


Many-Body Quantum State Diffusion for Non-Markovian Dynamics in Strongly Interacting Systems

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Capturing non-Markovian dynamics of open quantum systems is generally a challenging problem, especially for strongly interacting many-body systems. In this Letter, we combine recently developed non-Markovian quantum state diffusion techniques with tensor network methods to address this challenge. As a first example, we explore a Hubbard-Holstein model with dissipative phonon modes, where this new approach allows us to quantitatively assess how correlations spread in the presence of non-Markovian dissipation in a 1D many-body system. We find regimes where correlation growth can be enhanced by these effects, offering new routes for dissipatively enhancing transport and correlation spreading, relevant for both solid state and cold atom experiments.

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Introduction.—In open quantum system dynamics, it is becoming increasingly crucial to consider the effects of non-Markovian dissipation, i.e., dissipation into a spectrally structured environment which remembers past interactions with the system [1], as demonstrated in many recent quantum devices which are non-Markovian in nature [2–4]. While there has been great progress in treating these features computationally [5–11], there has so far been difficulty in generalizing these methods for strongly interacting many-body systems, even in 1D. Here, by hybridizing tensor network and non-Markovian stochastic techniques, we show how to capture the effects of non-Markovian dissipation on the generation of long-range correlations in strongly interacting one-dimensional many-body systems. As an example, we consider a damped form of the Hubbard-Holstein model, which introduces electron-phonon interactions to strongly correlated systems [12–14]. We find that the growth of pairing correlations can be enhanced by going beyond the Markovian regime and that by controlling the properties of the environment we can tune the correlation spreading in the (electron) system. Our results demonstrate the capabilities of these methods to explore dissipative many-body systems beyond the Born-Markov limit and quantitatively capture their out-of-equilibrium dynamics, as motivated by experimental advances with many-body cavity quantum electrodynamics (QED) [15–17] and with cold atoms immersed in reservoir gases [18–22].

Large separations of frequency scales in quantum optical systems coupled to their environment have made theoretical tools such as the Gorini, Kossakowski, Sudarshan, Lindblad master equation [23,24] invaluable for quantitatively capturing many important experiments. There, the system and environment are weakly coupled and the

environment is memory less, satisfying the Born-Markov approximation [25,26]. Reservoir engineering in recent quantum optics experiments, such as using impurities immersed in Bose-Einstein Condensates (BEC) to produce spin-boson models [18–22] or with multimode cavity QED systems [15–17], has made it possible to go beyond the Born-Markov regime in systems where microscopic models can still be derived from first principles. This has motivated interest in creating theoretical tools to compute dynamics in these cases. The large size of these systems makes it necessary to trace out the BEC in the former scenario and the cavity modes in the latter, which results in open quantum system descriptions that are generally non-Markovian [14,27–30]. Simulating these situations is particularly challenging due to the combination of strong interactions generating strongly correlated phases, the many-body system giving rise to an exponentially large Hilbert space and the non-Markovian features requiring the use of an equation of motion that is nonlocal in time.

Finding the best way to deal with non-Markovian dynamics, the most natural kind of open system dynamics occurring in the solid state from which our example originates, is an old and difficult problem, and a number of approaches have been developed over the past decades, ranging from non-Markovian master equations [26] to non-Markovian collapse theories [31], collisional models [32], and stochastic Schrödinger equations [33,34] (see Ref. [1] for a detailed review). More recently, time-evolving matrix product operators (TEMPO) [7–9] or hierarchical equations of motion (HEOM) [5,6] have shown remarkable potential for systems with a small Hilbert space, but so far have not been generalized to many-body systems.

To address this challenge here we employ the hierarchy of pure states (HOPS) [10,11], a non-Markovian quantum

state diffusion method, which we have combined with matrix product state (MPS) techniques [35]. We demonstrate applications for this method by exploring dynamics in a modified Hubbard-Holstein model [12,13], where we couple strongly interacting fermions to local harmonic oscillator modes that are damped, representative of phonons that have dispersion. We show that non-Markovian dissipation can enhance the short-time dynamical growth of the pairing correlations where we find a qualitative difference compared to the Markovian, but also the phononless cases. This demonstrates that this method allows us to quantitatively simulate the dynamics of strongly correlated one-dimensional open many-body systems well into the non-Markovian and strong coupling regimes.

