

Time evolution of controlled many-body quantum systems with matrix product operators

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We present a method for describing the time evolution of many-body controlled quantum systems using matrix product operators (MPOs). Existing techniques for solving the time-dependent Schrödinger equation with an MPO Hamiltonian often rely on time discretization. In contrast, our approach uses the Magnus expansion and Chebyshev polynomials to model the time evolution and the MPO representation to efficiently encode the system's dynamics. This results in a scalable method that can be used efficiently for many-body controlled quantum systems. We apply this technique to quantum optimal control, specifically for a gate synthesis problem, demonstrating that it can be used for large-scale optimization problems that are otherwise impractical to formulate in a dense matrix representation.

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I. INTRODUCTION

The time-dependent Schrödinger equation (TDSE) is fundamental in quantum mechanics, as it governs the time evolution of quantum systems. Solving the TDSE accurately is crucial for the development of quantum technologies, understanding quantum dynamics, and simulating physical processes. In fields such as quantum computing [1], quantum simulation [2], and quantum control [3], precise solutions to the TDSE are required for the manipulation and generation of quantum states and unitary transformations. Furthermore, solving the TDSE is crucial for the understanding of many-body quantum physics [4], where the interactions between particles give rise to emergent phenomena such as entanglement or quantum phase transitions [5].

However, this is a challenging task due to the exponential growth of the Hilbert space with the system size. As a result, storing and manipulating state vectors and Hamiltonians become infeasible for large systems. If the system presents localized interactions, we can encode the information of the system's Hamiltonian in a tensor network like a matrix product operator (MPO) [6–14], which allows for a scalable representation of the system.

Tensor networks have been used widely [15–24] in the study of the time evolution of quantum systems, focusing mainly on the manipulation of high-dimensional quantum states. These methods make use of matrix product states (MPSs) to efficiently represent the state and reduce computational complexity, allowing them to address multiple problems in condensed-matter physics and quantum chemistry. In this work we extend this approach by developing a method that encodes the unitary evolution of a controlled quantum system

in a tensor network, an MPO, which is useful for applications like quantum control, where the unitary evolution operator is essential for the design of gates in quantum computers.

The current uses of MPO Hamiltonians to model the time evolution of many-body quantum systems often rely on time-independent Hamiltonians in order to use methods like Trotter-Suzuki decomposition or commutator-free Magnus expansion [25–30], which generally consider efficient state evolution instead of the unitary evolution. In this work we develop a fundamentally different method to solve the TDSE using tensor networks by representing the Hamiltonian as an MPO. Our method considers the continuous time interval and uses the Magnus expansion and Chebyshev polynomials to approximate the unitary operator that solves the TDSE in a scalable manner.

We apply our method to quantum optimal control problems, where finding the optimal control pulses to synthesize unitary gates or to prepare quantum states is crucial. Traditional quantum optimal control methods like the gradient ascent pulse engineering (GRAPE) [31] and chopped random basis (CRAB) algorithms [32] are also limited by the exponential scaling, although tensor network approaches have been explored to mitigate this issue [33–36]. By integrating the method developed in this paper with the quantum control via polynomial optimization (QCPOP) method [37,38], which reformulates control problems as polynomial optimization problems, we achieve a scalable and efficient framework for solving quantum optimal control problems.

II. SOLUTION OF THE TDSE

We want to solve the Schrödinger equation (where we let $\hbar = 1$)

$$\frac{\partial}{\partial t}U(t) = -iH(t)U(t), \quad U(0) = I. \quad (1)$$

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We study a time-dependent Hamiltonian that is subject to a control function $u(t)$. Therefore, we have

$$H(t) = H_0 + u(t)H_c, \quad (2)$$

where H_0 is the free Hamiltonian and H_c the control Hamiltonian.

