Simulating Bosonic Baths with Error Bars

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(Received 19 May 2015; published 22 September 2015)

We derive rigorous truncation-error bounds for the spin-boson model and its generalizations to arbitrary quantum systems interacting with bosonic baths. For the numerical simulation of such baths, the truncation of both the number of modes and the local Hilbert-space dimensions is necessary. We derive superexponential Lieb-Robinson-type bounds on the error when restricting the bath to finitely many modes and show how the error introduced by truncating the local Hilbert spaces may be efficiently monitored numerically. In this way we give error bounds for approximating the infinite system by a finite-dimensional one. As a consequence, numerical simulations such as the time-evolving density with orthogonal polynomials algorithm (TEDOPA) now allow for the fully certified treatment of the system-environment interaction.

DOI: 10.1103/PhysRevLett.115.130401 PACS numbers: 03.65.Yz, 03.70.+k

Introduction.—Ideal quantum systems may be considered closed, undergoing textbook unitary evolution. In any realistic experimental setup, however, a quantum system is open; that is, it interacts with an environment composed of those degrees of freedom that are not under the control of the experimenter. Hence, the numerical and analytical description of the dynamics of a quantum system in interaction with its environment is of fundamental importance in quantum physics. The precise nature and composition of the system-environment interaction is generally not known, but for a wide range of systems encountered in physics, chemistry, and biology, it is common to model the environment as a continuum of harmonic oscillators which interact linearly with the system. This results in the paradigmatic spin-boson model that captures many aspects of the system-environment interaction [1]. The spin-boson model is exactly solvable only in the rarest of special cases, and one is therefore compelled to employ a variety of approximations and numerical descriptions in order to obtain the reduced dynamics of the quantum system in question. Notable examples include those cases in which the environment possesses a correlation time that is much shorter than the system dynamics *and* the system-environment interaction is weak. Under these assumptions, it is then well justified and customary to resort to the so-called Markov approximation, which permits the derivation of completely positive and linear differential equations, the Lindblad equation, for the quantum system alone [2].

However, settings of considerable practical importance may violate either or both of these assumptions and require a more sophisticated treatment. The recently emerging interest in quantum effects in biological systems provides a case in point [3]. For instance, in typical pigment-protein complexes the dynamical time scales of the vibrational environment can be comparable or even slower than the quantum mechanical excitation energy transfer dynamics. Moreover, in the limit of slow bath dynamics, perturbative treatments of the coupling between system and environment cannot be used even if the system-bath coupling is intrinsically weak. Consequently, steps have been taken towards the development of nonperturbative and non-Markovian approaches for the description of the quantum system-environment interaction (see Refs. [3,4] for overviews of recent developments). However, the majority of these approaches have in common that they exploit approximations that are not well controlled, in the sense that no rigorous error bounds on the simulation results are available. Hence, these methods are not certified.

The time-evolving density with orthogonal polynomials algorithm (TEDOPA) for the spin-boson model presents a notable exception, as will be demonstrated in the present Letter. It makes use of an exact transformation of the standard representation of the spin-boson model onto a spin interacting with the first site of a semi-infinite nearest-neighbor coupled chain [5–9], which renders the system particularly amenable to time-adaptive density matrix renormalization group (t-DMRG) simulations. The structure of the resulting system is such that excitations tend to propagate along the chain away from the system towards infinity, leading to irreversible system dynamics for long times. This approach has been used with success in the simulation of a number of highly non-Markovian system-environment interactions [6,10,11].