Dissipative Hubbard-Holstein model.—We consider the model shown in Fig. 1(a), with fermions in an M site lattice, described by a many-body system Hamiltonian \hat{H}_s where each site is coupled to a local phonon mode similar to the (Hubbard)-Holstein model [12,13]. The total Hamiltonian is given by

$$\hat{H} = \hat{H}_s + \omega \sum_{n=1}^M \hat{a}_n^\dagger \hat{a}_n + g \sum_{n=1}^M (\hat{L}_n \hat{a}_n^\dagger + \hat{L}_n^\dagger \hat{a}_n), \quad (1)$$

where \hat{a}_n^\dagger and \hat{a}_n create and destroy a phonon in the n th mode and \hat{L}_n are system operators acting on site n . We modify the usual Holstein model by going beyond the approximation of dispersionless phonons, taking a next step in better modeling realistic situations with this toy model [36]. We incorporate these effects by modeling each phonon mode as a damped harmonic oscillator, such that we can write the phonon correlation function as

$$\alpha_n(t-t') = \langle \hat{a}_n(t) \hat{a}_n^\dagger(t') \rangle = e^{-\kappa|t-t'| - i\omega(t-t')}, \quad (2)$$

where ω and κ are the phonon frequency and damping rate, respectively.

Non-Markovian quantum state diffusion.—Non-Markovian dynamics arise when we trace out part of the system where we do not have a strong separation of frequency scales that satisfy the conditions for the Born-Markov approximation. In principle it is always possible to place the boundary of the system where the dynamics are Markovian. In this case, we could take the fermions and phonon modes as the *system* [dashed black box in Fig. 1(a)], with the phonon damping remaining Markovian [37]. However, in many relevant situations (such as multimode cavities described above), it becomes prohibitively expensive computationally to make this choice because of the large local basis. In this particular case, we find it much more convenient to trace out the phonon modes and work with an effective equation of motion for the Hubbard system only [dashed blue box in Fig. 1(a)]. For finite κ the resulting correlation function

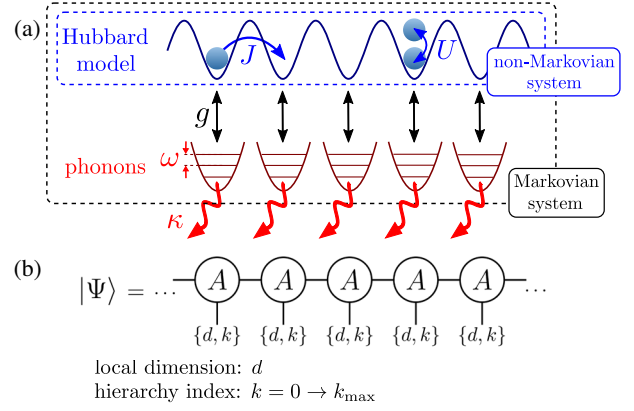


FIG. 1. (a) Illustration of the Hubbard model coupled with strength g to independent identical local phonon modes of frequency ω and damping rate κ . While the dissipative dynamics of the system made up of the fermions and the phonons (dashed black box) is Markovian, the one of the Hubbard system alone (dashed blue box) is generally non-Markovian. (b) Matrix product state (MPS) representation of the many-body HOPS equations [see Eq. (6)], with local dimension d and hierarchy dimension $k_{\max} + 1$ in the usual form but now with an enlarged local dimension $d + k_{\max} + 1$.

for the phonon modes, Eq. (2), cannot be approximated as a delta function, and so we must use the non-Markovian quantum state diffusion equation for the dynamics of the reduced system $|\psi(t)\rangle$ [1,33],

$$\begin{aligned} \partial_t |\psi(t)\rangle &= -i\hat{H}_s |\psi(t)\rangle + g \sum_{n=1}^M \hat{L}_n z_n^*(t) |\psi(t)\rangle \\ &\quad - g \sum_{n=1}^M \hat{L}_n^\dagger \int_0^t ds \alpha_n^*(t-s) \frac{\delta |\psi(t)\rangle}{\delta z_n^*(s)}, \end{aligned} \quad (3)$$

where we have introduced a set of stochastic *colored* noise terms $z_n^*(t)$ which upon taking an ensemble average give the correlation function $\mathcal{E}[z_n(t) z_n^*(t')] = \delta_{n,n'} \alpha_n(t-t')$.