The solution to Eq. (1) can be written as the Magnus expansion [39,40]

$$U(T) = \exp[\Omega^{(\infty)}(T)], \quad (3)$$

where

$$\Omega^{(\infty)}(T) = \sum_{i=1}^{\infty} \Omega_i(T). \quad (4)$$

If we let $H_j \equiv H(t_j)$ we can write the first terms of this sum as

$$\Omega_1(T) = -i \int_0^T dt_1 H_1, \quad (5)$$

$$\Omega_2(T) = \frac{-1}{2} \int_0^T dt_1 \int_0^{t_1} dt_2 [H_1, H_2], \quad (6)$$

$$\begin{aligned} \Omega_3(T) = & \frac{i}{6} \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 [[H_1, [H_2, H_3]] \\ & + [[H_1, H_2], H_3]]. \end{aligned} \quad (7)$$

The nested commutators enclose the time-ordering effects of the system, and absolute convergence is ensured [41] if

$$\int_0^T \|H(t)\|_2 dt < \pi. \quad (8)$$

Furthermore, we can approximate the exponential of the Magnus series truncated to a certain order n through a Chebyshev polynomial [42] as

$$U(T) \approx \exp(\Omega^{(n)}) \approx J_0(1)\mathbb{I} + 2 \sum_{i=1}^p J_i(1)T_i, \quad (9)$$

where p is the truncation order, $J_i(x)$ is the Bessel function, and T_i is the Chebyshev polynomial element defined recursively as

$$T_0 = \mathbb{I}, \quad T_1 = \Omega^{(n)}, \quad T_{i+1} = 2\Omega^{(n)}T_i + T_{i-1}. \quad (10)$$

III. MATRIX PRODUCT OPERATORS

In this section we will go through the main concepts underlying matrix product operators to see how their structure changes when we do operations with them. For a more detailed introduction to tensor networks, and MPOs specifically, we recommend Refs. [6,7,10].

If we assume the physical system we are controlling is an N -body system and has some type of localized interactions, we can write the Hamiltonian terms as MPOs in an efficient manner. By localized interactions we mean that each site interacts only with neighboring sites, typically those adjacent or within a short range. This characteristic leads to sparse operator structure, with low entanglement, which results in a small MPO bond dimension, which makes the MPO representation

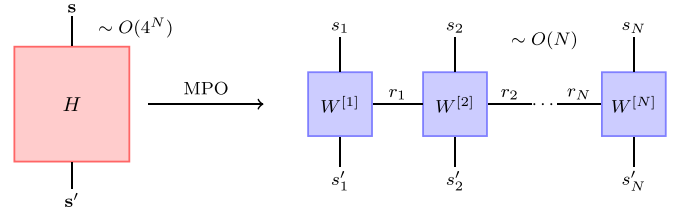


FIG. 1. MPO decomposition of an N -qubit Hamiltonian.

efficient. We let

$$H_0 = \sum_{\mathbf{s}, \mathbf{s}'} W_{s_1 s'_1}^{[1]} \cdots W_{s_N s'_N}^{[N]} |\mathbf{s}\rangle \langle \mathbf{s}'|, \quad (11)$$

where $|\mathbf{s}\rangle \equiv |s_1 s_2 \cdots s_N\rangle$. For $i \in \{2, \dots, N-1\}$, $W^{[i]}$ are order 4 tensors with dimensions $d_i \times d'_i \times r_i \times r'_i$; $W^{[1]}$ has dimensions $d_1 \times d'_1 \times 1 \times r_1$ and $W^{[N]}$ has dimensions $d_N \times d'_N \times r_N \times 1$, both of which impose the boundary conditions.

We will work with qubits so we let the physical dimensions be $d_i = d'_i = 2$ for all tensors, which implies $s_i, s'_i \in \{0, 1\}$ for all i . The artificial bond dimensions r_i and r'_i represent the interactions between sites and they can change depending on the system.

