

Simulation Complexity of Open Quantum Dynamics: Connection with Tensor Networks

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The difficulty to simulate the dynamics of open quantum systems resides in their coupling to many-body reservoirs with exponentially large Hilbert space. Applying a tensor network approach in the time domain, we demonstrate that effective small reservoirs can be defined and used for modeling open quantum dynamics. The key element of our technique is the timeline reservoir network (TRN), which contains all the information on the reservoir's characteristics, in particular, the memory effects timescale. The TRN has a one-dimensional tensor network structure, which can be effectively approximated in full analogy with the matrix product approximation of spin-chain states. We derive the sufficient bond dimension in the approximated TRN with a reduced set of physical parameters: coupling strength, reservoir correlation time, minimal timescale, and the system's number of degrees of freedom interacting with the environment. The bond dimension can be viewed as a measure of the open dynamics complexity. Simulation is based on the semigroup dynamics of the system and effective reservoir of finite dimension. We provide an illustrative example showing the scope for new numerical and machine learning-based methods for open quantum systems.

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Introduction.—One of the most challenging and important problems of modern theoretical physics is the accurate simulation of an interacting many-body system. As the dimension of its Hilbert space grows exponentially with the system size, direct simulations become impossible. Exactly solvable models exist nonetheless [1]; they provide some insights into the properties of actual physical systems. Perturbation theory can be used only for problems that can be split into an exactly solvable part and a perturbative one provided that a relevant small parameter (e.g., weak interaction strength with respect to other energy scales) can be defined. For strongly interacting many-body systems, a range of techniques including, e.g., the Bethe ansatz [2], the dynamical mean field theory [3,4], or the slave boson techniques [5,6] have been developed and applied to problems like the diagonalization of the Kondo Hamiltonian or the Anderson impurity model [7–11]. Numerical approaches, which may significantly go beyond the range of applicability of analytical methods, have been also developed and proved quite successful, though they suffer from limits. For example, methods based on tensor networks [12–14] and the density matrix renormalization group [15–17] work well mainly for one-dimensional models. Quantum Monte Carlo (QMC) methods provide reliable ways to study the many-body problem [18], but for interacting fermion systems these approaches are plagued by the sign problem [19].

Unitary evolution of a many-body system is completely out of reach: dynamical versions of QMC calculations or efficient methods like the time-evolving block decimation algorithm cannot predict long-term time dynamics because of the Lieb-Robinson bound [20–23]. Having experimental access only to a part of a many-body system, one in fact deals with an *open* quantum dynamics of the subsystem (S), whereas the rest of the particles (modes) play the role of environment also referred to as reservoir (R); see Fig. 1(a). The subsystem is described by a density operator $\rho_S(t) = \text{tr}_R[U(t)\rho(0)U^\dagger(t)]$, the evolution of which is still challenging to determine though the subsystem is relatively small compared to the environment [24,25]: the partial trace, tr_R , disregards the environment degrees of freedom (d.o.f.) but $\rho(0)$ is the initial state of the *whole* many-body system and its evolution operator is $U(t) = e^{-itH}$. There exist particular exactly solvable models of open quantum dynamics [26–28]; however, without the Markov

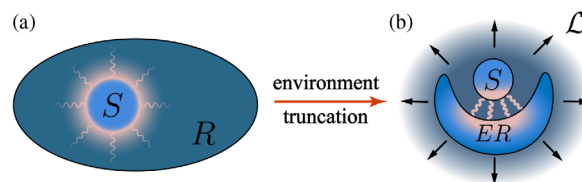


FIG. 1. Schematic of reservoir truncation.

approximation the problem of open dynamics is typically impossible to solve directly because of the exponentially large dimension of the reservoir's Hilbert space [25,29,30]. Examples of complex open dynamics in structured reservoirs, where it is necessary to go beyond the Markov approximation, are presented in Refs. [31–42]. Therefore, new, numerically tractable approaches permitting significant progress in the field of open quantum dynamics simulation are highly desirable, and their development constitutes a timely challenge, especially in the study of quantum control and dynamical decoupling [40–42], and quantum dynamics induced by many-body reservoirs [43–46].

