is best understood from right to left: $\mathbf{X}$ transforms from the Krylov ONB to the original time-evolved states, while $\mathbf{E}$ maps them onto the basis used for ED. Then, the overlap is calculated by acting with the right eigenvectors in this basis from the left. We use Appendix (F1) to calculate the overlaps with the exact right and left eigenvectors in Figs. 4(b) and 4(c) in the main text.

APPENDIX G: QUANTIFYING ACCURACY BEYOND ED COMPARISONS

When considering small systems, the accuracy of the CLIK-MPS framework can be tested straight away as outlined in Appendix F. Instead, for large-scale systems lacking exact reference data, it becomes imperative to develop alternative checks to assess the precision of the computed quantities.

Our main objective is to quantify the deviations from the exact steady state when using CLIK-MPS. We formulate the following theorem:

Denote by $|\rho_{\text{SS}}^K\rangle\rangle$ the approximate steady state from CLIK-MPS. Then we have

$$|\langle\langle \rho_{\text{SS}}^K | \rho_{\text{SS}} \rangle\rangle|^2 \geq 1 - \frac{\langle\langle \rho_{\text{SS}}^K | \hat{\mathcal{L}}^\dagger \hat{\mathcal{L}} | \rho_{\text{SS}}^K \rangle\rangle}{|\sigma_2|^2}. \quad (\text{G1})$$

For the proof, notice that $\hat{\mathcal{L}}^\dagger \hat{\mathcal{L}}$ is Hermitian with a non-negative spectrum. Furthermore, the steady state is its only eigenstate with eigenvalue 0. The gap of this Hermitian operator is given by $\mu_2 = |\sigma_2|^2$, where σ_2 is the second lowest singular value of $\hat{\mathcal{L}}$. We may diagonalize $\hat{\mathcal{L}}^\dagger \hat{\mathcal{L}}$, denote its increasingly ordered eigenvalues by μ_k and its eigenvectors by $|v_k\rangle\rangle$. Going into the eigenbasis we find $|\rho_{\text{SS}}^K\rangle\rangle = \sum_m a_m |v_m\rangle\rangle$ and

$$\langle\langle \rho_{\text{SS}}^K | \hat{\mathcal{L}}^\dagger \hat{\mathcal{L}} | \rho_{\text{SS}}^K \rangle\rangle = \sum_{m \geq 2} \mu_m |a_m|^2. \quad (\text{G2})$$

Combining this with the normalization constraint $1 = \sum_m |a_m|^2$, we find the bound

$$|a_1|^2 = 1 - \sum_{m \geq 2} |a_m|^2 \geq 1 - \frac{1}{\mu_2} \sum_{m \geq 2} \mu_m |a_m|^2, \quad (\text{G3})$$

where we used that $\mu_m/\mu_2 \geq 1$ if $m \geq 2$. Since $|a_1|^2 = |\langle\langle \rho_{\text{SS}}^K | \rho_{\text{SS}} \rangle\rangle|^2$, the lower bound follows immediately.

Although we do not know the singular value σ_2 , the accuracy of the two approximate steady states can nevertheless be compared with only the knowledge of the variance. In some cases, the second-lowest singular value may also be approximated within the Krylov space. Notice that it is possible to calculate $\langle\langle \rho_{SS}^K | \hat{\mathcal{L}}^\dagger \hat{\mathcal{L}} | \rho_{SS}^K \rangle\rangle$ directly inside the Krylov subspace similar to Appendix D. A nontrivial upper bound can be obtained using $\mu_m/\mu_{D^2} \leq 1$, where μ_{D^2} denotes the highest eigenvalue. Following the same steps as above, this implies

$$|\langle\langle \rho_{SS}^K | \rho_{SS} \rangle\rangle|^2 \leq 1 - \frac{\langle\langle \rho_{SS}^K | \hat{\mathcal{L}}^\dagger \hat{\mathcal{L}} | \rho_{SS}^K \rangle\rangle}{|\sigma_{D^2}|^2}. \quad (\text{G4})$$

Interestingly, it is now possible to quantify the accuracy of the bounds. It is governed by the ratio σ_{D^2}/σ_2 , which is connected to the condition number of the Lindbladian (on the subspace orthogonal to the steady state).

Unfortunately, it is hard to derive error bounds for other parts of the spectrum, but there are other ways to check if a spectral feature is sufficiently converged. A simple yet effective approach is to compare approximated spectra from different Krylov spaces with each other. We suggest varying the maximal evolution time T used to construct the Krylov space, while the sampling interval δt remains fixed. In the following, we refer to the Krylov space with larger T as the big Krylov space (having T_{big}), and to the other as the small one (T_{small}). This construction ensures that the second Krylov space contains the first, so the big Krylov space is expected to yield a more accurate spectrum than the small one. If $T_{\text{big}} - T_{\text{small}} \gg \delta t$, but an eigenvalue is the same in both Krylov spaces, we may say that this eigenvalue is sufficiently converged. Notice that if the Gram matrix $\mathbf{M}$ and effective Lindbladian $\mathbf{L}$ have been calculated for the big Krylov space, then the ones in the small Krylov space are trivially known by restricting the matrices to the time-evolved states contained in the small one, and no further overlaps or expectations need to be calculated. This makes convergence analysis particularly easy.