We can also see the tensors as matrices $W_{s_2 s'_2}^{[2]}, \dots, W_{s_{N-1} s'_{N-1}}^{[N-1]}$ of size $r_i \times r'_i$, a row vector $W_{s_1 s'_1}^{[1]}$ of size $1 \times r_1$, and a column vector $W_{s_N s'_N}^{[N]}$ of size $r_N \times 1$. We illustrate the MPO decomposition in Fig. 1, where we show at a high level how we reduce the number of elements from $O(4^N)$ to $O(N)$ if we fix the physical and bond dimensions needed to describe the Hamiltonian by finding local tensors $W^{[i]}$ for each site. The sizes of s_i and s'_i are fixed as they are physical quantities, but the size of the bond dimensions r_i can vary; consequently, the accuracy of the MPO representation also varies.

If we let the bond dimension for all tensors be $r = 3$, then we can visualize the central tensors as

$$W_{s_i s'_i}^{[i]} = \begin{pmatrix} \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} & \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} & \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} \\ \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} & \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} & \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} \\ \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} & \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} & \begin{pmatrix} * & * \\ * & * \end{pmatrix}_{s_i s'_i} \end{pmatrix}.$$

The initial and final tensors follow similarly but in the shape of row and column vectors.

We also let

$$H_c = \sum_{\mathbf{s}, \mathbf{s}'} V_{s_1 s'_1}^{[1]} \cdots V_{s_N s'_N}^{[N]} |\mathbf{s}\rangle \langle \mathbf{s}'|. \quad (12)$$

Let us now look at how to perform operations with MPOs. We consider scalar products, sums, and products, which are all the necessary ingredients to do the Magnus expansion and the Chebyshev approximation, as we show in Appendix A.

The scalar product only affects one of the tensors, the first one, for example, so for a scalar a we write

$$aH_0 = \sum_{\mathbf{s}, \mathbf{s}'} a W_{s_1 s'_1}^{[1]} \cdots W_{s_N s'_N}^{[N]} |\mathbf{s}\rangle \langle \mathbf{s}'|. \quad (13)$$

TABLE I. Bond dimensions for different orders of the Magnus expansion and Chebyshev approximations, for initial bond dimension of 3 for both H_0 and H_c .

Magnus order	Chebyshev order			
	First	Second	Third	Fourth
First	7	43	2599	1.55×10^3
Second	25	601	1.44×10^4	3.46×10^5
Third	187	3.47×10^4	6.46×10^6	1.20×10^9
Fourth	1.15×10^3	1.34×10^6	1.55×10^9	1.79×10^{12}

For the sum of two MPOs we write

$$\begin{aligned}
 H_0 + H_c &= \sum_{\mathbf{s}, \mathbf{s}'} W_{s_1 s'_1}^{[1]} \cdots W_{s_N s'_N}^{[N]} |\mathbf{s}\rangle \langle \mathbf{s}'| \\
 &\quad + \sum_{\mathbf{s}, \mathbf{s}'} V_{s_1 s'_1}^{[1]} \cdots V_{s_N s'_N}^{[N]} |\mathbf{s}\rangle \langle \mathbf{s}'| \\
 &= \sum_{\mathbf{s}, \mathbf{s}'} (W_{s_1 s'_1}^{[1]} \oplus V_{s_1 s'_1}^{[1]}) \cdots \\
 &\quad \times (W_{s_N s'_N}^{[N]} \oplus V_{s_N s'_N}^{[N]}) |\mathbf{s}\rangle \langle \mathbf{s}'|. \quad (14)
 \end{aligned}$$

For the product we have

$$\begin{aligned}
 H_0 H_c &= \sum_{\mathbf{s}, \mathbf{s}'} W_{s_1 s'_1}^{[1]} \cdots W_{s_N s'_N}^{[N]} |\mathbf{s}\rangle \langle \mathbf{s}'| \\
 &\quad \times \sum_{\mathbf{s}, \mathbf{s}'} V_{s_1 s'_1}^{[1]} \cdots V_{s_N s'_N}^{[N]} |\mathbf{s}\rangle \langle \mathbf{s}'| \\
 &= \sum_{\mathbf{s}, \mathbf{s}'} \left(\sum_{l_1} W_{s_1 l_1}^{[1]} \otimes V_{l_1 s'_1}^{[1]} \right) \cdots \\
 &\quad \times \left(\sum_{l_N} W_{s_N l_N}^{[N]} \otimes V_{l_N s'_N}^{[N]} \right) |\mathbf{s}\rangle \langle \mathbf{s}'|. \quad (15)
 \end{aligned}$$