The errors that accumulate in the t-DMRG simulation can be bounded rigorously [12,13]. Nevertheless, the numerical TEDOPA simulation employs two as yet uncertified assumptions: (i) the semi-infinite chain needs to be truncated to a finite length, and (ii) the local dimension associated with each harmonic oscillator of the chain needs to be truncated to a finite dimensional Hilbert space; see Fig. 1. The errors that are introduced in this manner are usually estimated by increasing both the chain length and

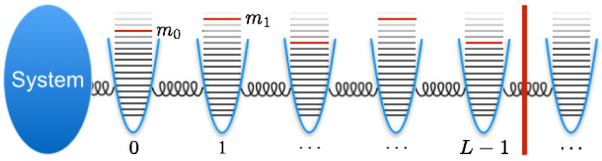

FIG. 1 (color online). A system coupled to a bosonic bath. Red lines indicate the truncations: the spatial truncation to a chain of finite length L and the truncation of the local Hilbert space dimensions to m_i.

the Hilbert space cutoff until the change in the result drops below a predefined threshold. However, in practice this somewhat inelegant approach can become highly challenging numerically, and it can lead to erroneous numerical predictions [14]. A more rigorous approach is therefore desirable.

Here we employ techniques that lead to Lieb-Robinson-type bounds to achieve this goal by deriving bounds for the errors arising from approximations (i) and (ii). As the errors arising in each step of the t-DMRG integration can also be bounded, we arrive at a method that possesses rigorous error bounds on the results that it delivers. This extends significantly the existing recent results in the literature that apply to the finite dimensional setting of spin systems [15] and therefore allows the fully certified treatment of the system-environment interaction for both harmonic oscillator and spin environments.

The system under consideration.—We will consider the Hamiltonian of an arbitrary system $\hat{H}_S$ coupled via $\hat{V}$ to a bosonic bath described by $\hat{H}_B$, so that the total Hamiltonian reads

$$\hat{H} = \hat{H}_S + \hat{V} + \hat{H}_B. \tag{1}$$

For simplicity and to directly connect to the TEDOPA approach [6,7,10,11], we assume that $\hat{H}_B$ describes a one-dimensional nearest-neighbor Hamiltonian (the higher dimensional case with more general couplings will be published elsewhere [16]) and takes the form

$$\hat{H}_B = \frac{1}{2}\sum_{i,j=0}^{\infty} (\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j), \tag{2}$$

where we assume that only nearest neighbors are coupled, $X_{i,j} = P_{i,j} = 0$ for $|i-j| > 1$, and we let without loss of generality $X_{i,j} = X_{j,i} \in \mathbb{R}$, $P_{i,j} = P_{j,i} \in \mathbb{R}$. We consider system-bath couplings of the form $\hat{V} = \hat{h} \otimes \hat{x}_0$ (see the Supplemental Material [17] for systems coupled to several baths), where $\hat{h}$ acts on the system and we assume that it is bounded in operator norm, $\|\hat{h}\| < \infty$. The system with Hamiltonian $\hat{H}_S$ has no restrictions: it can correspond to any system—bosons, fermions, and/or spins, all in arbitrary dimensions. As we will see later, the generalized spin-boson model can be written in this form.

Spatial truncation of the bath.—For bounded system observables $\hat{O}$, $\|\hat{O}\| < \infty$, we are interested in the quantity

$$\Delta(t, L) = |\mathrm{tr}[\hat{O} e^{-i\hat{H}t} \hat{\varrho}_0 e^{i\hat{H}t}] - \mathrm{tr}[\hat{O} e^{-i\hat{H}_L t} \hat{\varrho}_0 e^{i\hat{H}_L t}]|, \tag{3}$$

i.e., the error introduced when, instead of simulating the full Hamiltonian $\hat{H}$, we simulate the time evolution of system observables $\hat{O}$ with the truncated bath Hamiltonian

$$\hat{H}_B^L = \frac{1}{2}\sum_{i,j=0}^{L-1} (\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j) \tag{4}$$

and the corresponding total Hamiltonian $\hat{H}_L = \hat{H}_S + \hat{V} + \hat{H}_B^L$. Our first main result is the following.