In the insets of Fig. 12(a) [Fig. 2(b)], such an analysis is shown for the dissipative Bose-Hubbard system with 20 sites and ten particles at $J = 1$, $\kappa/J = 2$, and $U/J = 0.16$ ($U/J = 0.5$), respectively. The spectra obtained by CLIK-MPS with complex angles $\alpha = 0$ and $\alpha = 0.02$, with spacing $dt = 0.2/J$ are shown for many different maximal times T . While the slowest-decaying mode $\lambda_2^K(T)$ is almost constant for $T \geq 25$, indicating sufficient convergence, λ_3 needs until $T = 40$ to converge. Additionally, λ_4 seems converged out after $T \geq 35$, while λ_5 would need time evolutions way beyond $T = 45$ to converge out. In total, we conclude that maximal time $T = 42$ suffices for $U/J = 0.16$ and $U/J = 0.5$ to resolve both Δ_3 and Δ_4 . In Fig. 12(a), we furthermore show the whole spectrum for $U/J = 0.16$ at identical parameters as in the inset, for two maximal times, underscoring the convergence of the low-lying spectrum.

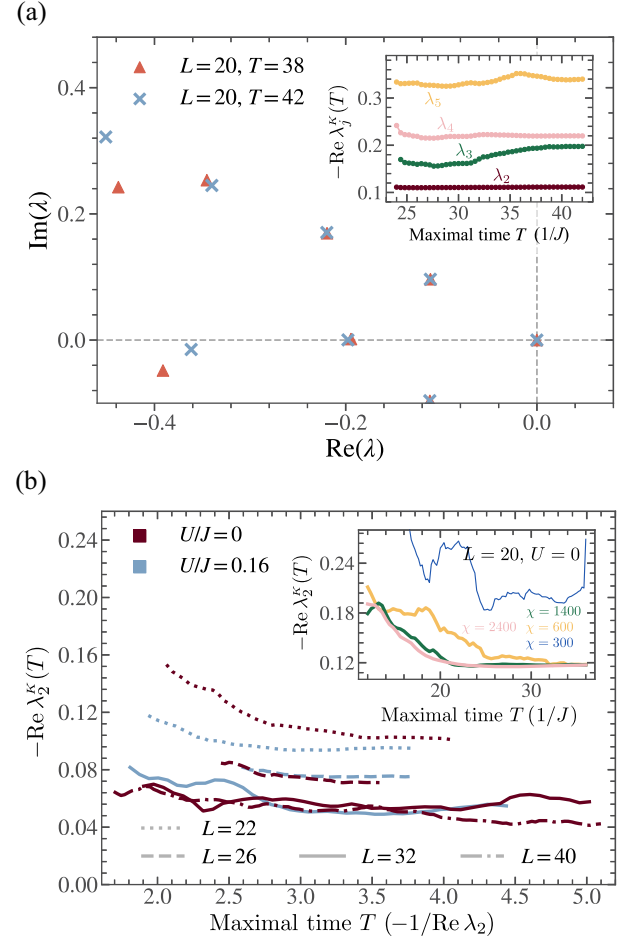


FIG. 12. Convergence analysis for large-scale systems. (a) CLIK-MPS generated spectrum of the Bose-Hubbard system with $U/J = 0.16$ with $L = 20$ at half filling, depending on the maximal evolution time T . We fix the Krylov sampling step at $\delta t = 0.2$, and evolve to $T = 34$ (orange) and $T = 38$ (blue), getting Krylov spaces of dimensions 340 and 380, respectively. By varying the maximal time T taken into the Krylov space, we can see if a spectral point is sufficiently converged (see also inset). Inset: maximal time T dependence of the first four nonzero eigenvalues. We set the maximal bond dimension to $\chi = 2400$. (b) Dissipative gap from CLIK-MPS for system sizes $L = 22, 26$ at $\delta t = 0.4$ and $L = 32, 40$ at $\delta t = 0.6$ depending on the maximal evolution time T at two different U/J . T is given in units of the gap to best display the damping rates the states experience. We set the maximal bond dimension to $\chi = 1600$ for $L = 40$ and $\chi = 1400$ for all other system sizes. Inset: dissipative gap depending on T for $L = 20$, $U = 0$ at half filling with $\delta t = 0.2$ with four different maximal bond dimensions during time evolution. While $\chi \geq 600$ eventually converge to the same dissipative gap, $\chi = 300$ (thin blue line) misses the correct value. Note that deviations in the intermediate-time regime might also originate from the stochastically chosen initial states. For all data shown here, we chose $J = 1$, $\kappa = 2J$, a local dimension $d = N + 1$.

We conducted the same analysis for all data shown in Fig. 7, and we chose $T = 38$ for $U = 0$, $T = 42$ for $U = 0.16, 0.33, 0.5$, and lastly $T = 44$ for $U = 0.66$.

In Fig. 12(b), we lastly show a part of the convergence analysis for the dissipative gaps provided in Fig. 6. We again show the dissipative gap for various system sizes (line style) and on-site interactions U/J (color) at half filling, depending on the maximal time T for the Krylov space. Since convergence times strongly depend on the system parameters, we express T in orders of the inverse dissipative gap $-1/\text{Re}\lambda_2$. We see that all data is sufficiently converged between $T = 3.5$ and 5 in orders of the inverse dissipative gap. Nevertheless, for $L = 32$ we evolve further to be sure and finally take the maximal times $T = 87$ for $U = 0$, $T = 81$ for $U = 0.16$, and $T = 84$ for $U = 0.66$ for CLIK-MPS and the analysis provided in Fig. 6. For $L = 40$, we evolve up to $T = 120.0$ with a step $\delta t = 0.6$, resulting in 400 time-evolved states.