In this work, we show that the actual infinite environment can be replaced by a *finite*-dimensional effective reservoir (ER) in such a way that the aggregate “S + ER” experiences semigroup dynamics, see Fig. 1(b). This approach resembles the idea of Markovian embedding of non-Markovian dynamics [47–50] and the pseudomode method [51–53]. Our main result is the estimation of the minimal (sufficient) dimension d_{ER} of the effective reservoir expressed through a reduced set of parameters. Knowledge of d_{ER} enables one to efficiently simulate the complex dynamics of a subsystem of dimension d_S via $\rho_S(t) = \text{tr}_{\text{ER}}[e^{\mathcal{L}t}\rho_{S+\text{ER}}(0)]$, where the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) generator \mathcal{L} [54,55] is easy to parametrize in this case: \mathcal{L} acts on $d_S d_{\text{ER}} \times d_S d_{\text{ER}}$ matrices and can be numerically found via machine learning techniques provided a sequence of measurements on the subsystem is performed [56]. Another machine learning algorithm [57] estimates d_{ER} within the training range $d_{\text{ER}} = 1, 2, 8, 16$ based on interventions in the open qubit evolution at 4 time moments.

Open quantum systems properties.—Let \mathcal{H}_S and \mathcal{H}_R be Hilbert spaces of subsystem and reservoir, respectively. Typically $\dim(\mathcal{H}_S) \ll \dim(\mathcal{H}_R)$ as \mathcal{H}_S could be associated with, e.g., a qubit or other small system, and \mathcal{H}_R with a many-body quantum environment of a huge dimension. The total Hilbert space is $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_R$. As the environment is assumed to be in the thermodynamic limit, the dynamics of $\rho_S(t)$ is irreversible; i.e., the Poincaré recurrence time is infinite. When the subsystem and reservoir exchange energy, thermalization is expected on a long timescale [58], though the dynamics can be strongly non-Markovian at finite times [59].

The total Hamiltonian reads $H = H_0 + H_{\text{int}}$, where $H_0 = H_S \otimes \mathbb{1} + \mathbb{1} \otimes H_R$ involves individual Hamiltonians of subsystem and reservoir, $H_{\text{int}} = \gamma \sum_{i=1}^n A_i \otimes B_i$ is the interaction part with characteristic interaction strength γ ; n is the effective subsystem's number of d.o.f. interacting with the reservoir. Denote $B_i(t) = U^\dagger(t) B_i U(t)$, then $g_{ij}(t, t-s) = \text{tr}[B_i^\dagger(t) B_j(t-s) \rho(0)] - \text{tr}[B_i^\dagger(t) \rho(0)] \text{tr}[B_j(t-s) \rho(0)]$ is the reservoir correlation function [60]. Suppose $g_{ij}(t, t-s)$ decays exponentially with the growth of s over a characteristic time s_{ij} (see examples in Refs. [61,62]), then $T = \max_{ij} s_{ij}$ is the reservoir correlation time. Suppose the

Fourier transform of the reservoir correlation function decays significantly at the characteristic frequency Ω_{ij} , then $\tau = (\max_{ij} \Omega_{ij})^{-1}$ defines the minimal timescale in the dynamics. In the case of a bosonic bath, $\tau = \omega_c^{-1}$, where ω_c is the cutoff frequency of the spectral function [63]. Our approach to determine the dimension d_{ER} of the truncated environment is based on tensor network formalism in the time domain, where the building blocks are responsible for evolution during time τ and the ancillary space is capable of transferring temporal correlations for the period T . Therefore, d_{ER} depends only on the following few physical parameters: γ , n , τ , and T .