Theorem: Let $\hat{H}$ and $\hat{H}_L$ be as above. Let $X, P > 0$ or $X = P$ (see the Supplemental Material [17] for a bound when neither of these conditions is satisfied). Let c be such that $\|XP\|^{1/2} \leq c$. Then,

$$\frac{\Delta^2(t, L)}{4\|\hat{O}\|^2 \|\hat{h}\|/c} \leq C\left(\|\gamma_0\|^{1/2} + t\|\hat{h}\|\right) \frac{(ct)^{L+1}(e^{ct}+1)}{(L+1)!}, \tag{5}$$

where $C = \|P_L\||X_{L-1,L}|/c^2 + |P_{L-1,L}|/c$ and

$$\gamma_0 = \begin{pmatrix} \gamma_{xx} & \gamma_{xp} \\ \gamma_{px} & \gamma_{pp} \end{pmatrix}, \qquad [\gamma_{ab}]_{i,j} = \mathrm{tr}[\hat{a}_i \hat{b}_j \hat{\varrho}_0], \tag{6}$$

collects the two-point bath correlations in the initial state. If $P \propto \mathbb{1}$, we may replace L by $2L$ in Eq. (5).

If the initial two-point correlation functions (the matrix elements of γ_0) are unbounded, then one can still achieve bounds; see the Supplemental Material [17] for details. The rhs of Eq. (5) describes the Lieb-Robinson-type light cone [18]. Outside the light cone (so, for $\tau := ect < L$), one finds superexponential decay in L: $(ct)^L e^{ct}/L! \leq e^{ct - L|\ln(L/\tau)|}$. This makes rigorous the physical intuition that for all finite times only a chain of *finite* length is required to simulate the dynamics of local observables to within a prescribed precision. Our bound applies to *any* system Hamiltonian, unbounded or otherwise, and depends only linearly on the operator norm of the system coupling $\|\hat{h}\|$. The proof relies on Lieb-Robinson bounds for harmonic systems [19–21] (see also Ref. [22]) and may be found in the Supplemental Material [17]. Before stating our second main result, we discuss the above bound in light of the generalized spin-boson model.

Generalized spin-boson model.—In this section we will investigate Hamiltonians of the form

$$\hat{H} = \hat{H}_S + \int d\boldsymbol{k} g(\boldsymbol{k}) a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \hat{A}_S \int d\boldsymbol{k} h(\boldsymbol{k})(a_{\boldsymbol{k}}^\dagger + a_{\boldsymbol{k}}). \tag{7}$$

This describes a quantum system with Hamiltonian $\hat{H}_S$ interaction with a bath of bosons; it is described in more detail in terms of second quantized operators in Ref. [23]. This model has received renewed interest in recent years due to its importance in the theoretical study of quantum effects in biology (see Ref. [3] for a review). An important quantity that describes the bath and its coupling to the system is the spectral density, which, for invertible g, is defined as

$$J(\omega) = \pi h^2[g^{-1}(\omega)]\left|\frac{dg^{-1}(\omega)}{d\omega}\right|, \tag{8}$$

with g^{-1} being the inverse of g (see Ref. [9] for instances where g takes vector arguments). The smallest closed interval containing the support of g^{-1} is denoted $[\omega_{\min}, \omega_{\max}]$. The case $\omega_{\min} = 0$ is called massless, whereas $\omega_{\min} > 0$ is known as massive.

Building on the work of Refs. [5,7,8], it was shown using the theory of orthogonal polynomials in Ref. [9] that Eq. (7) can be written in the form of Eqs. (2) and (1) and that there are two ways to do this. Both choices

$$\hat{h} = \mu_0 \hat{A}_S, \qquad X = P, \tag{9}$$

and

$$\hat{h} = \mu_1 \hat{A}_S, \qquad P = \omega_{\max}\mathbb{1}, \tag{10}$$

with an appropriate X (given in terms of the spectral density in the Supplemental Material [17]) are equivalent to Eq. (7). Here,

$$\mu_0^2 = \frac{2}{\pi}\int d\omega J(\omega), \qquad \mu_1^2 = \frac{1}{\pi\omega_{\max}}\int d\omega J(\sqrt{\omega}), \tag{11}$$