Error bounds on the steady-state approximation quality have been put forward for Krylov methods in the past. For exponential Krylov spaces, they typically depend on the exponential of the dissipative gap Δ , as well as the maximal evolution time T as $\|\rho_0\|/\|\langle l_1|\rho_0\rangle\|e^{-\Delta T}$, where the prefactor may vary, but the asymptotic behavior is the same [97]. This, however, also means that at least the asymptotic behavior of the error bound is not sharper than normal time-evolution methods. In our case, however, the Krylov space $\mathcal{K}$ is actually a block Krylov space consisting of two independent blocks of Krylov basis vectors coming from the traceless and traceful initial states. To understand the impact of the second time evolution on the approximation quality, we need to first consider the basis vectors again. They are given by $|\rho_k\rangle\rangle, |\sigma_k\rangle\rangle$ and can be written as time evolutions of the initial vectors as

$$\begin{aligned}\mathcal{K} &= \text{span}\{|\rho_k\rangle\rangle, |\sigma_k\rangle\rangle \text{ for } k = 1, \dots, m\}, \\ |\rho_k\rangle\rangle &= e^{k\delta t \hat{L}}|\rho_0\rangle\rangle, |\sigma_k\rangle\rangle = e^{k\delta t \hat{L}}|\sigma_0\rangle\rangle.\end{aligned}\quad (\text{G5})$$

Written in the right eigenbasis of the Lindbladian, the states are

$$\begin{aligned}|\rho_k\rangle\rangle &= a_1|\rho_{\text{SS}}\rangle\rangle + \sum_{j=2} e^{k\delta t \lambda_j} a_j |r_j\rangle\rangle, \\ |\sigma_k\rangle\rangle &= \sum_{j=2} e^{k\delta t (\lambda_j - \lambda_2)} b_j |r_j\rangle\rangle,\end{aligned}\quad (\text{G6})$$

where the coefficients a_j, b_j depend on the left eigenvectors. Since the joint Krylov space contains all linear combinations of these states by definition, we can change the basis of the space and instead look at the states

$$|\gamma_k\rangle\rangle = |\rho_k\rangle\rangle - \frac{a_2}{b_2} e^{\lambda_2 k \delta t} |\sigma_k\rangle\rangle. \quad (\text{G7})$$

The Krylov space can be rewritten in terms of these states as

$$\mathcal{K} = \text{span}\{|\gamma_k\rangle\rangle, |\sigma_k\rangle\rangle \text{ for } k = 1, \dots, m\}, \quad (\text{G8})$$

where $|\gamma_0\rangle\rangle = |\rho_0\rangle\rangle - (a_2/b_2)|\sigma_0\rangle\rangle$. Now, notice that the approximation quality of the steady state is better in $\mathcal{K}$ than in the smaller Krylov space

$$\mathcal{K}_\gamma = \text{span}\{|\gamma_k\rangle\rangle \text{ for } k = 1, \dots, m\} \quad (\text{G9})$$

since it is a subset of $\mathcal{K}$. Crucially, this Krylov space contains no contributions from the fastest eigenmode $|r_2\rangle\rangle$, making the convergence speed at least $-\text{Re}\lambda_3$. This directly leads to the bound

$$\|(\mathbb{1} - P_{\mathcal{K}})|\rho_{\text{SS}}\rangle\rangle\| \leq \frac{\|\rho_0\|}{a_1} e^{\lambda_3 m \delta t} + \mathcal{O}(e^{(\lambda_3 + \lambda_2) m \delta t}), \quad (\text{G10})$$

which is exponentially sharper than an error bound depending on the dissipative gap. Note that we introduced the projector onto the Krylov space $P_{\mathcal{K}}$ here.

By applying the same logic to another Krylov subspace

$$\mathcal{K}_\sigma = \text{span}\{|\sigma_k\rangle\rangle \text{ for } k = 1, \dots, m\}, \quad (\text{G11})$$

one gets a similar bound for the slowest-decaying eigenvector given by

$$\|(\mathbb{1} - P_{\mathcal{K}})|r_2\rangle\rangle\| \leq \frac{\|\sigma_0\|}{a_2} e^{(\lambda_3 - \lambda_2) m \delta t}. \quad (\text{G12})$$

Of course, the complex-time step in the second time evolution has some effects on these bounds. Note, however, that while the complex angle may affect the exponential scalings by a $\mathcal{O}(\alpha)$ correction (not too severe because α is in general chosen quite small), it most importantly lifts degeneracy of the real part of the eigenvalues. This makes it especially important for systems with degenerate slowest-decaying modes.

APPENDIX H: NUMERICAL DETAILS

In this section, we present the details of the numerical implementation used for the dissipative time evolution. All calculations were performed using the SyTen toolkit [93,94]. To employ the MPS representation [51] in the context of mixed states, we need to vectorize density matrices, which is done by doubling the system size, alternating physical and auxiliary sites, as shown schematically in Fig. 13(a). In the same way, as shown in Fig. 13(b) we recast the Lindbladian as an operator acting on the vectorized space according to Eq. (2) in the main text [19]. Importantly, alternating physical and auxiliary sites ensures that local Hamiltonians and dissipators remain local in the vectorized description [62]. In the specific case of the dissipative Bose-Hubbard model considered in the main text, the vectorized Lindbladian features at most next-nearest-neighbor terms.