Using these operations, we can write the solution of the TDSE in an MPO form

$$U(T) = \sum_{\mathbf{s}, \mathbf{s}'} T_{s_1 s'_1}^{[1]} \cdots T_{s_N s'_N}^{[N]} |\mathbf{s}\rangle \langle \mathbf{s}'|. \quad (16)$$

We note that, by taking sums and products, the bond dimension of the resulting MPO $U(T)$ increases. In Table I we see how the bond dimension of $U(T)$ increases with the higher truncation orders we make in the Magnus and Chebyshev approximations.

From Table I we see that to keep the bond dimension of the tensors around 10^4 , which would be enough to do computations with a laptop, we can use a Magnus expansion of order 2 and Chebyshev approximation of order 3 or vice versa. However, the characteristics of the physical system we are considering will be the main indicator to know the order at which we should truncate the approximations.

If we use a dense matrix method, where we operate with matrices of 4^N elements, we reach a computational limit relatively fast. Our method, on the other hand, uses MPOs storing $4Nr^2$ elements, which scale linearly in N instead of exponentially. This allows for the use of the MPO method for very large systems.

As we see, the biggest limitation of this method is the growth of the bond dimension, but this is a recurring theme when working with MPOs, as there is no physically sensitive method to reduce the bond dimension of the unitary operator written as an MPO [26], in the same sense that we can use bond dimension reduction algorithms for MPS. Currently existing methods [25–30] are based on building the unitary operator as an MPO for each time step, then applying it to the MPS, and finally reducing the bond dimension to make the full time evolution computationally feasible. We can also consider the time evolution of the unitary operator and limit the number of time steps according to the maximum bond dimension we can have for the resulting MPO. Our method lies on this line as it does not (and it cannot) depend on bond dimension reduction algorithms, first, because we work with operators, not states, and second, because this allows us to work with variables symbolically in the tensor network entries, which will help us formulate the quantum optimal control problem. The bond dimension reduction algorithms are numerical and therefore cannot work symbolically.

IV. EXAMPLE

Let us look at the controlled Ising model, for which we have

$$H(t) = \sum_{i=1}^{N-1} J \sigma_i^z \sigma_{i+1}^z + u(t) \sum_{i=1}^N \sigma_i^x. \quad (17)$$

To ensure convergence of the Magnus expansion through Eq. (8) we will set the maximum time evolution for this Hamiltonian to be $T_{\max} = \frac{1}{2N}$, considering its norm scales with N . We take the control function to be the polynomial $u(t) = 1 - t + t^2$ and $J = 1$. Note that $u(t)$ can take any form as long as it is integrable.

We write the free Hamiltonian H_0 as an MPO with boundary tensors

$$W^{[1]} = \begin{pmatrix} 0 & J\sigma^z & I \end{pmatrix}, \quad W^{[N]} = \begin{pmatrix} I \\ \sigma^z \\ 0 \end{pmatrix} \quad (18)$$

and central tensors, for $i = 2, \dots, N-1$, of the form

$$W^{[i]} = \begin{pmatrix} I & 0 & 0 \\ \sigma^z & 0 & 0 \\ 0 & J\sigma^z & I \end{pmatrix}. \quad (19)$$

Similarly, for the control Hamiltonian H_c we have boundary tensors

$$W^{[1]} = \begin{pmatrix} I & \sigma^x \end{pmatrix}, \quad W^{[N]} = \begin{pmatrix} \sigma^x \\ I \end{pmatrix} \quad (20)$$

and core tensors, for $i = 2, \dots, N-1$, of the form

$$W^{[i]} = \begin{pmatrix} I & \sigma^x \\ 0 & I \end{pmatrix}. \quad (21)$$

We note that the initial bond dimensions are 3 and 2, so the total bond dimension will increase at a slightly slower pace than in Table I. We now look at the error between the dense representation ($2^N \times 2^N$ matrix) of the unitary and the one