and one finds $\|X\| = \|P\| = \omega_{\max}$ for both cases and $X > 0$ if and only if $\omega_{\min} > 0$. Because of the form of their elementary excitations, the mappings leading to couplings as in Eqs. (9) and (10) were named *particle mapping* and *phonon mapping*, respectively, and we will adopt this denomination here. Crucially, in both cases, X couples nearest neighbors only, such that the bound in Eq. (5) is readily applicable to the particle and the massive phonon case, setting $c = \omega_{\max}$ for both (similar results hold for the massless case; see the Supplemental Material [17] for full details). For the particle mapping, we find $C \leq 2$ and for the phonon mapping $C \leq 1$ such that, up to the constants $\mu_{0/1}$, we obtain the same behavior of the bound in both cases, but by replacing L by $2L$ in the massive phonon case. Hence, for the phonon mapping with a chain of only half the length, one has approximately the same chain truncation error as for the particle mapping.

If the maximum frequency of the bath $\omega_{\max} = \infty$, the chain coefficients are unbounded [9] and our bounds diverge. This divergence is not surprising in light of the observation that certain one-dimensional infinite harmonic lattice models with nearest-neighbor interactions and unbounded coefficients have been proven *not* to have a light cone bound [24]. It is noteworthy that similar results can be derived for the case of a fermionic bath since the chain mapping is still valid and Lieb-Robinson bounds for fermions are well known [25].

Truncating local Hilbert spaces.—We now consider the error introduced when the local Hilbert space dimensions of the harmonic oscillators making up the bath are truncated. To this end, we define the projector

$$\mathbb{1}_{\boldsymbol{m}} = \mathbb{1}_{m_0} \otimes \cdots \otimes \mathbb{1}_{m_{L-1}}, \qquad \mathbb{1}_m = \sum_{n=0}^{m} |n\rangle\langle n|, \tag{12}$$

where $\mathbb{1}_{m_i}$ acts on the ith site of the bath and truncates the local Hilbert space according to $\mathbb{1}_m$. For bounded observables acting on the system $\hat{O}$, $\|\hat{O}\| < \infty$, we consider

$$\Delta_{\boldsymbol{m}}(t) = |\mathrm{tr}[\hat{O}e^{-it\hat{H}}\hat{\varrho}_0 e^{it\hat{H}}] - \mathrm{tr}[\hat{O}e^{-it\hat{H}_{\boldsymbol{m}}}\hat{\varrho}_0 e^{it\hat{H}_{\boldsymbol{m}}}]|, \tag{13}$$

i.e., the error introduced by evolving the system according to

$$\hat{H}_{\boldsymbol{m}} = \mathbb{1}_{\boldsymbol{m}}\hat{H}\mathbb{1}_{\boldsymbol{m}} \tag{14}$$

instead of $\hat{H}$. Here, $\hat{H}$ is as in Eq. (4) and we omit the index L for notational clarity. The truncated Hamiltonian reads $\hat{H}_{\boldsymbol{m}} = \hat{H}_S + \hat{H}_B^{\boldsymbol{m}} + \hat{h} \otimes \mathbb{1}_{\boldsymbol{m}}\hat{x}_0\mathbb{1}_{\boldsymbol{m}}$, where

$$\hat{H}_B^{\boldsymbol{m}} = \frac{1}{2}\sum_{i,j=0}^{L-1}[X_{i,j}\mathbb{1}_{\boldsymbol{m}}\hat{x}_i\hat{x}_j\mathbb{1}_{\boldsymbol{m}} + P_{i,j}\mathbb{1}_{\boldsymbol{m}}\hat{p}_i\hat{p}_j\mathbb{1}_{\boldsymbol{m}}]. \tag{15}$$