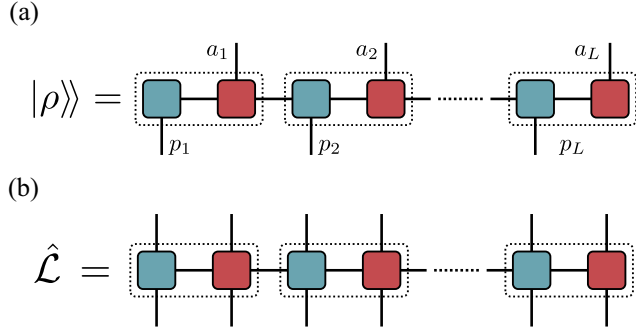


FIG. 13. The MPS representation of a vectorized density matrix (a) and the MPO representation of a vectorized Lindbladian (b) on a doubled lattice. Here, p_j labels the j th physical site (blue) and a_j the corresponding auxiliary site (red).

We utilize the TDVP method for MPS to simulate dissipative dynamics [64,65]. For bosonic systems with a large local physical dimension d , as discussed in the main text, the most suitable approach is the LSE TDVP [66,67]. This method relies on single-site updates in combination with a local subspace expansion [98], offering a speed advantage of a factor of d over the standard two-site time-dependent variational principle. Applying TDVP to Lindbladian dynamics poses additional difficulties due to the non-Hermitian nature of the generator. To address this, we adopt a straightforward approach: We perform a brute-force Taylor expansion of the exponentials of the local site tensors, which are then used for the time evolution, as explained in Ref. [68]. For all calculations provided in this paper, we chose the time step $dt = 0.01$ for time evolutions, unless otherwise stated.

The dissipative Bose-Hubbard model possesses a strong $U(1)$ symmetry associated with the conservation of the total particle number. In the vectorized representation, this single $U(1)$ symmetry maps onto two $U(1)$ symmetries corresponding to particle number conservation on each sublattice. We take advantage of both symmetries within the MPS structure to achieve a block decomposition of the Lindbladian. The second $U(1)$ symmetry arises because the full vectorized Hilbert space includes unphysical states, and the Lindbladian adopts a block diagonal form that separates the physical from the unphysical sectors. Therefore, explicitly incorporating this symmetry in the implementation is crucial; failing to do so may allow truncation errors to shift weight into the unphysical subspace, potentially introducing unphysical vectors into the Krylov space. Thanks to the presence of both symmetries, the system can be exactly represented using a local Hilbert-space dimension of $d = N + 1$. Moreover, dissipation suppresses the growth of entanglement in time. Nonetheless, when fixing a maximal bond dimension χ for the time evolution, severe truncation errors might occur. In Fig. 14, we show the truncation error and bond dimension for one exemplary time evolution. We see that the bond dimension quickly

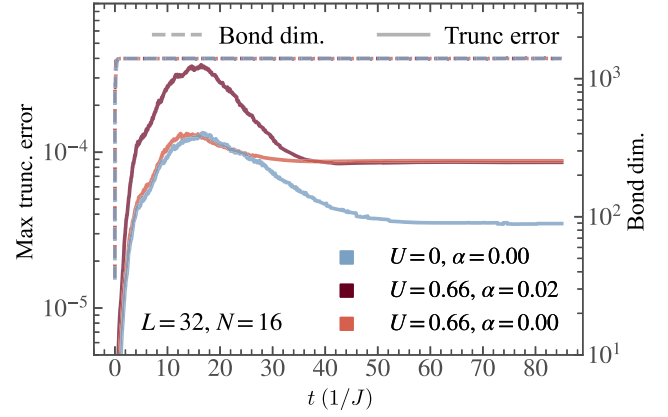


FIG. 14. Truncation error and right bond dimension during time evolution for large-scale calculations. We consider the Bose-Hubbard model with 32 sites at half filling with $\kappa/J = 2$ and $U/J = 1$ and $U/J = 0$, respectively. We show both the physical time evolution at $\alpha = 0$ (blue) for $U = 0$ and $U = 0.66$ and the complex-time evolution with traceless initial state at $\alpha = 0.02$ (orange) for $U = 0.66$. In all cases, the bond dimension increases strongly in the first time steps up to the maximal bond dimension of χ . Similarly, the truncation error increases in the beginning before decreasing and saturating. The maximal bond dimension χ is set to 1400 for all calculations. To accurately capture the behavior in the first steps, the time step was initially set to 1×10^{-3} , and after ten steps it was increased to 0.01.

saturates to the maximal bond dimension of $\chi = 1400$, while the truncation errors remain moderate. Interestingly, low maximal bond dimension χ seems not to be a problem at all, as we see in the inset of Fig. 12(b). We employ CLIK-MPS for a fixed parameter set for four different maximal bond dimensions, and look at the approximated dissipative gap depending on the maximal evolution time. Although at intermediate times, there are large deviations between the different data, the ones with $\chi \geq 600$ converge to the same value. This is perfectly explained by the effective bond dimension χ_{eff} in the Krylov space [cf. Eq. (B2)], which is the bond dimension that is reachable within the Krylov space. Crucially, besides scaling linearly in χ , it also scales linearly in the Krylov-space dimension D_K . Thus, while at mediocre times $\chi = 600$ does not have a sufficient χ_{eff} due to low D_K , the Krylov space with $\chi = 2400$ already has, and it can render the slowest-decaying mode correctly. This advantage is diminished by adding more time-evolved states to the Krylov space, eventually increasing the effective bond dimension strongly enough to render the eigenmode correctly. Note that this analysis is only true in a bond dimension window: For $\chi = 300$, the Krylov space completely misses the dissipative gap, shows strong discontinuities, and convergence is never reached. This is traced back to projection errors completely obscuring the actual dynamics generated by the Lindbladian. Also, in Fig. 3 we found that if the bond dimension during time evolution is chosen much too small, the Krylov space can

nevertheless fail in resolving the spectrum accurately, which happened when choosing a bond dimension of $\chi \leq 400$. This observation suggests a simple heuristic to use bond dimensions as small as possible: One simply runs a few CLIK-MPS in parallel with different bond dimensions and monitors the convergence of the low-lying eigenstates. As soon as the quantities of interest (e.g., dissipative gap, target observable) do not change upon further increasing the bond dimension, this run is converged, and all other calculations can be terminated.

