Suppressing the entanglement growth in TD-DMRG simulations of quantum systems

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Introduction

Dynamical simulations of quantum systems suffer from rapid entanglement growth during real-time evolution. We examine the possibility of using similarity transformations to alter dynamical entanglement growth in matrix-product-state simulations of quantum systems.

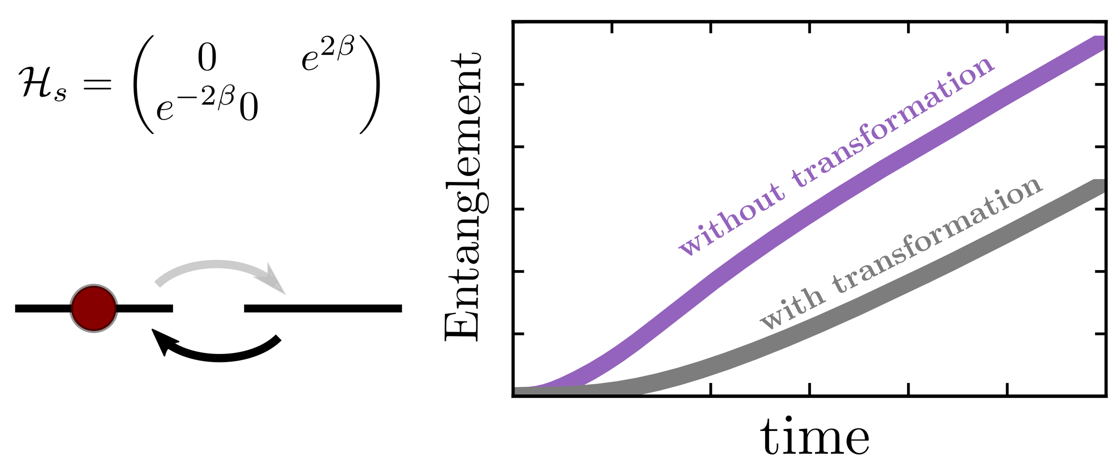

Figure 1: Non-unitary transformations can reduce entanglement growth speed.

By appropriately choosing the similarity transformation, the entanglement growth rate is suppressed, improving the numerical efficiency. It can be applied to general quantum-many-body systems.

Theory

A prototypical model to investigate electron and energy transfer in condensed media:

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

We can obtain a new Hamiltonian $\mathcal{H}$ using a similarity transformation: $\mathcal{H} = e^{\hat{S}}\hat{H}e^{-\hat{S}}$. $\hat{S}$ is Hermitian which makes $e^{\hat{S}}$ non-unitary: $(e^{\hat{S}})^\dagger = e^{\hat{S}}$. Using an evolution operator in the transformed frame $\mathcal{U}_t = e^{-i\mathcal{H}t}$, the evolution of the of an observable (which is transformation-invariant) $\hat{A}$ is

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

$e^{-\hat{S}}\mathcal{U}_t e^{\hat{S}} |\psi_0\rangle$ 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 in the transformed frame.

A good $\hat{S}$ can change the nature of the Hamiltonian and favors the numerical efficiency. The simplest choice is $\hat{S} = \beta\hat{\sigma}_z$. The transformed Hamiltonian is then:

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

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

After the transformation, the transition from $|\downarrow\rangle$ to $|\uparrow\rangle$ is enhanced, and the reverse transition is weakened. The dynamics of the system can be obtained by

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

Numerical results

The spin-boson model with a Debye bath is used to illustrate the effect of the nonunitary transformation.

