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Suppressing the entanglement growth in matrix-product-state evolution of quantum systems through nonunitary similarity transformations

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In strong-coupling regimes, quantum dynamical effects can alter conventional physics described by perturbation theories, but the dynamical simulations of these quantum systems using matrix product states—such as multi-level vibronic systems that are relevant to energy and electron transfer reactions—suffer from rapid entanglement growth during their real-time evolution, impeding explorations of spectra, dynamics, and kinetics. We examine the possibility of using non-unitary transformations to alter dynamical entanglement growth in matrix-product-state simulations of quantum systems, using the spin-Boson model to showcase the reduced entanglement. By appropriately choosing the transformation, the entanglement growth rate is suppressed, improving the efficiency of quantum dynamical simulations. Entanglement control is achieved by the transformation-induced biased transitions among the system quantum states, and by “projecting” (approximately) the system quantum state to one of the eigenstates of the system-bath coupling operator, thus controlling the energy exchange between the system and bath. The transformation can be applied to quantum many-body systems, including spin chains and multi-level vibronic systems; the approach improves the numerical efficiency of the MPS simulations.

I. INTRODUCTION

Understanding and controlling quantum dynamics are important for many areas ranging from many-body physics to quantum computations [1–8]. While numerical techniques based on matrix product states (MPS) are a powerful tool to study the time evolution of quantum systems, accurate determination of the dynamics of quantum systems remains a long-standing problem, due to the complexities caused by quantum entanglement [9–17]. In the low-entanglement regime, quantum dynamics can be simulated efficiently using tensor-network techniques [18–25] if the components of the system are not strongly coupled or if the system is close to its ground state (assuming no phase transition occurs). However, when the system is far from equilibrium the entanglement entropy may grow linearly in time [26–29], necessitating exponentially growing dimensions for the MPS, and impeding numerically accurate simulations. Unfortunately, many important physical processes exhibit high-entanglement during their dynamical evolution. For example, the study of quantum thermalization is an important challenge in theoretical physics. Recent studies found that the thermalization dynamics requires a description beyond the semi-classical Boltzmann theory, and requires long-time dynamical simulations that are obstructed by the linear growth of entanglement [30]. Also, in the field of cavity quantum electrodynamics [31–34], where light and matter are strongly coupled, the electronic-vibronic degrees of freedom of a

molecular ensemble are strongly coupled to multiple cavity modes, producing highly-entangled dynamical evolution and strongly-perturbed chemical reactivity [35–37]. Molecular and solid-state nano-junctions provide another example, where strong electronic-vibrational entanglement can significantly change the transport kinetics and device performance. For example, the low-bias current in single-molecule junctions and single-walled nanotube quantum dots can be suppressed [38], and this effect is known as the Franck-Condon (FC) blockade [39, 40].

Using MPS to study the quantum dynamics of these highly-entangled systems has attracted intense interest [25, 41–47]. Most proposed methods use global basis transformations to reduce entanglement in the MPS, since local on-site unitary transformations cannot change the entanglement of a quantum state. These proposed methods that use global basis transformations, however, require that the Hamiltonians have some specific properties (e.g., linear couplings and a harmonic bath for a system-bath model).

In this paper, we introduce a general local non-unitary similarity transformation for open-system Hamiltonians and examine its influence on the entanglement growth rate during the real-time evolution of the open quantum system. The transformation produces a family of Hamiltonians characterized by a continuous parameter that controls the entanglement growth rate. By adjusting the parameter, one can suppress the entanglement growth in matrix product states during the real-time evolution of highly entangled quantum systems. This method is general and can be applied to almost any Hamiltonian, including open quantum system Hamiltonians with an anharmonic bath or non-linear system-bath couplings. The approach has the potential to enable efficient non-

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Markovian simulations of large open quantum systems, including multi-chromophore exciton chains in strong-coupling regimes [48, 49]. The effect of non-unitary similarity transformations on the simulation efficiency has been explored extensively in the electronic-structure literature [50–53], but is much less-well explored for quantum dynamics. Such a transformation not only sheds light on improving the efficiency of numerical simulations by tuning the entanglement growth in *time-dependent* simulations, but also provides a promising way to explore the hidden structure of the entanglement growth.