To speed up the calculations, we can employ parallelization at multiple stages of the framework. First, the two time evolutions needed in CLIK-MPS are independent of each other, so they can be trivially parallelized. A similar procedure can be adopted when calculating the overlaps and expectations needed for the effective Lindbladian $\mathbf{L}$ and Gram matrix $\mathbf{G}$. Here, each overlap and expectation is independent of all the others, and thus the $(N_K)^2$ calculations can also be trivially parallelized. Similarly, expectation values and overlaps for observable calculation in the steady state as described in Appendix D is amenable to parallelization in the same manner.

Regarding the truncation of the MPS during the dynamics [65], one has to be careful that truncation errors do not introduce contributions on unphysical states into the Hilbert space. This problem typically arises if not all the system's symmetries are exploited in the numerics. Furthermore, truncation strongly affects the time evolutions with traceless states. These states are orthogonal on the steady-state sector, which is conserved during time evolution, if there is no truncation. However, if the state is truncated, in each step a small mass is shifted into the steady-state sector, which is enhanced due to the normalization done in each time step, leading to

$$\langle\langle l_1 | \rho(t) \rangle\rangle \sim \beta e^{|\operatorname{Re}(\lambda_2)|t}, \quad (\text{H1})$$

where the prefactor β is proportional to the truncation error. The exponential increase originates from the exponential decay of the contribution of the slowest-decaying mode, which enhances the weight on the steady-state sector during the normalization of $|\rho(t)\rangle\rangle$ at every time step.

[1] E. Altman *et al.*, *Quantum simulators: Architectures and opportunities*, *PRX Quantum* **2**, 017003 (2021).
 [2] F. Gyger, M. Ammenwerth, R. Tao, H. Timme, S. Snigirev, I. Bloch, and J. Zeiher, *Continuous operation of large-scale atom arrays in optical lattices*, *Phys. Rev. Res.* **6**, 033104 (2024).
 [3] L. S. Madsen, F. Laudenbach, M. F. Askarani, F. Rortais, T. Vincent, J. F. F. Bulmer, F. M. Miatto, L. Neuhaus, L. G. Helt, M. J. Collins, A. E. Lita, T. Gerrits, S. W. Nam, V. D. Vaidya, M. Menotti, I. Dhand, Z. Vernon, N. Quesada, and J. Lavoie, *Quantum computational advantage with a*

programmable photonic processor, *Nature (London)* **606**, 75 (2022).
 [4] A. *et al.*, *Quantum error correction below the surface code threshold*, *Nature (London)* **638**, 920 (2025).
 [5] D. G. Baranov, M. Wersäll, J. Cuadra, T. J. Antosiewicz, and T. Shegai, *Novel nanostructures and materials for strong light-matter interactions*, *ACS Photonics* **5**, 24 (2018).
 [6] W. Qin, A. F. Kockum, C. S. Muñoz, A. Miranowicz, and F. Nori, *Quantum amplification and simulation of strong and ultrastrong coupling of light and matter*, *Phys. Rep.* **1078**, 1 (2024).
 [7] J. Zribi, L. Khalil, B. Zheng, J. Avila, D. Pierucci, T. Brulé, J. Chaste, E. Lhuillier, M. C. Asensio, A. Pan, and A. Ouerghi, *Strong interlayer hybridization in the aligned SnS₂/WSe₂ hetero-bilayer structure*, *npj 2D Mater. Appl.* **3**, 27 (2019).
 [8] S. Duan, Y. Cheng, W. Xia, Y. Yang, C. Xu, F. Qi, C. Huang, T. Tang, Y. Guo, W. Luo, D. Qian, D. Xiang, J. Zhang, and W. Zhang, *Optical manipulation of electronic dimensionality in a quantum material*, *Nature (London)* **595**, 239 (2021).
 [9] T. Prosen, *Third quantization: A general method to solve master equations for quadratic open fermi systems*, *New J. Phys.* **10**, 043026 (2008).
 [10] G. T. Landi, D. Poletti, and G. Schaller, *Nonequilibrium boundary-driven quantum systems: Models, methods, and properties*, *Rev. Mod. Phys.* **94**, 045006 (2022).
 [11] F. Verstraete, J. J. García-Ripoll, and J. I. Cirac, *Matrix product density operators: Simulation of finite-temperature and dissipative systems*, *Phys. Rev. Lett.* **93**, 207204 (2004).
 [12] T. Prosen and M. Žnidarič, *Matrix product simulations of non-equilibrium steady states of quantum spin chains*, *J. Stat. Mech.* (2009) P02035.
 [13] J. Cui, J. I. Cirac, and M. C. Bañuls, *Variational matrix product operators for the steady state of dissipative quantum systems*, *Phys. Rev. Lett.* **114**, 220601 (2015).
 [14] E. Mascarenhas, H. Flayac, and V. Savona, *Matrix-product-operator approach to the nonequilibrium steady state of driven-dissipative quantum arrays*, *Phys. Rev. A* **92**, 022116 (2015).
 [15] A. H. Werner, D. Jaschke, P. Silvi, M. Kliesch, T. Calarco, J. Eisert, and S. Montangero, *Positive tensor network approach for simulating open quantum many-body systems*, *Phys. Rev. Lett.* **116**, 237201 (2016).
 [16] A. Kshetrimayum, H. Weimer, and R. Orús, *A simple tensor network algorithm for two-dimensional steady states*, *Nat. Commun.* **8**, 1291 (2017).
 [17] A. A. Gangat, T. I, and Y.-J. Kao, *Steady states of infinite-size dissipative quantum chains via imaginary time evolution*, *Phys. Rev. Lett.* **119**, 010501 (2017).
 [18] A. D. Somoza, O. Marty, J. Lim, S. F. Huelga, and M. B. Plenio, *Dissipation-assisted matrix product factorization*, *Phys. Rev. Lett.* **123**, 100502 (2019).
 [19] S. Wolff, A. Sheikhan, and C. Kollath, *Numerical evaluation of two-time correlation functions in open quantum systems with matrix product state methods: A comparison*, *SciPost Phys. Core* **3**, 010 (2020).
 [20] C. Guo, *Density matrix renormalization group algorithm for mixed quantum states*, *Phys. Rev. B* **105**, 195152 (2022).