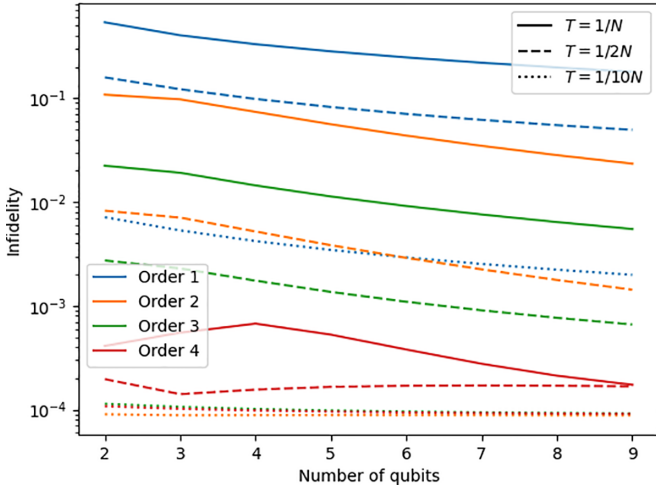


FIG. 2. Infidelity between the dense and the MPO method. We fix a Magnus expansion of order 1 and vary the Chebyshev order. We compare different time evolutions.

resulting from the Magnus and Chebyshev approximations using MPOs.

To look at the error $|\varepsilon|$ between the dense unitary U_{dense} and the approximate unitary in MPO form U_{MPO} , we compute the infidelity between them, defined as

$$\varepsilon = 1 - \frac{1}{d^2} |\text{Tr}(U_{\text{dense}}^\dagger U_{\text{MPO}})|^2, \quad (22)$$

where d is the dimension of the system. We consider the infidelity instead of other error measures because we are interested in the gate synthesis problem, and the infidelity is directly related to the error probabilities we see in experiments.

The error results only from the approximations and it is independent of the use of MPO representations which, in this case, is exact. We plot the error for different orders of truncation of the Chebyshev approximation and for different time evolutions in Fig. 2.

We only consider Magnus expansions of order 1 because, for this Hamiltonian, higher orders do not improve the accuracy. From Fig. 2 we note that to get an error of less than 1%, for $T = \frac{1}{N}$, we need a Chebyshev approximation of at least order 3. Similarly, we see how the shorter the evolution time, the better the infidelity. From these, we decide the truncation orders of the unitary calculation for this example to be 1 for the Magnus expansion and 3 for the Chebyshev approximation. We will let the time evolution be $T = \frac{1}{2N}$.

To see how the MPO representation provides an advantage compared to the full matrix representation we look at the time and memory required to compute both the dense and MPO solutions and plot these in Fig. 3.

We use the library qutip [43] in python to calculate the dense evolution, which can be solved almost exactly. In Fig. 3 we see that for a small number of qubits ($N < 8$) it takes fewer resources to compute the evolution using a dense representation. However, as the number of qubits increases, the resources required for the unitary evolution increase exponentially, making the computation infeasible for large N . On the other hand, the resources required for the MPO method only increase linearly. Therefore, for more