Tensor network representation of open quantum dynamics.—For simplicity, we resort to the vector representation of a density operator:

$$\rho = \sum_{jk} \rho_{jk} |j\rangle\langle k| \rightarrow |\rho\rangle = \sum_{jk} \rho_{jk} |j\rangle \otimes |k\rangle, \quad (1)$$

which implies $Q\rho P \rightarrow Q \otimes P^T |\rho\rangle$. The dynamics of the whole system reads

$$|\rho(t)\rangle = \exp[-itH] \otimes \exp[itH^T] |\rho(0)\rangle. \quad (2)$$

The initial state $\rho(0)$ can be correlated in general, i.e., $\rho(0) = \sum_i \sigma_S^{(i)} \otimes \sigma_R^{(i)}$. The subsystem state $\rho_S(t) = \text{tr}_R \rho(t)$ in terms of vectors reads $|\rho_S(t)\rangle = \langle \psi_+ | |\rho(t)\rangle$, where $\langle \psi_+ | = \sum_{j=1}^{d_R} \mathbb{1}_S \otimes \langle j | \otimes \mathbb{1}_S \otimes \langle j |$. For further convenience we introduce a new order of Hilbert spaces: $\mathcal{H}_{\mathcal{H}} \otimes \mathcal{H}_{\mathcal{H}} \otimes \mathcal{H}_{\mathcal{H}}^\dagger \otimes \mathcal{H}_{\mathcal{H}}^\dagger \rightarrow \mathcal{H}_{\mathcal{H}} \otimes \mathcal{H}_{\mathcal{H}}^\dagger \otimes \mathcal{H}_{\mathcal{H}} \otimes \mathcal{H}_{\mathcal{H}}^\dagger$.

The minimal timescale τ is a time step in discretized evolution; τ can always be reduced in such a way that $\gamma\tau \ll 1$, which permits application of the Trotter decomposition [64]. Note that we do not restrict our framework to a weak coupling between a subsystem and reservoir ($\gamma \ll \|H_0\|$); we rather adjust the minimal timescale τ in accordance with the interaction strength, which yields

$$|\rho(t)\rangle = \underbrace{\Phi_0(\tau) \Phi_{\text{int}}(\tau) \cdots \Phi_0(\tau) \Phi_{\text{int}}(\tau)}_{t/\tau \text{ times}} |\rho(0)\rangle + O(\gamma\tau), \quad (3)$$

where $\Phi_0(\tau)$ and $\Phi_{\text{int}}(\tau)$ are responsible for the non-interactive and interactive evolutions of the subsystem and environment:

$$\begin{aligned} \Phi_0(\tau) &= \exp[-i\tau H_S] \otimes \exp[i\tau H_S^T] \\ &\otimes \exp[-i\tau H_R] \otimes \exp[i\tau H_R^T], \end{aligned} \quad (4)$$

$$\Phi_{\text{int}}(\tau) = \sum_{i=0}^{2n} \mathcal{A}_i(\tau) \otimes \mathcal{B}_i(\tau), \quad (5)$$

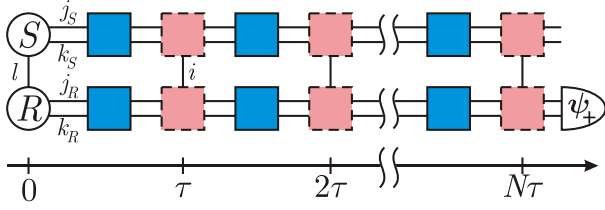


FIG. 2. Tensor network for open system dynamics.

$$A_i(\tau) = \begin{cases} 1 \otimes 1 & \text{if } i = 0, \\ \sqrt{\gamma\tau} A_i \otimes 1 & \text{if } 1 \leq i \leq n, \\ \sqrt{\gamma\tau} 1 \otimes A_{i-n}^T & \text{if } i \geq n + 1, \end{cases} \quad (6)$$

$$B_i(\tau) = \begin{cases} 1 \otimes 1 & \text{if } i = 0, \\ -i\sqrt{\gamma\tau} B_i \otimes 1 & \text{if } 1 \leq i \leq n, \\ i\sqrt{\gamma\tau} 1 \otimes B_{i-n}^T & \text{if } i \geq n + 1. \end{cases} \quad (7)$$