HOPS + MPS algorithm.—The insight which leads to the HOPS algorithm [10,11] is to introduce a set of auxiliary states which absorb the numerically intractable functional derivatives $\delta/\delta z_n^*(s)$,

$$|\psi^{(1,n)}(t)\rangle = D_n(t) |\psi(t)\rangle \equiv \int_0^t ds \alpha_n^*(t-s) \frac{\delta |\psi(t)\rangle}{\delta z_n^*(s)}. \quad (4)$$

Deriving an equation of motion for this auxiliary state requires the introduction of further auxiliary states defined through $|\psi^{(k,n)}(t)\rangle = [D_n(t)]^k |\psi(t)\rangle$ which give rise to a hierarchical set of equations. In order to write this hierarchy, we find it convenient to include the hierarchy index into the basis states and write a total state for the combined system and auxiliary Hilbert space,

$$|\Psi(t)\rangle = \sum_{\vec{k}} C_{\vec{k}}(t) |\psi^{(\vec{k})}(t)\rangle \otimes |\vec{k}\rangle, \quad (5)$$

where the $C_{\vec{k}}(t)$ are time-dependent complex numbers and $|\vec{k}\rangle = |k_1, k_2, \dots, k_M\rangle = |k_1\rangle \otimes |k_2\rangle \otimes \dots \otimes |k_M\rangle$ with each of the k_n running from $0, 1, \dots, \infty$, as we have a hierarchy index for each of the M phonon environment modes. Each hierarchy index is represented as an independent boson mode, see Supplemental Material for details [38]. Note that the $|\psi^{(0)}(t)\rangle \otimes |0\rangle = |\psi(t)\rangle$ is the physical system state. This allows us to write the equation of motion for the total state as

$$\begin{aligned} \partial_t |\Psi(t)\rangle = & -i\hat{H}_s |\Psi(t)\rangle + \sum_{n=1}^M [\tilde{z}_n^*(t) g \hat{L}_n - (\kappa + i\omega) \hat{K}_n \\ & + g \hat{L}_n \otimes \hat{K}_n \hat{b}_n^\dagger - g(\hat{L}_n^\dagger - \langle \hat{L}_n^\dagger \rangle_t) \otimes \hat{b}_n] |\Psi(t)\rangle. \end{aligned} \quad (6)$$

Note that we time-dependently modify the colored noise according to $\tilde{z}_n^*(t) = z_n^*(t) + g \int_0^t ds \alpha_n^*(t-s) \langle \hat{L}_n^\dagger \rangle_s$ with $\langle \hat{L}_n^\dagger \rangle_s = \langle \psi^{(0)}(s) | \hat{L}_n^\dagger | \psi^{(0)}(s) \rangle$ thus explicitly taking into account previous states of the system. Note that one has to consider sufficiently small time steps in the numerical resolution of the equation so that the time-dependent terms in Eq. (6) can be approximated as constant in time. In this way the nonlinear terms $\tilde{z}_n^*(t)$ and $\langle \hat{L}_n^\dagger \rangle_t$ are calculated using the state before the time increment.

In the above equation we have introduced the bare operators (omitting the index n) $\hat{b}^\dagger |k\rangle = |k+1\rangle$, $\hat{b} |k\rangle = |k-1\rangle$ (see Refs. [45,46]) and $\hat{K} = \sum_k k |k\rangle \langle k|$. We initialize the hierarchy with $C_0(0) = 1$ and $C_{|\mathbf{k}|>0}(0) = 0$ and in order to extract observables we use the (normalized) physical system state $O(t) = \langle \psi^{(0)}(t) | \hat{O} | \psi^{(0)}(t) \rangle$ which we must average over many trajectories with different realizations of the random numbers $z_n^*(t)$, similar to conventional QSD equations [1,25,37].

Formally the hierarchy depth is infinite, but the populations of the auxiliary states typically decrease with the hierarchy indices k_n , which makes it possible in practice to truncate each hierarchy to some index k_{\max} (chosen such that the results have converged to a given precision) to render the problem numerically feasible. In general, the stronger the violation of the Born-Markov approximations the larger the number of auxiliary states we must retain. Note that this hierarchy truncation still results in an exponential number of equations: if each hierarchy index can run from $0, 1, \dots, k_{\max}$ then in total we have $(k_{\max} + 1)^M$ auxiliary states. This motivates the incorporation of MPS techniques which allow us to time evolve many-body states of one-dimensional Hamiltonians without explicitly working with the full Hilbert space [35]. As each hierarchy only couples locally with a system operator of site n this allows us to efficiently write this problem as an MPS simply with an enlarged local Hilbert space consisting of the physical local dimension of the system, but now also an effective