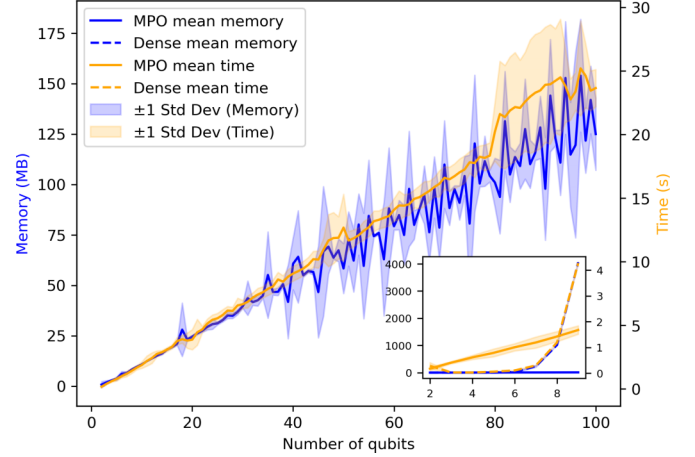


FIG. 3. Time and memory required to compute the dense and MPO unitary evolutions using a first-order Magnus expansion, a Chebyshev approximation of third order, and an evolution time $T = \frac{1}{2N}$. We do five repetitions for each N to look at the mean and standard deviation.

than eight qubits we have an advantage by using the MPO representation.

We can also compare our method with a Trotterization method, where we build an MPO following a discrete time approach, dividing the time interval into K segments such that $T = \Delta t K$. Therefore, we write the total time evolution of the unitary operator as $U(T) = U_K U_{K-1} \cdots U_2 U_1$, where $U_j = e^{-i\Delta t H(\Delta t j)}$. If we consider the controlled Ising model, we can approximate this by considering almost-commuting parts of the Hamiltonian

$$H(t) = H_Z + H_X(t) \quad (23)$$

$$= \sum_{i=1}^{N-1} J \sigma_i^z \sigma_{i+1}^z + u(t) \sum_{i=1}^N \sigma_i^x \quad (24)$$

such that $U_j \approx e^{-i\Delta t H_X(\Delta t j)} e^{-i\Delta t H_Z}$, with an error of $O(\Delta t^2)$.

The terms of the sums of these two components all commute with themselves, which allows us to write

$$e^{-i\Delta t H_X(\Delta t j)} = \prod_i e^{-i\Delta t u(\Delta t j) \sigma_i^x}, \quad (25)$$

$$e^{-i\Delta t H_Z} = \prod_i e^{-i\Delta t J \sigma_i^z \sigma_{i+1}^z}. \quad (26)$$

These factorizations allow for simple MPO representations (see Appendix B for more details). The MPOs have bond dimensions of 1 and 2, respectively, which means one time step of the unitary operator will be an MPO of bond dimension 2. The total bond dimension for the MPO of $U(T)$ will then be 2^K , and if we want to keep the bond dimension below computational limits, then we can have a maximum of around seven time steps per interval.

We compare the accuracy of this Trotterization of first order with our Magnus method of first order and Chebyshev approximation of third order and illustrate the results in Fig. 4. We let $T = \frac{1}{2N}$ and $J = 1$ and compare two different control functions.