II. THEORY

The Hamiltonian of a system-bath quantum system is

$$\hat{H} = \hat{H}_s + \hat{H}_{sb} + \hat{H}_b \quad (1)$$

where $\hat{H}_b$ describes a collection of bosons (interacting or non-interacting) and $\hat{H}_{sb}$ contains couplings between the system and the bosons, it is possible to obtain a new Hamiltonian $\mathcal{H}$ using a similarity transformation: $\mathcal{H} = e^{\hat{S}} \hat{H} e^{-\hat{S}}$. Here, we choose $\hat{S}$ to be Hermitian, in contrast to the usual choice that $\hat{S}$ is anti-Hermitian. Thus, $e^{\hat{S}}$ is non-unitary: $(e^{\hat{S}})^\dagger = e^{\hat{S}}$. In the similarity-transformed frame, using an evolution operator $\mathcal{U}_t = e^{-i\mathcal{H}t}$ ($\hbar = 1$), the time evolution of the expectation value (which is transformation-invariant) for an observable $\hat{A}$ is given by

$$\langle \hat{A} \rangle(t) = \langle \psi_0 | e^{\hat{S}} \mathcal{U}_t^\dagger e^{-\hat{S}} \hat{A} e^{-\hat{S}} \mathcal{U}_t e^{\hat{S}} | \psi_0 \rangle. \quad (2)$$

We recognize that $e^{-\hat{S}} \mathcal{U}_t e^{\hat{S}} | \psi_0 \rangle$ is the state at time t in the original frame (i.e., without the similarity transformation), and $\mathcal{U}_t e^{\hat{S}} | \psi_0 \rangle$ is the state at time t in the transformed frame.

A judiciously chosen $\hat{S}$ can alter the nature of the Hamiltonian and favor the simulations. We will use the zero-bias spin-boson model as an example. This Hamiltonian is a prototypical model to investigate electron and energy transfer in condensed media:

$$\hat{H} = \Delta \hat{\sigma}_x + \sum_n c_n \hat{A} \otimes (\hat{a}_n^\dagger + \hat{a}_n) + \sum_n \omega_n \hat{a}_n^\dagger \hat{a}_n. \quad (3)$$

Δ is the coupling between the two spin states $|\uparrow\rangle$ and $|\downarrow\rangle$, and c_n and ω_n are the coupling strength and the vibrational frequency associated with the n -th boson, respectively. We use $\hat{A} = \hat{\sigma}_z$ below. The simplest choice of $\hat{S}$ is $\hat{S} = \beta \hat{\sigma}_z$ with β constant. Other forms of $\hat{S}$ are possible (e.g., $\beta \sum_n \hat{a}_n^\dagger \hat{a}_n$). We choose $\beta \hat{\sigma}_z$ as a proof of principle. The transformed Hamiltonian is then:

$$\mathcal{H}(\beta) = e^{\beta \hat{\sigma}_z} \hat{\sigma}_x e^{-\beta \hat{\sigma}_z} + \sum_n c_n \hat{\sigma}_z \otimes (\hat{a}_n^\dagger + \hat{a}_n) + \sum_n \omega_n \hat{a}_n^\dagger \hat{a}_n. \quad (4)$$

To better understand the effect of the similarity transformation, we explicitly specify the matrix elements of

$$e^{\beta \hat{\sigma}_z} \hat{\sigma}_x e^{-\beta \hat{\sigma}_z}:$$

$$e^{\beta \hat{\sigma}_z} \hat{\sigma}_x e^{-\beta \hat{\sigma}_z} = \begin{pmatrix} 0 & e^{2\beta} \\ e^{-2\beta} & 0 \end{pmatrix}. \quad (5)$$

This matrix indicates that, after the transformation, the transition from $|\downarrow\rangle$ to $|\uparrow\rangle$ is enhanced, while the reverse transition is weakened. These incommensurate transition strengths are reminiscent of the Aubry-André-Harper model [54, 55], which can be realized in optical-lattice experiments.