local dimension for the auxiliary state of that effective environment mode [see Fig. 1(b)] modeled as a boson Hilbert space. This is particularly convenient as we can then apply standard MPS techniques for time evolution [47]. This does result in an MPS with a large local dimension but in the following sections we show that it can be used to make important quantitative predictions with practical numerical values for the size of the hierarchy dimension k_{\max} and also the bond dimension of the MPS D (see Supplemental Material for a detailed error analysis [38]). Note finally that providing k_{\max} and D are large enough, Eq. (6) numerically converges to the *exact* dynamics of the system (as well as of the environment via monitoring of the noises as we will discuss below), as it does not directly rely on any approximation (neither Born nor Markov).

Benchmarking.—We first consider the out-of-equilibrium dynamics of a Holstein model [12,13]. We use

$$\hat{H}_s = -J \sum_n (\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{c}_{n+1}^\dagger \hat{c}_n), \quad (7)$$

as the system Hamiltonian in Eq. (6), where J describes the tunneling of the (spinless) electrons. Additionally, we use the number operator as our system-environment coupling operators $\hat{L}_n = \hat{n}_n = \hat{c}_n^\dagger \hat{c}_n$, and as mentioned we include dissipation on the phonons yielding the damped correlation functions, Eq. (2).

We begin with the initial state $|1, 0, 1, 0, \dots\rangle$ and time-dependently calculate a charge density wave (CDW) correlations $O_{\text{CDW}}(t) = (1/M) \sum_n (-1)^n \langle \hat{n}_n(t) \rangle$. We plot this in Figs. 2(a) and 2(b) for different coupling strengths g and phonon dispersions κ . Comparing to the results obtained in Ref. [48], which analyzes this system in the limit of dispersionless phonons ($\kappa \rightarrow 0$), we find the same qualitative behavior, where for $g = J$ the dynamics are similar to the closed system ($g = 0$) case where there are oscillations but the CDW *melts* into a homogeneous steady state. Increasing the coupling strength to $g = 5J$ we can see that the CDW melting is slowed for short times and the oscillations become completely damped.

Born-Markov limit.—We also compare our results to that of a conventional quantum state diffusion (QSD) equation valid in the Born-Markov limit [37]. This is achieved by setting $k_{\max} = 1$ and $\alpha_n(\tau) = \delta(\tau)$ (see Ref. [10] and Supplemental Material [38]) which physically corresponds to the approximation that the phonon dispersion κ goes to infinity. From Fig. 2 we see that for strong coupling ($g = 5J$) this model completely fails to predict the suppression of the CDW correlations at short times.

Finite temperature.—Within the framework of HOPS it is also possible to efficiently include finite temperature effects of the environment (see Ref. [11]). In Figs. 2(c) and 2(d) we plot the dependence on the CDW correlations upon increasing the initial temperature of the environment modes. We see that the suppression of the CDW melting is