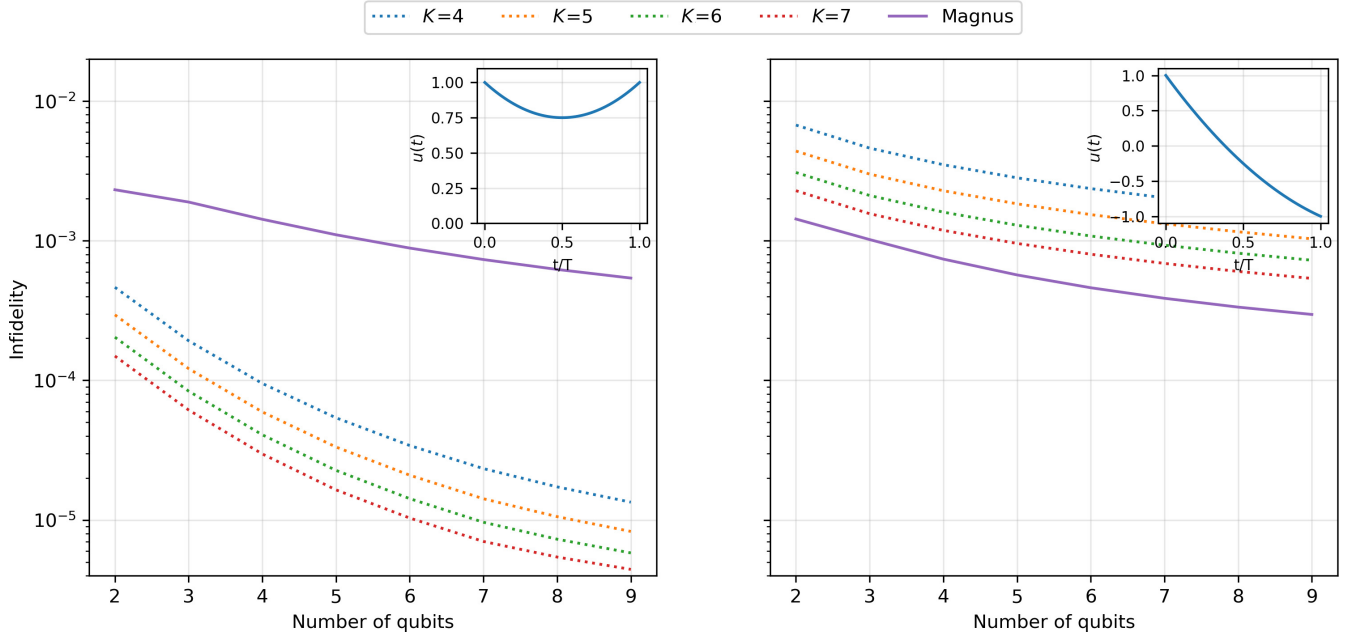


FIG. 4. Comparison of the accuracy of the Magnus and Chebyshev methods with Trotterization of K time steps for two different controls $u(t)$.

Trotterization provides better accuracy for controls with not much steepness or with oscillations, while the Magnus and Chebyshev methods perform better for steeper controls that Trotterization might undersample due to the low number of time steps. This indicates that both approaches can still be used to find the unitary evolution of systems that can be represented with low bond dimensions, and depending on the characteristics of the system, we might prefer one or the other. In the next section we show how for an application like quantum optimal control of many body systems, our approach might provide even a larger advantage.

The limitations of our method are illustrated by the results in Table I and Fig. 2. In the former we see that the bond dimension increases very fast as we improve the order of approximations, which means that for Hamiltonians with higher starting bond dimension (or equivalently longer-range interactions) we might not be able to have an accurate approximate solution to the unitary operator. In the latter we consider the other limiting factor, the total time evolution T , which has to be very small in order for the Magnus expansion to fulfill its convergence properties. In what follows we will improve the fast bond dimension growth by avoiding the Chebyshev polynomial approximation, leading to accurate results for quantum optimal control.

V. QUANTUM OPTIMAL CONTROL

We now consider a quantum optimal control problem following from the previous example to show the power of the MPO representation method. We take the Hamiltonian of the system to be

$$H(t, \mathbf{x}) = \sum_{i=1}^{N-1} J \sigma_i^z \sigma_{i+1}^z + u(t, \mathbf{x}) \sum_{i=1}^N \sigma_i^x, \quad (27)$$

with $J = 1$ and a control function

$$u(t, \mathbf{x}) = \sum_{i=1}^m x_i t^{i-1}, \quad (28)$$

where $\mathbf{x} = \{x_1, \dots, x_m\}$ are unknown control coefficients we want to optimize. Now we represent the Hamiltonian terms as MPOs using the tensors defined in Eqs. (18)–(21).

We want to synthesize a unitary gate, for example, the global rotation

$$U^* = \exp \left(-i \frac{\pi}{4} \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z \right), \quad (29)$$

which is a multiqubit controlled-Z gate.

There are several requirements the target unitary must have for a good formulation of the problem. The most important one is that we can write it as the exponential of an MPO, even for large bond dimension r . Further, if we want to synthesize the specific target and not just minimize the error, we require the unitary target to be reachable for our defined system. This means that there exists a control function $u(t)$ and finite time T such that the Schrödinger equation evolves the system from the identity to U^* . This restricts the choice, which is why we pick U^* such that we can reach it and write it as the exponential of an MPO.