- [21] H. Pichler, J. Schachenmayer, A. J. Daley, and P. Zoller, *Heating dynamics of bosonic atoms in a noisy optical lattice*, *Phys. Rev. A* **87**, 033606 (2013).
- [22] S. Sarkar, S. Langer, J. Schachenmayer, and A. J. Daley, *Light scattering and dissipative dynamics of many fermionic atoms in an optical lattice*, *Phys. Rev. A* **90**, 023618 (2014).
- [23] M. Moroder, M. Grundner, F. Damanet, U. Schollwöck, S. Mardazad, S. Flannigan, T. Köhler, and S. Paeckel, *Stable bipolarons in open quantum systems*, *Phys. Rev. B* **107**, 214310 (2023).
- [24] Z. Xie, M. Moroder, U. Schollwöck, and S. Paeckel, *Photo-induced dynamics with continuous and discrete quantum baths*, *J. Chem. Phys.* **161**, 074109 (2024).
- [25] D. A. Hryniuk and M. H. Szymańska, *Tensor-network-based variational Monte Carlo approach to the non-equilibrium steady state of open quantum systems*, *Quantum* **8**, 1475 (2024).
- [26] M. J. Hartmann and G. Carleo, *Neural-network approach to dissipative quantum many-body dynamics*, *Phys. Rev. Lett.* **122**, 250502 (2019).
- [27] F. Vicentini, A. Biella, N. Regnault, and C. Ciuti, *Variational neural-network ansatz for steady states in open quantum systems*, *Phys. Rev. Lett.* **122**, 250503 (2019).
- [28] J. Mellak, E. Arrigoni, and W. von der Linden, *Deep neural networks as variational solutions for correlated open quantum systems*, *Commun. Phys.* **7**, 268 (2024).
- [29] R. Cleve and C. Wang, *Efficient quantum algorithms for simulating Lindblad evolution*, *arXiv:1612.09512*.
- [30] N. Yoshioka, Y. O. Nakagawa, K. Mitarai, and K. Fujii, *Variational quantum algorithm for nonequilibrium steady states*, *Phys. Rev. Res.* **2**, 043289 (2020).
- [31] H.-Y. Liu, T.-P. Sun, Y.-C. Wu, and G.-P. Guo, *Variational quantum algorithms for the steady states of open quantum systems*, *Chin. Phys. Lett.* **38**, 080301 (2021).
- [32] Z. Ding, X. Li, and L. Lin, *Simulating open quantum systems using Hamiltonian simulations*, *PRX Quantum* **5**, 020332 (2024).
- [33] S. Santos, X. Song, and V. Savona, *Low-rank variational quantum algorithm for the dynamics of open quantum systems*, *Quantum* **9**, 1620 (2025).
- [34] X.-D. Xie, Z.-Y. Xue, and D.-B. Zhang, *Variational quantum algorithm for solving the Liouvillian gap*, *Chin. Phys. Lett.* **42**, 080605 (2025).
- [35] J. Tosca, F. Carnazza, L. Giacomelli, and C. Ciuti, *Efficient variational dynamics of open quantum bosonic systems via automatic differentiation*, *arXiv:2507.14076* [Phys. Rev. X (to be published)].
- [36] F. Carollo, A. Lasanta, and I. Lesanovsky, *Exponentially accelerated approach to stationarity in Markovian open quantum systems through the Mpemba effect*, *Phys. Rev. Lett.* **127**, 060401 (2021).
- [37] P. Westhoff, S. Paeckel, and M. Moroder, *Fast and direct preparation of a genuine lattice bec via the quantum mpemba effect*, *Phys. Rev. A* **112**, L061304 (2025).
- [38] F. Minganti, A. Biella, N. Bartolo, and C. Ciuti, *Spectral theory of Liouvillians for dissipative phase transitions*, *Phys. Rev. A* **98**, 042118 (2018).
- [39] F. Minganti, V. Savona, and A. Biella, *Dissipative phase transitions in n-photon driven quantum nonlinear resonators*, *Quantum* **7**, 1170 (2023).