The tensor network representation to calculate $|\rho_S(t)\rangle$ is presented in Fig. 2. It is a particular case of the general quantum circuits [65–69]. Each building block with m arms corresponds to a tensor of rank m . Connecting links denote contractions over the same indices. The vector $|\rho(t)\rangle$ has two multi-indices $j = (j_S, j_R)$ and $k = (k_S, k_R)$, so it is represented as a tensor of rank 4. The upper (bottom) row corresponds to the d.o.f. of subsystem S (reservoir R). The operator $\Phi_0(\tau)$ is depicted by solid squares. The dashed squares with a link between them denote the operator $\Phi_{\text{int}}(\tau)$, with the link being responsible for summation $\sum_{i=0}^{2n}$ in formula (5). Concatenation with the building block ψ_+ in the right bottom of Fig. 2 corresponds to the partial trace over R and will be further denoted by connecting link \triangleright .

A key object in our study is the tensor in Fig. 3(c), which we call a timeline reservoir network (TRN). The TRN contains all the information on the reservoir and controls all features of open dynamics, including dissipation, Lamb shift, and memory effects like revivals [25]. From the computational viewpoint, for a fixed time t , TRN is a tensor with t/τ indices. Since the physical reservoir has a finite

memory depth T , the considered tensor must have vanishing correlations between apart indices. Tensors of such a type can be effectively approximated by one-dimensional tensor networks of matrix-product (MP) form.

The TRN is closely related to the recent reformulations of the Feynman-Vernon path integrals [63,73–76] and the process tensor [68,70–72], see Figs. 3(a)–3(b). In fact, the influence functional in Fig. 3(b) can be explicitly calculated in the case of a bosonic bath linearly coupled to the system [77] but it remains difficult to contract with the system initial state and unitary evolution tensors, so in Refs. [73–75] the contraction calculation is approximated by fixing a finite memory depth $K = T/\tau$. References [63,76] further use MP approximation of the influence functional (with rank λ_{max} and accuracy λ_c), which allows us to deal with longer memory depths. Since λ_{max} is d_{ER}^2 in our model, we actually estimate the complexity (λ_{max}) of the algorithm in Ref. [63].

MP approximation of the TRN.—From a mathematical viewpoint, the constructed TRN can be treated as a pure multipartite quantum state $|\psi\rangle$, where summation index $i_m = 0, \dots, 2n$ at time moment $t_m = m\tau$ plays the role of the physical index assigned to the m th particle:

$$|\psi\rangle = \sum_{l, i_1, i_2, \dots, i_N} \psi_{l i_1 i_2 \dots i_N} |l\rangle \otimes |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_N\rangle. \quad (8)$$

The only difference between the TRN and $|\psi\rangle$ is the normalization: $\text{TRN} \propto |\psi\rangle$, $\langle\psi|\psi\rangle = 1$.

A multipartite quantum state $|\psi\rangle$ with a finite correlation length L can be effectively described via MP approximation [12]. The benefit of such an approximation is that it is able to reproduce spatial correlations among particles within the characteristic length L . The effectiveness of approximation means that the bond dimension r of the ancillary space (rank of MP state) is rather small. Similarly, the TRN is able to effectively reproduce temporal correlations within the period T with a rather small dimension d_{ER} of effective reservoir. Since we deal with matrices, d_{ER}^2 is equivalent to the rank of corresponding MP state. The dimension of the physical space in the MP state is $2n + 1$, where n is the number of the subsystem’s d.o.f. involved in the interaction with environment. Note that $n \leq d_S^2$. The physics of MP approximations for states and TRN is summarized in Table I.