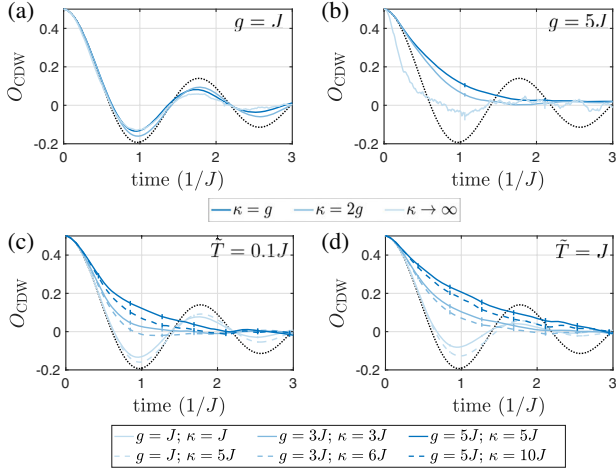


FIG. 2. Dynamics in the dissipative Holstein model [Eq. (1) with the system Hamiltonian (7), $\hat{L}_n = \hat{n}_n$ and the environment correlation functions (2)] upon beginning in an initial state $|1, 0, 1, 0, \dots\rangle$. (a),(b) The evolution of the CDW correlations $O_{\text{CDW}}(t) = (1/M) \sum_n (-1)^n \langle \hat{n}_n(t) \rangle$ for different coupling strengths g ($g = 0$ in black dotted) and phonon dispersion rates $\kappa = [g, 2g, \infty]$ (dark to light blue). The Born-Markov limit ($\kappa \rightarrow \infty$) was calculated using a conventional quantum trajectory method [37]. (c),(d) Finite temperature analysis for different coupling strengths $g = [1, 3, 5]J$ (light to dark blue, $g = 0$ in black dotted) and phonon dispersion rates κ . See Ref. [11] on how to adapt the algorithm for finite temperature environments. In all cases we average the observables over $N_{\text{traj}} = 100$ trajectories and use $\omega = J$ and $M = 20$ lattice sites. For our hybridized HOPS + MPS algorithm, we use the numerical parameters $k_{\text{max}} = 8$, $D = 128$, and $Jdt = 0.01$.

enhanced for increasing temperatures which is due to a nonzero population of phonons in the initial state, allowing for a greater effect on the short time dynamics. Including finite temperature effects in the Born-Markov QSD simply increases the effective system-environment coupling strength (see Supplemental Material [38]) which as seen from Figs. 2(a) and 2(b) predicts an increased decay of the CDW. Increasing the temperature of the phonon modes in this model therefore results in further deviations from the Born-Markov regime, in contrast to the more common cases where larger temperatures suppress non-Markovian features [1, 14].

Correlation spreading.—We move on and consider the Hubbard-Holstein model describing two-species fermions coupled to phonon modes and now with an on-site interaction U . Explicitly our system Hamiltonian is given by

$$\hat{H}_s = -J \sum_{n,\sigma} (\hat{c}_{n,\sigma}^\dagger \hat{c}_{n+1,\sigma} + \hat{c}_{n+1,\sigma}^\dagger \hat{c}_{n,\sigma}) + U \sum_n \hat{n}_{n,\uparrow} \hat{n}_{n,\downarrow}, \quad (8)$$

where $\hat{n}_{n,\sigma} = \hat{c}_{n,\sigma}^\dagger \hat{c}_{n,\sigma}$ and our system-environment coupling operators are $\hat{L}_n = \hat{n}_{n,\uparrow} + \hat{n}_{n,\downarrow}$. As earlier, we go beyond the usual case and include phonon dissipation.

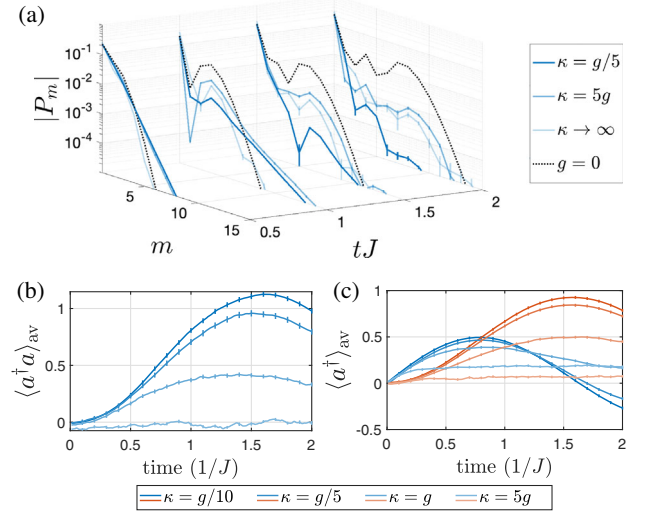


FIG. 3. Dynamics in the dissipative Hubbard-Holstein model [Eq. (1) with the system Hamiltonian (8), $\hat{L}_n = \hat{n}_{n,\uparrow} + \hat{n}_{n,\downarrow}$ and the environment correlation functions (2)], upon beginning in an initial CDW state $|\uparrow, \downarrow, \uparrow, \downarrow, \dots\rangle$. (a) The pair correlation function [Eq. (9)], where we use $g = J$ ($g = 0$ in black) and compare different phonon dispersion rates $\kappa = [g/5, 5g, \infty]$ (dark to light blue). (b) Dynamics of the average phonon mode occupation, $\langle a^\dagger a \rangle_{\text{av}} = (1/M) \sum_n \langle a_n^\dagger a_n \rangle = (1/M) \sum_n (|z_n^*(t)|^2 - 1)$. (c) The real (blue) and imaginary (red) part of the phonon coherences $\langle a^\dagger \rangle_{\text{av}} = (1/M) \sum_n \langle a_n^\dagger \rangle = (1/M) \sum_n z_n^*(t)$. For our hybridized HOPS + MPS algorithm, we use the parameters $k_{\text{max}} = 6$, $D = 300$, and $Jdt = 0.01$ where we also have incorporated conserved quantum numbers into the MPS algorithm [52]. We average the observables over $N_{\text{traj}} = 100$ trajectories. In all cases we use $U = J$, $\omega = 2J$, and $M = 50$ sites.