- [40] M. Moroder, O. Culhane, K. Zawadzki, and J. Goold, *Thermodynamics of the quantum Mpemba effect*, *Phys. Rev. Lett.* **133**, 140404 (2024).
- [41] F. Song, S. Yao, and Z. Wang, *Non-Hermitian skin effect and chiral damping in open quantum systems*, *Phys. Rev. Lett.* **123**, 170401 (2019).
- [42] S. Lieu, M. McGinley, and N. R. Cooper, *Tenfold way for quadratic Lindbladians*, *Phys. Rev. Lett.* **124**, 040401 (2020).
- [43] T. Yoshida, K. Kudo, H. Katsura, and Y. Hatsugai, *Fate of fractional quantum Hall states in open quantum systems: Characterization of correlated topological states for the full liouvillian*, *Phys. Rev. Res.* **2**, 033428 (2020).
- [44] K. Macieszczak, M. Guță, I. Lesanovsky, and J. P. Garrahan, *Towards a theory of metastability in open quantum dynamics*, *Phys. Rev. Lett.* **116**, 240404 (2016).
- [45] A. Nagy, *Quantum Monte Carlo approach to the non-equilibrium steady state of open quantum systems*, Ph.D. thesis, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, 2020.
- [46] L. Xu, *A quantum kinetic Monte Carlo method for Lindblad equation*, *arXiv:2306.05102*.
- [47] G. Almeida, P. Ribeiro, M. Haque, and L. Sá, *Universality, robustness, and limits of the eigenstate thermalization hypothesis in open quantum systems*, *Phys. Rev. E* **113**, L012101 (2026).
- [48] J. Richter, L. Sá, and M. Haque, *Integrability versus chaos in the steady state of many-body open quantum systems*, *Phys. Rev. E* **111**, 064103 (2025).
- [49] S. R. White, *Density matrix formulation for quantum renormalization groups*, *Phys. Rev. Lett.* **69**, 2863 (1992).
- [50] S. R. White, *Density-matrix algorithms for quantum renormalization groups*, *Phys. Rev. B* **48**, 10345 (1993).
- [51] U. Schollwöck, *The density-matrix renormalization group in the age of matrix product states*, *Ann. Phys. (Amsterdam)* **326**, 96 (2011).
- [52] G. K.-L. Chan and T. Van Voorhis, *Density-matrix renormalization-group algorithms with nonorthogonal orbitals and non-Hermitian operators, and applications to polyenes*, *J. Chem. Phys.* **122**, 204101 (2005).
- [53] L. Vanderstraeten, J. Haegeman, P. Corboz, and F. Verstraete, *Gradient methods for variational optimization of projected entangled-pair states*, *Phys. Rev. B* **94**, 155123 (2016).
- [54] P. Zhong, W. Pan, H. Lin, X. Wang, and S. Hu, *Density matrix renormalization group algorithm for non-Hermitian systems*, *Phys. Rev. Lett.* **135**, 106502 (2025).
- [55] Y. Zhan, Z. Ding, J. Huhn, J. Gray, J. Preskill, G. K.-L. Chan, and L. Lin, *Rapid quantum ground state preparation via dissipative dynamics*, *Phys. Rev. X* **16**, 011004 (2026).
- [56] F. Minganti and D. Huybrechts, *Arnoldi-Lindblad time evolution: Faster-than-the-clock algorithm for the spectrum of time-independent and Floquet open quantum systems*, *Quantum* **6**, 649 (2022).
- [57] M. Grundner, P. Westhoff, F. B. Kugler, O. Parcollet, and U. Schollwöck, *Complex time evolution in tensor networks and time-dependent Green's functions*, *Phys. Rev. B* **109**, 155124 (2024).
- [58] S. Paeckel, *Spectral Decomposition and high-accuracy Green's Functions: Overcoming the Nyquist-Shannon limit*