Suppose $|\psi^{(r)}\rangle$ is a rank- r MP approximation of the pure state $|\psi\rangle$. The approximation error $\epsilon(r)$ equals the Frobenius distance between $|\psi^{(r)}\rangle$ and $|\psi\rangle$. Consider $|\psi\rangle$ as a bipartite state, with parties being separated by a cut between the m th and $(m + 1)$ th particle. MP approximation effectively disregards low-weight contributions in the Schmidt decomposition of $|\psi\rangle$ with respect to such a cut. The approximation error $\epsilon(r)$ is related to the Rényi entropy of order α ($0 < \alpha < 1$), S_α of a single reduced density operator as follows [78]:

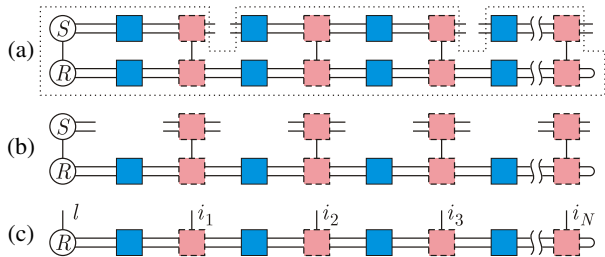

 FIG. 3. (a) Process tensor $\mathcal{T}(t_1; t_3; t_n)$ [68,70–72]. (b) Influence functional [63,73–76]. (c) Timeline reservoir network.

TABLE I. Correspondence between physical descriptions of pure quantum states and TRN in MP approximation.

MP approximation of states	MP approximation of TRN
Position of m th particle in space	Time moment $t_m = m\tau$ on timeline
Dimension of a particle's Hilbert space	Twice the number of subsystem's d.o.f. plus one, $2n + 1$
Rank, bond dimension r (dimension of ancillary space)	Square of dimension of effective reservoir, d_{ER}^2
Correlation length, L	Reservoir correlation time, T

$$\ln[\epsilon(r)] \leq \frac{1-\alpha}{\alpha} \left[S_\alpha - \ln\left(\frac{r}{1-\alpha}\right) \right], \quad (9)$$

from which one readily obtains the sufficient bond dimension guaranteeing the arbitrary desired accuracy ϵ :

$$r_{\text{suff}}(\epsilon) = \min_{0 < \alpha < 1} (1-\alpha) e^{-\alpha/(1-\alpha)} \exp(S_\alpha). \quad (10)$$

In the language of TRN, the sufficient rank is the square of minimal dimension of effective reservoir, d_{ER}^2 , which can reproduce all temporal correlations with error ϵ . Therefore, to find d_{ER} one needs to estimate the Rényi entropy S_α of tensor in Fig. 4 considered as a matrix M with 2 multi-indices (l, i_1, \dots, i_m) and (l', i'_1, \dots, i'_m) :

$$M_{(l, i_1, \dots, i_m), (l', i'_1, \dots, i'_m)} = \sum_{i_{m+1}, \dots, i_N} \Psi_{l, i_1, \dots, i_m, i_{m+1}, \dots, i_N} \Psi_{l', i'_1, \dots, i'_m, i_{m+1}, \dots, i_N}^* \quad (11)$$

The Rényi entropy reads [79]:

$$S_\alpha \lesssim \frac{1}{1-\alpha} \ln \frac{[1 + 2n(\gamma\tau)^\alpha]^{T/\tau}}{(1 + 2n\gamma\tau)^{\alpha T/\tau}} \approx 2n\gamma T \frac{(\gamma\tau)^{\alpha-1} - \alpha}{1-\alpha}. \quad (12)$$

The entropy S_α is a measure of the time correlations in TRN. Substituting Eq. (12) in Eq. (10), we obtain the sufficient rank r_{suff} of MP approximation of TRN with desired physical properties (parameters γ , n , T , τ) and accuracy ϵ . On the other hand, the rank of MP approximation is the square of the dimension d_{ER} of the *effective*