Actual density matrix dynamics

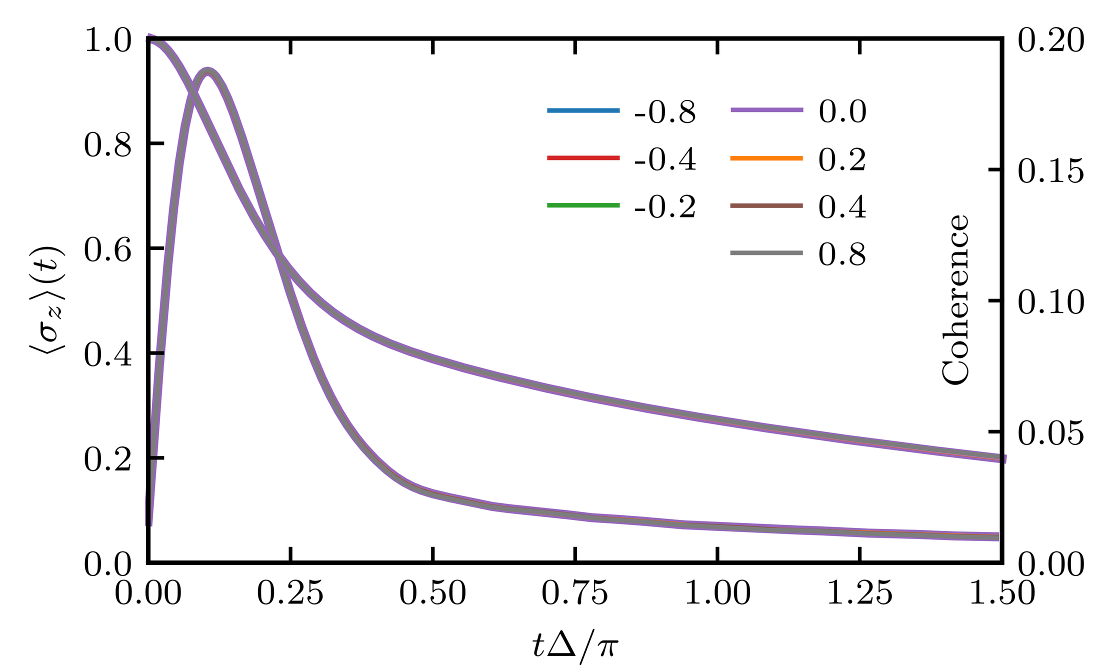

Figure 2: The dynamics of the polarization $\langle\sigma_z\rangle$ and coherence of $\rho(t)$ with different βs.

Fig. 2 shows the agreement of the dynamics between the transformed and non-transformed Hamiltonian.

Transformed population dynamics

The fictitious dynamics (i.e., $\mathrm{tr}(\rho_f(t)\sigma_z)$) in Fig. 3 shows a freezing effect: with $\beta > 0$, the population on $|\uparrow\rangle$ in the fictitious system has slower transfer than the actual system. A large enough 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.