If the initial state of the spin is an eigenstate of $\hat{\sigma}_z$ (e.g., $|\uparrow\rangle$), which is the case for most open quantum system simulations, the effect of the non-unitary transformation $e^{\beta \hat{\sigma}_z}(\cdot)e^{-\beta \hat{\sigma}_z}$ is, to some extent, to freeze the spin in its initial eigenstate. This freezing effect is favorable for matrix-product-state simulations of open quantum systems, since the initial state often has the lowest entanglement. The parameter β characterizes a family of Hamiltonians $\mathcal{H}(\beta)$, which are related to each other by the non-unitary transformation. It is expected that some of the Hamiltonians (i.e., for some special values of β) in this family can show slower growth of entanglement during the evolution than the original Hamiltonian $\mathcal{H}(0)$.

The transformed Hamiltonian (Eq. (4)) describes a fictitious system which is related to the actual system (Eq. (3)) by the non-unitary transformation $e^{\beta \hat{\sigma}_z}(\cdot)e^{-\beta \hat{\sigma}_z}$. The dynamics of the fictitious system can be back-transformed to the dynamics of the actual system by the reverse transformation $e^{-\beta \hat{\sigma}_z}(\cdot)e^{\beta \hat{\sigma}_z}$. The density matrix of the fictitious system $\rho_f(t) = \mathcal{U}_t e^{\hat{S}} | \psi_0 \rangle \langle \psi_0 | e^{\hat{S}} \mathcal{U}_t^\dagger$ is related to the density matrix of the actual system $\rho(t)$ by

$$\rho(t) = \frac{e^{-\beta \hat{\sigma}_z} \rho_f(t) e^{\beta \hat{\sigma}_z}}{\text{tr}[e^{-\beta \hat{\sigma}_z} \rho_f(t) e^{\beta \hat{\sigma}_z}]}. \quad (6)$$

This relation indicates that the fictitious reduced density matrix of the spin $\text{tr}_B \rho_f(t)$ is still a legitimate density matrix—after a normalization: $\rho_f(t) \rightarrow \rho_f(t)/\text{tr}(\rho_f(t))$. The entanglement of the fictitious system density matrix can still be defined by the singular value decomposition of the wave function expansion coefficient tensor in an orthonormal basis. The entanglement of the fictitious system wave functions has no simple relationship to the entanglement of the actual wave function, in contrast to the simple equation (6) that describes the relationships for the wave functions themselves. This necessitates numerical simulations to explore the properties of entanglement growth for the Hamiltonian family $\{\mathcal{H}(\beta)\}$. We will use the zero-bias spin-boson model to show the entanglement growth for different $\mathcal{H}(\beta)$ s in the result section.

III. NUMERICAL RESULTS

We use the Debye spectral density $J(\omega) = \frac{\eta \omega_c \omega}{\omega_c^2 + \omega^2}$ for the spin-boson model where η and ω_c describe the coupling strength and the characteristic frequency of the

Parameter	Physical Quantity
Δ	spin coupling
$\eta = 4\Delta$	system-bath coupling
$\omega_c = 1\Delta$	characteristic bath frequency
$k_B T = 2\Delta$	bath temperature
$\pm\omega_{\max} = \pm 12.7324\Delta$	frequency cutoffs in the discretization
$N_{\text{mode}} = 200$	the number of discretized bath modes

TABLE I. The reduced Planck constant $\hbar$ is set to be 1. η , ω , T and $\omega_{\max}$ are in the unit of Δ (spin coupling). $\pm\omega_{\max}$ are the upper and lower limits used in the discretization of the Debye spectral density.