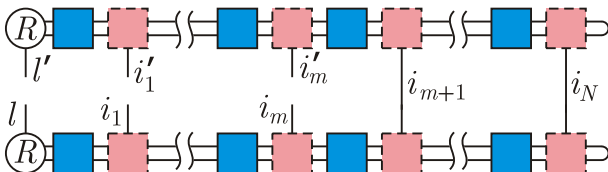


FIG. 4. Reduced matrix of TRN.

reservoir that can reproduce all the features of open dynamics (including memory effects) with accuracy ϵ . Therefore, it is possible to simulate the complex open system dynamics by using the effective reservoir of dimension

$$d_{\text{ER}}(\epsilon) = \min_{0 < \alpha < 1} \frac{\sqrt{1-\alpha}}{\epsilon^{\alpha/2(1-\alpha)}} \exp\left(n\gamma T \frac{(\gamma\tau)^{\alpha-1} - \alpha}{1-\alpha}\right). \quad (13)$$

Once the effective reservoir is constructed, the aggregate $S + \text{ER}$ experiences the semigroup dynamics. This follows from the tensor network representation in Fig. 2. The TRN has a homogeneous structure and so does its MP approximation. The regular structure of building blocks in the time scale means that the same transformation $\mathbb{1} + \tau\mathcal{L}$ acts on $S + \text{ER}$ between the successive times $m\tau$ and $(m+1)\tau$. The GKSL generator \mathcal{L} [54,55] acts on $d_S d_{\text{ER}} \times d_S d_{\text{ER}}$ density matrices and guarantees complete positivity of evolution.

Discussion.—Although the actual environment consists of infinitely many modes, the developed theory facilitates the simulation of complex open system dynamics with a finite dimensional effective reservoir. The sufficient dimension d_{ER} depends on two combinations of physical parameters: $n\gamma T$ and $\gamma\tau$. Figure 5 shows that one can simulate the open dynamics on a classical computer for a wide range of parameters: $n\gamma T$ and $\gamma\tau$, accounting for all potential initial correlations between the system and its environment.

The first illustrative example is a decay of the two-level system (qubit) in a multimode environment [79]. We compare the exactly solvable qubit dynamics, the Markov approximation ($d_{\text{ER}}' = 1$), and the approximation obtained with the reservoir of fixed dimension ($d_{\text{ER}}'' = 2$). Figure 6 shows that the best Markovian approximation cannot reproduce oscillations in the exact dynamics, whereas the approximation with the fixed dimension $d_{\text{ER}}'' = 2$ fits well the exact dynamics when the simulation complexity $d_{\text{ER}} \sim d_{\text{ER}}''$. However, if d_{ER} is several orders of magnitude larger than d_{ER}'' , then the approximation is not able to reproduce memory effects present in the exact solution. Thus, d_{ER} does quantify the complexity of dynamics.

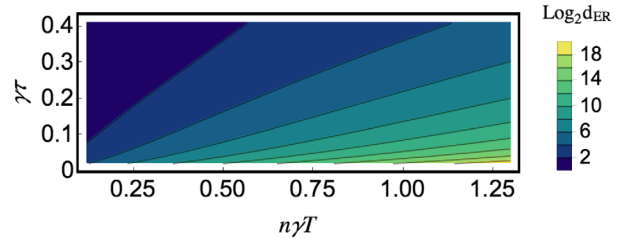


FIG. 5. Number of qubits $\log_2(d_{\text{ER}})$ in effective reservoir, which is sufficient for simulation of open dynamics with accuracy $\epsilon = 0.05$. $n\gamma T$ is dimensionless memory time and $\gamma\tau$ is dimensionless minimal timescale.