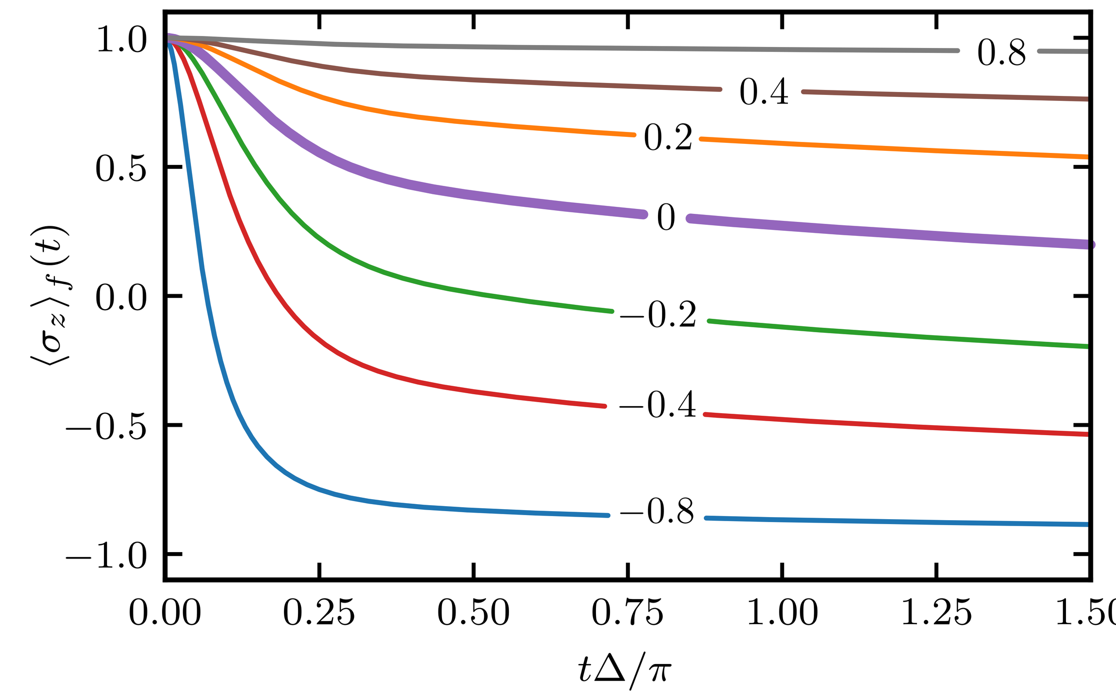

Figure 3: The dynamics of $\mathrm{tr}[\sigma_z\rho_f(t)]$ without the reverse transformation with different β values.

Suppressed entanglement growth

Fig. 4 shows the transformed Hamiltonians ⊙ have different entanglement growth rates. Positive βs cause entanglement to grow slowly while Negative βs cause the entanglement growth of the fictitious systems to be faster, but such an acceleration reaches its maximum at a critical value of β (at $\beta \sim -0.4$).

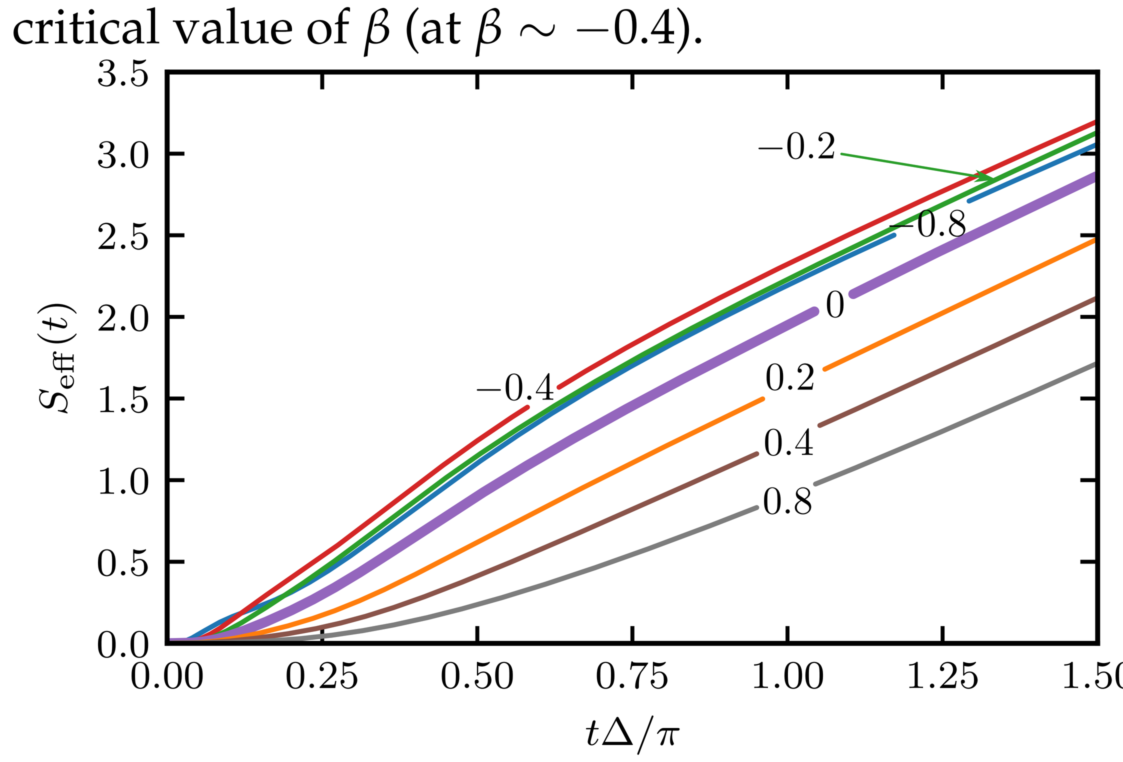

Figure 4: The entanglement growth dynamics for different βs.