bath modes, respectively. To include finite-temperature effects, the spectral density is thermalized by using a temperature-dependent factor and extending the frequency axis to negative infinity following Refs [56, 57]. The thermalized spectral density is discretized (with maximum and minimum frequencies $\omega_{\max}$ and $-\omega_{\max}$) to generate the Hamiltonian in Eq. (3), which is then transformed to the β -dependent Hamiltonian in Eq. (4). No further basis transformation (e.g., the chain transformation [41, 42]) is used. Thus, the topology of the Hamiltonian is a “star” [46] which is known to have a rapidly growing entanglement with time [46]. The parameters used for the spin-boson model are shown in Table I. The parameters used have values typical for open quantum system simulations. The initial state of the system and the bath is set to be $|\uparrow\rangle \otimes |0, 0, \dots\rangle$. The second-order time-evolving-block-decimation (TEBD2) method [58] with swap gates [59] is used to propagate the wave function. Note that the evolution operators used in TEBD2 are nonunitary, since the Hamiltonian itself is non-Hermitian. The non-unitary evolution operators destroy the canonical form of a MPS. To restore the canonical form and to obtain the correct singular values, we perform a canonicalization procedure after each evolution step [58].

Fig. 1 shows the time-dependent polarization $\langle\hat{\sigma}_z\rangle$ obtained by the reverse transformation of Eq. (6). The results generated from the fictitious systems using the reverse transformation agree well with the actual dynamics ($\beta = 0$, the thick line), validating the similarity-transformation formalism. The lines with $\beta > 0.8$ and $\beta < -0.8$ are not shown in Fig. 1, since they begin to deviate from the correct dynamics.

We also plot the fictitious dynamics (i.e., $\text{tr}(\rho_f(t)\sigma_z)$) in Fig. 2 to demonstrate the freezing effect: with $\beta > 0$, the population on $|\uparrow\rangle$ in the fictitious system has slower transfer than in the actual system. A sufficiently large β (0.8) completely freezes the spin in its initial state ($|\uparrow\rangle$). With $\beta < 0$, the transfer from $|\uparrow\rangle$ to $|\downarrow\rangle$ is accelerated and the reverse transfer is obstructed. These results are consistent with the analysis in the Introduction.

Fig. 3 shows that members of the Hamiltonian family $\{\mathcal{H}(\beta)\}$ have different entanglement growth rates. For positive β s, the entanglement grows more slowly with

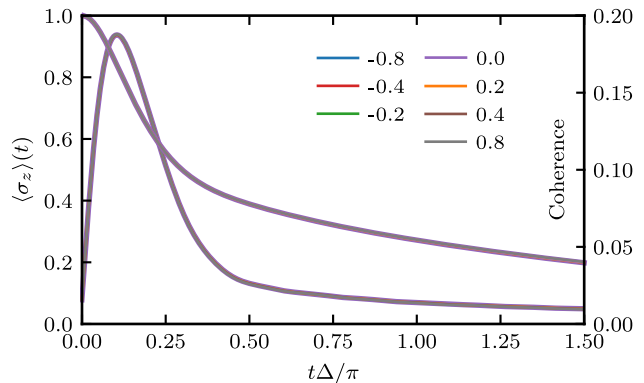


FIG. 1. The dynamics of the polarization $\langle\sigma_z\rangle$ and the real part of non-diagonal $\rho(t)$ elements for different β values. The threshold for singular values is 10^{-5} . The time step is 0.005. If β is larger than 0.8 (or smaller than -0.8), the dynamics begin to deviate from the exact line ($\beta = 0$). All of the lines overlap.