In the Supplemental Material [17] we show that

$$\frac{\Delta_{\boldsymbol{m}}^2(t)}{4\|\hat{O}\|^2} \leq \mathrm{tr}[(\mathbb{1} - \mathbb{1}_{\boldsymbol{m}})\hat{\varrho}_0] + 2\int_0^t dx\sqrt{\epsilon_{\boldsymbol{m}}(x)}, \tag{16}$$

where

$$\epsilon_{\boldsymbol{m}}(x) = \mathrm{tr}[\hat{h}^2 e^{-ix\hat{H}_B^{\boldsymbol{m}}}\hat{X}^2(x)e^{ix\hat{H}_B^{\boldsymbol{m}}}\hat{\varrho}_{\boldsymbol{m}}(x)], \tag{17}$$

with

$$\hat{X}(x) = \mathbb{1}_{\boldsymbol{m}}e^{ix\hat{H}_B}\hat{x}_0 e^{-ix\hat{H}_B}\mathbb{1}_{\boldsymbol{m}} - e^{ix\hat{H}_B^{\boldsymbol{m}}}\hat{x}_0 e^{-ix\hat{H}_B^{\boldsymbol{m}}},$$
$$\hat{\varrho}_{\boldsymbol{m}}(x) = e^{-ix\hat{H}_{\boldsymbol{m}}}\hat{\varrho}_0 e^{ix\hat{H}_{\boldsymbol{m}}}. \tag{18}$$

Crucially, under the assumption that the system Hilbert space is finite dimensional, this error may be computed numerically, as it involves only observables acting on the truncated Hilbert space ($e^{ix\hat{H}_B}\hat{x}_0 e^{-ix\hat{H}_B}$ is a linear combination of the $\hat{x}_i$ and $\hat{p}_i$) and which are of a form amenable to t-DMRG simulations (see the Supplemental Material [17]

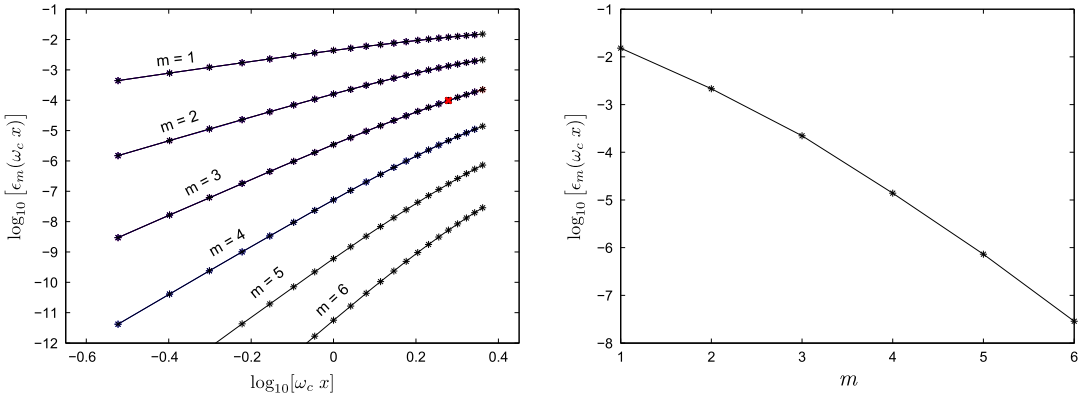

FIG. 2 (color online). Fock space truncation error [Eq. (17)] for the particle mapping and power-law spectral densities as in Eq. (19), with $\Delta/\omega_c = 1$, $\alpha = 0.8$, $s = 3$ for initial state $\hat{\varrho}_0 = \hat{\varrho}_S^0 \otimes \hat{\varrho}_B^0$, $\hat{\varrho}_S^0 = |\uparrow\rangle\langle\uparrow|$ and $\hat{\varrho}_B^0$ the vacuum. We truncate each local Hilbert space at the same value $m_i = m$ and L has the values 3 to 6, but they are indistinguishable (e.g., the difference between the $L = 6$ and $L = 3$ curve at the point denoted by a red square is 4.95×10^{-6}). Lines are guides for the eye. The log-log plot on the left suggests algebraic increase in time and the plot on the right (plotted for a constant time $t = 2.45/\omega_c$) suggests a better than exponential decrease with m.