- via complex-time Krylov expansion, *Phys. Rev. Lett.* **136**, 160401 (2026).
- [59] G. Preisser, D. Wellnitz, T. Botzung, and J. Schachenmayer, *Comparing bipartite entropy growth in open-system matrix-product simulation methods*, *Phys. Rev. A* **108**, 012616 (2023).
- [60] F. Caceffo and V. Alba, *Fate of entanglement in quadratic Markovian dissipative systems*, *Phys. Rev. A* **113**, 042436 (2026).
- [61] G. Lindblad, *On the generators of quantum dynamical semigroups*, *Commun. Math. Phys.* **48**, 119 (1976).
- [62] H. P. Casagrande, D. Poletti, and G. T. Landi, *Analysis of a density matrix renormalization group approach for transport in open quantum systems*, *Comput. Phys. Commun.* **267**, 108060 (2021).
- [63] In this work, we always refer to the bond dimension of a site tensor as the largest dimension of its set of virtual legs.
- [64] J. Haegeman, J. I. Cirac, T. J. Osborne, I. Pižorn, H. Verschelde, and F. Verstraete, *Time-dependent variational principle for quantum lattices*, *Phys. Rev. Lett.* **107**, 070601 (2011).
- [65] S. Paegel, T. Köhler, A. Swoboda, S. R. Manmana, U. Schollwöck, and C. Hubig, *Time-evolution methods for matrix-product states*, *Ann. Phys. (Amsterdam)* **411**, 167998 (2019).
- [66] M. Yang and S. R. White, *Time-dependent variational principle with ancillary Krylov subspace*, *Phys. Rev. B* **102** (2020).
- [67] M. Grundner, T. Blatz, J. Sous, U. Schollwöck, and S. Paegel, [arXiv:2308.13427](https://arxiv.org/abs/2308.13427).
- [68] M. Moroder, *Simulating quantum dissipative and vibrational environments*, Ph.D. thesis, LMU München, 2024.
- [69] Care must be taken in the presence of conserved quantities, under which the identity decomposes into sub-blocks. We address this issue in Appendix B.
- [70] E. M. Stoudenmire and S. R. White, *Real-space parallel density matrix renormalization group*, *Phys. Rev. B* **87**, 155137 (2013).
- [71] B. Kraus, H. P. Büchler, S. Diehl, A. Kantian, A. Micheli, and P. Zoller, *Preparation of entangled states by quantum markov processes*, *Phys. Rev. A* **78**, 042307 (2008).
- [72] S. Diehl, A. Micheli, A. Kantian, B. Kraus, H. P. Büchler, and P. Zoller, *Quantum states and phases in driven open quantum systems with cold atoms*, *Nat. Phys.* **4**, 878 (2008).
- [73] Y. Tanimura, *Numerically “exact” approach to open quantum dynamics: The hierarchical equations of motion (heom)*, *J. Chem. Phys.* **153**, 020901 (2020).
- [74] B. Debecker, J. Martin, and F. m. c. Damanet, *Spectral theory of non-Markovian dissipative phase transitions*, *Phys. Rev. A* **110**, 042201 (2024).
- [75] A. J. Daley, *Quantum trajectories and open many-body quantum systems*, *Adv. Phys.* **63**, 77 (2014).
- [76] M. Žnidarič, *Relaxation times of dissipative many-body quantum systems*, *Phys. Rev. E* **92**, 042143 (2015).
- [77] R. A. Hart, P. M. Duarte, T.-L. Yang, X. Liu, T. Paiva, E. Khatami, R. T. Scalettar, N. Trivedi, D. A. Huse, and R. G. Hulet, *Observation of antiferromagnetic correlations in the Hubbard model with ultracold atoms*, *Nature (London)* **519**, 211 (2015).
- [78] T. Mori and T. Shirai, *Resolving a discrepancy between Liouvillian gap and relaxation time in boundary-dissipated quantum many-body systems*, *Phys. Rev. Lett.* **125**, 230604 (2020).
- [79] Z. Lu and O. Raz, *Nonequilibrium thermodynamics of the Markovian Mpemba effect and its inverse*, *Proc. Natl. Acad. Sci. U.S.A.* **114**, 5083 (2017).
- [80] F. Ares, S. Murciano, and P. Calabrese, *Entanglement asymmetry as a probe of symmetry breaking*, *Nat. Commun.* **14**, 2036 (2023).
- [81] N. Beato and G. Teza, *Relaxation control of open quantum systems*, *Phys. Rev. Lett.* **136**, 070401 (2026).
- [82] A. Summer, M. Moroder, L. P. Bettmann, X. Turkeshi, I. Marvian, and J. Goold, *Resource-theoretical unification of Mpemba effects: Classical and quantum*, *Phys. Rev. X* **16**, 011065 (2026).
- [83] M. Schlosshauer, *Quantum decoherence*, *Phys. Rep.* **831**, 1 (2019).
- [84] A. Paulraj, R. Roy, and T. Kailath, *A subspace rotation approach to signal parameter estimation*, *Proc. IEEE* **74**, 1044 (1986).
- [85] W. Li, W. Liao, and A. Fannjiang, *Super-resolution limit of the esprit algorithm*, *IEEE Trans. Inf. Theory* **66**, 4593 (2020).
- [86] G. Park, Z. Huang, Y. Zhu, C. Yang, G. K.-L. Chan, and L. Lin, *Quasi-Lindblad pseudomode theory for open quantum systems*, *Phys. Rev. B* **110**, 195148 (2024).
- [87] Z. Huang, G. Park, G. K.-L. Chan, and L. Lin, *Coupled Lindblad pseudomode theory for simulating open quantum systems*, *Phys. Rev. Lett.* **136**, 090403 (2026).
- [88] N. Hatano, *Exceptional points of the Lindblad operator of a two-level system*, *Mol. Phys.* **117**, 2121 (2019).
- [89] F. Minganti, A. Miranowicz, R. W. Chhajlany, and F. Nori, *Quantum exceptional points of non-Hermitian Hamiltonians and Liouvillians: The effects of quantum jumps*, *Phys. Rev. A* **100**, 062131 (2019).
- [90] C. Booker, B. Buča, and D. Jaksch, *Non-stationarity and dissipative time crystals: Spectral properties and finite-size effects*, *New J. Phys.* **22**, 085007 (2020).
- [91] F. Carollo, I. Lesanovsky, M. Antezza, and G. De Chiara, *Quantum thermodynamics of boundary time-crystals*, *Quantum Sci. Technol.* **9**, 035024 (2024).
- [92] B. Debecker, J. Martin, and F. Damanet, *Controlling matter phases beyond markov*, *Phys. Rev. Lett.* **133**, 140403 (2024).
- [93] C. Hubig, F. Lachenmaier, N.-O. Linden, T. Reinhard, L. Stenzel, A. Swoboda, M. Grundner, S. Mardazad, S. Paegel, and F. Pauw, The SYTEN toolkit.
- [94] C. Hubig, *Symmetry-Protected Tensor Networks*, Ph.D. thesis, LMU München, 2017.
- [95] Philipp Westhoff, *Clik-mps data*, Version 1, <https://github.com/Philippmpsp/clik-mps-data> (2026).
- [96] Philipp Westhoff, *Clik-mps code*, Version 1, <https://github.com/Philippmpsp/clik-mps> (2026).
- [97] C. A. Beattie, M. Embree, and D. C. Sorensen, *Convergence of polynomial restart Krylov methods for eigenvalue computations*, *SIAM Rev.* **47**, 492 (2005).
- [98] C. Hubig, I. P. McCulloch, U. Schollwöck, and F. A. Wolf, *Strictly single-site DMRG algorithm with subspace expansion*, *Phys. Rev. B* **91**, 155115 (2015).