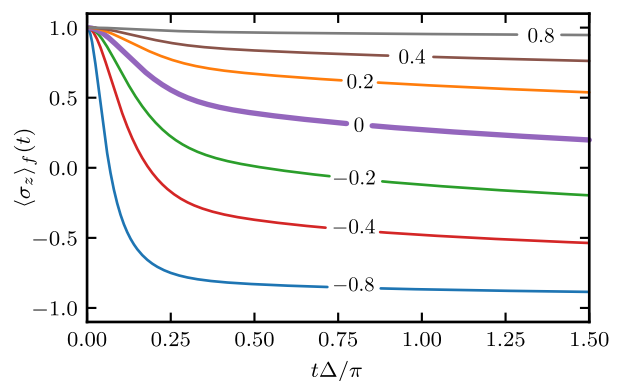


FIG. 2. The dynamics of $\text{tr}[\sigma_z \rho_f(t)]$ without the reverse transformation (Eq. (6)). The numbers indicate β values. The population transfer from $|\uparrow\rangle$ to $|\downarrow\rangle$ is slowed with $\beta > 0$, while negative β values accelerate the transfer. The thick purple curve indicates the population dynamics of the actual system with $\beta = 0$.

time when β is larger. For negative β values, a more negative β value (e.g., -0.2 to -0.4) causes the entanglement growth of the fictitious systems to be faster, but such an acceleration reaches its maximum at a critical value of β (in this example, at $\beta \sim -0.4$). If β continues to become more negative (e.g., $\beta = -0.8$), the entanglement growth can be slower than its maximum speed ($\beta \sim -0.4$). This is because, with a very negative β , the population in $|\uparrow\rangle$ is transferred quickly to $|\downarrow\rangle$, and it remains in $|\downarrow\rangle$, which disentangles the spin and the bath.

The similarity transformation presented here suppresses the entanglement growth rate in the evolving quantum systems by almost 50%. The singular values on the bonds (of the MPS) that are spatially close to the transformed site are significantly affected by the transformation: the singular values are localized on the first few eigenstates of the reduced density matrix. The bonds

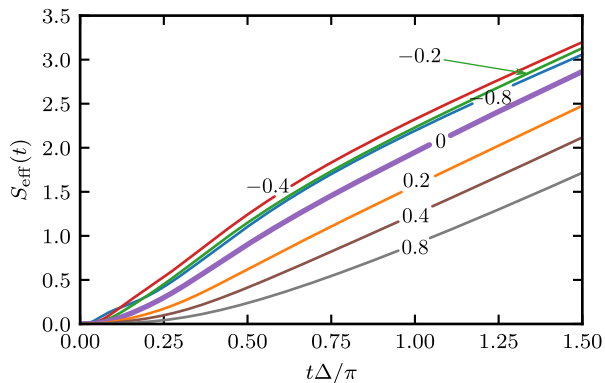


FIG. 3. Entanglement growth during the evolution of the spin-boson model for different β values. The effective entanglement S_{eff} is a function of the von Neumann entanglements $\{S_n\}$ on every bond of a matrix product state: $S_{\text{eff}} = \ln(\frac{1}{L-1} \sum_n e^{3S_n})^{1/3}$ where L is the number of bonds [44]. We use the binary logarithm to calculate the von Neumann entanglement entropy of each bond: $S_n = -\sum_i s_i^2 \log_2 s_i^2$ where s_i is the i -th singular value for the n -th bond.

far from the transformed site are less affected. We expect a more significant reduction of entanglement if a global transformation is applied to a quantum many-body Hamiltonian. For example, for a coupled spin chain, a global similarity transformation impacts every spin. Consequently, after the transformation, each bond connecting adjacent spins is dominated by a few large singular values, reducing the entanglement in the MPS more significantly than in single-spin systems. To show the advantage of the global transformation for multi-spin systems (or coupled chromophores for electron and energy transfer [60]), we use a GHZ [61] state of a 10-spin system as an example. The GHZ state is $\frac{|0\rangle^{\otimes 10} + |1\rangle^{\otimes 10}}{\sqrt{2}}$. Applying the transformation $e^{0.1\hat{\sigma}_z(\cdot)}e^{-0.1\hat{\sigma}_z}$ to the first 0, 1, 2, ..., 10 spins, the entanglement entropies (measured using the definition in the caption of Fig. 3) of the states obtained with different numbers of transformations are 1.04, 1.01, 0.93, 0.82, 0.69, 0.57, 0.45, 0.36, 0.28, 0.22, and 0.17. A relationship between the reduced entanglement and the number of transformed spins is clearly observed. The transformation is not limited to open quantum systems or spin systems, but may be useful for simulations of other quantum many-body systems, such as those that describe the dynamics of electron-phonon systems and correlated-electron systems [62].