More general system: a spin chain

A more significant reduction of entanglement can be achieved when applying a global transformation to a quantum many-body state. We consider a GHZ state of a 10-spin system and apply the transformation $e^{0.1\hat{\sigma}_z}$ to the first 0, 1, 2, ..., and 10 spins. The GHZ state is $\frac{|0\rangle^{\otimes 10} + |1\rangle^{\otimes 10}}{\sqrt{2}}$.

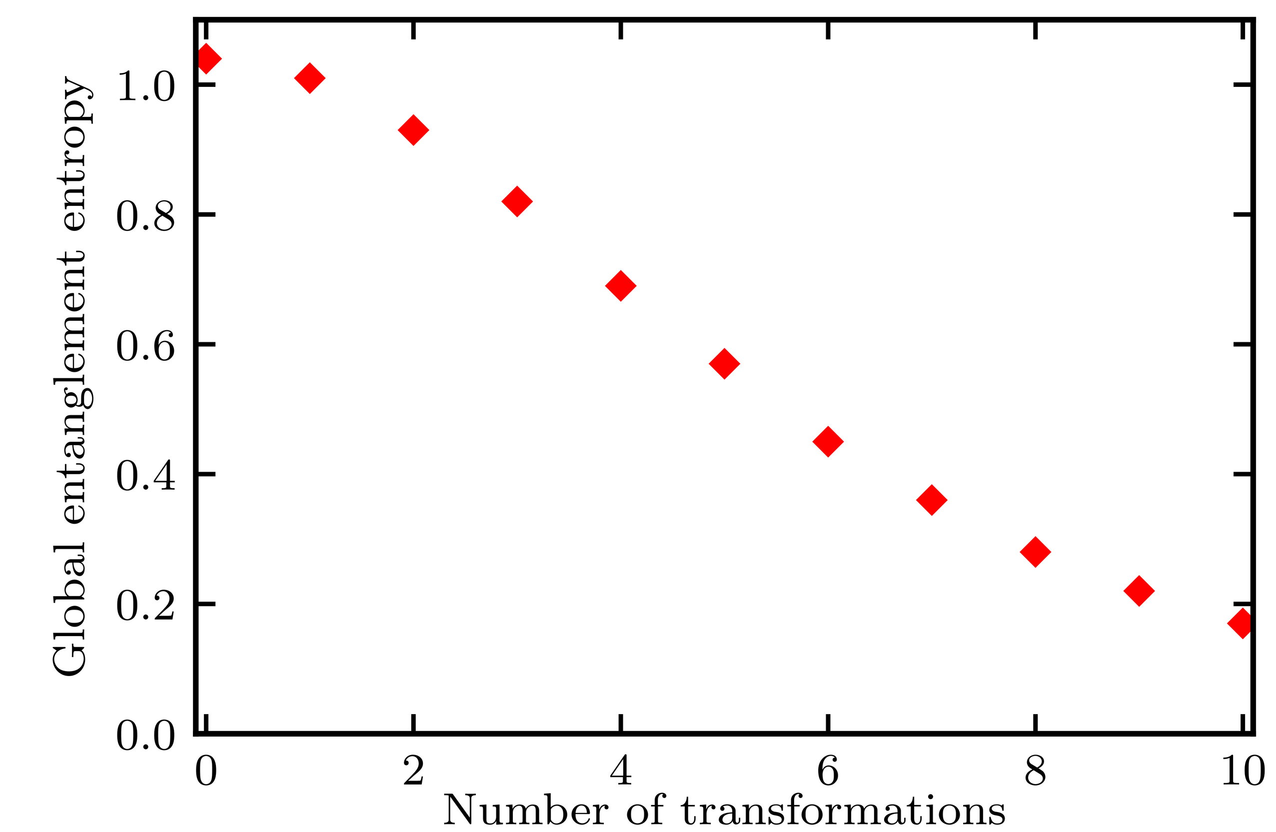

Figure 5: The entanglement reduction for different number of transformations.

Conclusions

Similarity transformations can control the transitions among the quantum states and the transition enhancement and suppression can be tuned so that the system and the bath are nearly disentangled, slowing down the growth of matrix product state entanglement.

References

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Acknowledgments

This material is based upon work supported by the National Science Foundation under Grant No. 1955138. We thank Jonathon L. Yuly for stimulating discussions.