In Fig. 3 we begin in the initial product state $|\uparrow, \downarrow, \uparrow, \downarrow, \dots\rangle$ and in (a) we analyze the fermionic pairing correlation functions

$$P_m = \frac{1}{M-m} \sum_{\tilde{m}} \langle \hat{c}_{\tilde{m},\uparrow}^\dagger \hat{c}_{\tilde{m},\downarrow}^\dagger \hat{c}_{\tilde{m}+m,\downarrow} \hat{c}_{\tilde{m}+m,\uparrow} \rangle. \quad (9)$$

For the case where there is no coupling to the phonons $g = 0$ we observe a peak in these correlations which spreads out in time, and beyond this the correlations decay exponentially which is the usual light cone spreading of correlations [49–51]. Including coupling to the phonon modes with $g = J$ we see similar behavior, although the dissipation damps the amplitude of this peak in time, gradually suppressing correlations in the steady state. For finite κ (i.e., non-Markovian environment behavior), we see a strong enhancement of the correlation length beyond the light cone at short times ($tJ \sim 0.5, 1$) which is qualitatively different to the case of purely Markovian dissipation ($\kappa \rightarrow \infty$) where the correlation length is unaffected.

These features of the non-Markovian dynamics can be understood by realizing that the coupling to the phonons *dresses* the electrons [53], modifying the quasiparticle

excitations and shifting the effective fermion-fermion interaction strength $U_{\text{eff}} \rightarrow U - 2g^2/\omega$. Here, there is a competition between a generated effective attractive interaction and then the dynamical generation of phonons in the environment, the presence of which can strongly suppress dynamics and correlation growth resulting in CDW order [53]. We can see the competition of these effects in Fig. 3(a), which are made even more clear by analyzing the phonon mode observables in Figs. 3(b) and 3(c) which we can directly calculate from HOPS using the time-dependent colored noise term $\tilde{z}_n^*(t)$ in Eq. (6) (see Supplemental Material [38]). We see that initially the phonon population is low and so the effective interaction between fermions dominates, enhancing the growth of pairing correlations, before the dynamical generation of phonons begins to dominate, suppressing correlations at later times, which for smaller κ is larger due to an increased phonon population.

Discussion and outlook.—Our combination of the HOPS algorithm with MPS techniques opens up the ability to explore a wide range of new and interesting regimes that were previously only possible to simulate qualitatively and/or through invoking some strong approximations. By considering the dispersive Hubbard-Holstein model we demonstrated that we can simulate the exact dynamics of open many-body systems well into the non-Markovian and strong coupling regimes and we are able to quantitatively analyze the dynamical properties of long-range correlation functions. In particular, we found strong qualitative differences in the dynamics of fermionic pairing correlations between the non-Markovian and Markovian cases. This work can be generalized to describe microscopic dynamics in a range of experimental settings, such as impurities immersed in BECs [18–22] or atoms in multimode cavities [15–17].

Other non-Markovian techniques could be adapted in order to probe the features investigated in our work, for example TEMPO [7–9] or HEOM [5,6]. It may similarly be possible to combine these methods with MPS, as we have done here with HOPS. The combination is particularly amenable to our case as it involves the evolution of a single 1D matrix product state to capture the strongly interacting open system. Alternatively, explicitly retaining the phonon basis states would result in an equivalent simulation with Markovian dissipation, allowing for the solution within a standard Born-Markov QSD [1,37]. However, we find that the number of phonon basis states required (the local dimension of the MPS) is generally larger than that required for the present HOPS algorithm. In addition, HOPS has two main additional advantages. First, it can simulate phonon modes initially at finite temperatures and then track the induced dynamics in real time as demonstrated here, whereas explicitly retaining the basis states in this case would further increase the complexity. But second, improvements and extensions to the MPS representation can be immediately implemented [48,54–57], allowing us

to generalize this approach and approximate the dynamics induced by, up to reasonable timescales, environments that have algebraically decaying correlations [10,11] such as those that arise from power law spectral densities [1,27,28].

All data underpinning this publication are openly available from the University of Strathclyde KnowledgeBase [58].

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