The similarity transformation $e^{\beta\hat{\sigma}_z(\cdot)}e^{-\beta\hat{\sigma}_z}$ has alternatives. The generator of the transformation can be $\sigma_+ = \sigma_x + i\sigma_y$, $\sigma_- = \sigma_x - i\sigma_y$, and any combination of their sum and product. These alternative transformations indicate the potential of the similarity-transformation method described here.

The entanglement suppression from the particular choice of the transformation $e^{\beta\hat{\sigma}_z(\cdot)}e^{-\beta\hat{\sigma}_z}$ used here arises from the suppressed transition between the two eigenstates of the system component of the system-bath inter-

action term $\hat{A} = \hat{\sigma}_z$ (see Eq. (5)). The transformed wave function of the entire system (spin and bath) $e^{\beta\hat{\sigma}_z}|\psi(t)\rangle$ is less entangled because the spin (the system) tends to remain in one of the eigenstates of $\hat{A} = \hat{\sigma}_z$. For general system-bath interactions, for example, $\hat{A} = x\hat{\sigma}_x + z\hat{\sigma}_z$ where x and z are scalars, the transformation $e^{\beta\hat{A}(\cdot)}e^{-\beta\hat{A}}$ can be an initial choice of the optimal similarity transformation, since it “projects” (approximately) the state of the spin to one of the eigenstates of the coupling operator $\hat{A} = x\hat{\sigma}_x + z\hat{\sigma}_z$, reducing the energy exchange between the spin and the bath. Our numerical tests show that this transformation ($e^{\beta\hat{A}}$) is better than other combinations of $\hat{\sigma}_z$ and $\hat{\sigma}_x$ for the suppression of growing entanglement.

Large $|\beta|$ values could increase the numerical errors in the simulations. A large $|\beta|$ values requires a smaller singular-value threshold to recover the original density matrix, as in Eq. (6). An empirical value for the optimal β is ~ 0.8 , which suppresses the population on $|\uparrow\rangle$ to $\sim 20\%$ of its original value.

IV. CONCLUSION

By applying a specific similarity transformation to a quantum system, we introduced a family of non-Hermitian Hamiltonians and explored the different growth rates of entanglement numerically for the evolution of open quantum systems. The similarity transformation controls the transitions among the quantum states of the system. The parameter (β) in the transformation determines how the transitions are diminished or enhanced. The quantum-state transition enhancement and suppression can be tuned so that the quantum states of the system and the bath are nearly disentangled during the evolution, suppressing the growth of matrix product state entanglement. Recent studies find that the dynamics from the $\mathcal{PT}$ (parity-time) and anti- $\mathcal{PT}$ symmetric Hamiltonians can produce reduced entanglement in the evolution of the system-bath dynamics [63, 64]. Our result is consistent with the findings in those studies. The similarity transformation introduced here is simple and produces pronounced effects on the growth rate of entanglement, even for a single-spin Hamiltonian. The numerical advantages can be further manifested in simulations of non-Markovian dynamics for large and strongly-coupled multi-state systems, where large entanglement prohibits long-time simulations [40, 44, 65]. The slow growth of entanglement is favorable for MPS simulations, but is not limited to open quantum systems.

Future studies can explore other similarity transformations that may further slow the growth of entanglement during a simulation. Combining the similarity transformation and basis transformations (e.g., chain transformations) [41, 44, 46, 66] is also possible to change the entanglement growth rate even further. It is also of interest to study the effects of similarity transformations on other exact and approximate numerical methods, including the hierarchical equation of motion, quasi-adiabatic

path integral, and quantum master equations.

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