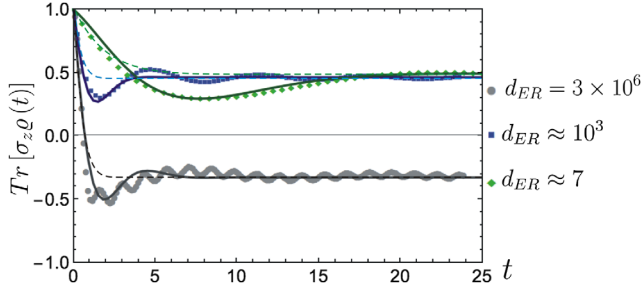


FIG. 6. Typical evolutions of parameter $\text{tr}[\sigma_z \rho(t)]$ of open qubit system $\rho(t)$ for different values of simulation complexity $d_{\text{ER}}(0.05)$ [79]. Dotted lines depict the exact dynamics. Dashed lines depict the best Markov approximations ($d'_{\text{ER}} = 1$). Solid lines are the approximations obtained with the reservoir of fixed dimension $d''_{\text{ER}} = 2$.

The second example is the double quantum dot charge qubit coupled to piezoelectric acoustic phonons [62]. Here, $n = 1$, $T \approx 4\tau$, $\tau = \omega_c^{-1}$, $\gamma = 0.05\omega_c$, and $\omega_c = 83$ GHz is the cutoff frequency of the spectral function. Equation (13) yields $\log_2 d_{\text{ER}} = 4$ for $\epsilon = 0.05$; i.e., the non-Markovian qubit dynamics can be embedded into a Markovian evolution of the very qubit and 4 auxiliary ones.

The third example is the non-Markovian evolution of the qubit due to interaction with the dissipative pseudomode [52,53]: $(d\rho/dt) = -i[H_0, \rho] + \Gamma(a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\})$, where $H_0 = \omega_0\sigma_+\sigma_- + \omega a^\dagger a + \Omega_0\sigma_x(a^\dagger + a)$ and ρ is the density operator for the qubit and the pseudomode. Physical parameters are $n = 1$, $T = \Gamma^{-1}$, $\tau = \omega^{-1}$, $\gamma = \Omega_0\sqrt{n_0 + 1}$, where n_0 is the effective number of photons in the pseudomode. Our result, Eq. (13), estimates where the pseudomode oscillator can be truncated (Fock states with number of photons less than d_{ER}) to reproduce the system dynamics with precision ϵ at any time despite the memory effects and the counterrotating terms in H_0 . In this example, construction of the effective reservoir reduces to the subspace spanned by d_{ER} lowest energy states of the pseudomode because the particular dissipator forces the pseudomode to the ground state.

There are physical scenarios in which the structure of the effective reservoir follows from the model. For instance, in a nitrogen-vacancy center in diamond, the inherent nitrogen (^{14}N) nuclear spin ($I = 1$) serves as an effective reservoir for the electronic spin qubit [42]. In this case, $d_{\text{ER}} = 3$. Similarly, in a composite bipartite collision model [83], d_{ER} is given by the size of an ancillary system. In general, however, the structure of the effective reservoir is to be determined from the experimental data. Reference [56] proposes a machine learning algorithm to reconstruct the generator \mathcal{L} based on a series of repeated measurements on the open system.

Finally, our result is applicable to the influence functional tensor networks in Refs. [63,76], where the analytical solution for open dynamics is not accessible, and provides

the upper bound on the maximum bond dimension, $\lambda_{\text{max}} < d_{\text{ER}}^2$. Conversely, for a fixed computationally tractable size of bond dimension, e.g., $\lambda_{\text{max}} \sim 10^3$, our result provides the region of physical parameters $\gamma\tau$ and $n\gamma T$, for which the algorithm in Ref. [63] definitely works well.

Importantly, the TRN is a multidimensional tensor, so it can be approximated with MP form but also with other constructions like multiscale entanglement renormalization ansatz [84,85] or artificial neural networks [86,87]. The benefit of such networks is that time correlations in the environment do not have to decay exponentially as for the MP approximation.

Conclusion.—We gave a definition of simulation complexity of open quantum dynamics in terms of a reservoir's effective dimension. We showed that the tensor networks' approach can be utilized to analyze memory effects in open dynamics. We provided an estimation of simulation complexity using a set of physical parameters. Our estimation is universal and fits well the arbitrary open quantum dynamics with finite memory.

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