for details). For all finite times, $\lim_{\{m_i\}\to\infty} \Delta_{\boldsymbol{m}} = 0$, and we study its behavior in $\boldsymbol{m}$ in numerical examples below. If the bath initially contains only a finite number of particles, $\mathrm{tr}[(\mathbb{1} - \mathbb{1}_{\boldsymbol{m}})\hat{\varrho}_0]$ vanishes for an appropriate $\boldsymbol{m}$. Such states include the vacuum state which is also the zero temperature thermal state for the particle mapping. For higher temperature thermal states of the bath, $\mathrm{tr}[(\mathbb{1} - \mathbb{1}_{\boldsymbol{m}})\hat{\varrho}_0]$ vanishes exponentially for a large $\{m_i\}$. The total error induced on the expectation value of $\hat{O}$ due to (i) truncating the chain to finite length and (ii) the truncation of the local dimensions is bounded by the sum of the two individual error bounds: $\Delta(t, L) + \Delta_{\boldsymbol{m}}(t)$. This rigorously bounds the error of approximating an infinite-dimensional bath of bosons by a chain of length L made up of finite-dimensional subsystems with nearest-neighbor interactions. If in addition we assume the system with Hamiltonian $\hat{H}_S$ to be a spin system, then the Hamiltonian is in the class which, as Ref. [15] shows, can be simulated with resources polynomial in L and error ϵ, and exponential in $|t|$.

Numerical example.—As an example, we consider the spin-boson model with a power-law spectral density,

$$J(\omega) = \pi\alpha\omega_c^{1-s}\omega^s\Theta(1 - \omega/\omega_c), \tag{19}$$

where Θ is the Heaviside step function. This model has been extensively probed numerically, and there has been controversy over the accuracy of numerically derived critical exponents. One of the issues with the results was the inability to verify the local Fock space truncation errors [14,26]. The system Hamiltonian and interaction part are $\hat{H}_S = -\Delta\hat{\sigma}_x/2$ and $\hat{A}_S = \sigma_z/2$. The dissipation is known as Ohmic for $s = 1$ and super-Ohmic for $s > 1$. This can be written in the chain representation using Eq. (9) (see the Supplemental Material [17] for details). In Fig. 2, the bound for the particle mapping is plotted for the super-Ohmic case and various L and $\boldsymbol{m}$. Constants used for the simulation (see the figure caption) are taken from the literature [27]. The initial state of the bath corresponds to the zero temperature thermal state. We probe the same initial state for the case of Ohmic dissipation and achieve qualitatively the same results (see the Supplemental Material [17]). Furthermore, we test the bound for a squeezed vacuum state of the bath, which is a highly populated state (see the Supplemental Material [17]).

Conclusion.—The detailed simulation of the interaction of a quantum system with a structured environment composed of harmonic oscillators has applications in a wide variety of scientific fields. The multitude of proposed algorithms to tackle this problem numerically lacked a method that delivers a simulation result with a rigorous error bound associated with it. In this Letter we derive error bounds that demonstrate that the recently developed TEDOPA can provide such a method. More specifically, obtaining Lieb-Robinson-type expressions, we provide complete error bounds on the simulation of observables of quantum systems coupled to a bosonic bath with infinitely many degrees of freedom, such as the spin-boson model. This includes the errors incurred due to the truncation of the local Hilbert spaces of the harmonic oscillators and due to the truncation of the length of the harmonic chain representing the environment. In this manner we provide a fully rigorous upper bound on the error for the numerical simulation of a spin-boson model and its generalization to multiple baths and more general systems.

M. P. W. would like to thank Gerald Teschl for discussions regarding Jacobi operators and M. B. P. acknowledges discussions with S. F. Huelga. This work was supported by the EPSRC CDT on Controlled Quantum Dynamics, the EU STREP projects PAPETS and EQUAM, the EU Integrating project SIQS, and the ERC Synergy grant BioQ, as well as the Alexander von Humboldt Foundation.

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