In order to optimize the control parameters of $u(t, \mathbf{x})$ to reach the desired unitary gate we have to solve the TDSE with the defined control Hamiltonian. If we pick a final evolution time T , we can find the solution $U(T, \mathbf{x})$ using the Magnus and Chebyshev approximations.

Once we have the evolution solution in terms of the unknown control coefficients $\mathbf{x}$ we want to find the optimal values for which we get as close as possible to the desired unitary gate. To find these we formulate the optimization

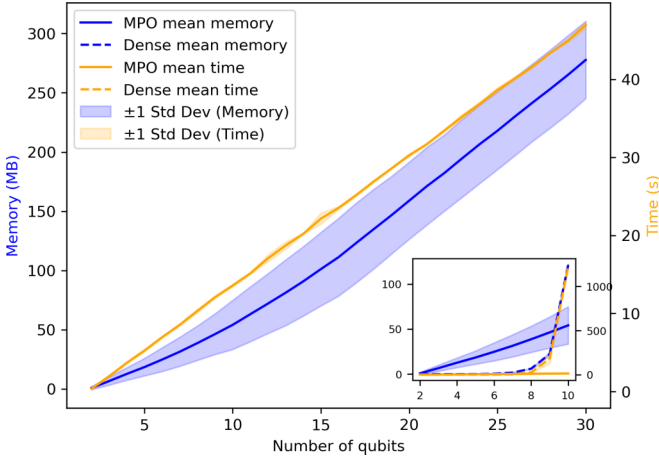


FIG. 5. Time and memory required to compute the polynomial to minimize for the dense and MPO representations. We use a second-order Magnus expansion, an evolution time $T = \frac{\pi}{4}$, and a control function with three unknown parameters. We do five repetitions per number of qubits to look at the mean and standard deviation.

problem

$$\min_{\mathbf{x}} 1 - \frac{1}{d^2} |\text{Tr}[U^{*†} U(T, \mathbf{x})]|^2, \quad (30)$$

where d is the dimension of the Hilbert space.

We want to find the global solution and recover the optimal control values that minimize this function. For this we use QCPOP, the method shown in [37,38], with which we can reformulate the problem (30) as a polynomial optimization problem of the form

$$\min_{\mathbf{x}} \|\Omega^{(n)}(T, \mathbf{x}) - i\Theta\|_F^2, \quad (31)$$

where $\Omega^{(n)}(T, \mathbf{x})$ is the truncated Magnus expansion at order n and Θ is the Hermitian matrix generating the unitary target, in our case $\Theta = -\frac{\pi}{4} \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z$.

Now we assume that Θ can be efficiently represented as an MPO and therefore we can use the MPO operations defined previously to reformulate (31) as

$$\min_{\mathbf{x}} \text{Tr}\{[-\Omega^{(n)}(T, \mathbf{x}) + i\Theta][\Omega^{(n)}(T, \mathbf{x}) - i\Theta]\}. \quad (32)$$

This is a polynomial that can then be minimized using the moment-sum of squares (moment-SOS) method [44], a series of relaxations of semidefinite programs that will generally converge to the global solution. To implement this numerically, and letting $m = 3$, we use the julia package tssos [45] in order to globally solve the polynomial optimization problem and extract the solution of the control parameters. In this example we find $\mathbf{x} = [0, 0, 0]$.

In QCPOP we also use the Magnus expansion and Chebyshev approximation, so the error in the approximation arises from the Magnus expansion only and not from the MPO representation. Therefore, we will obtain the same polynomial to minimize using both the MPO and dense methods. The only difference between both methods lies in the time and memory requirements to obtain the polynomial, and here is where we have the advantage of using the MPO representation.

In Fig. 5 we see how, for a control polynomial with $m = 3$ unknown parameters, the time and memory required to

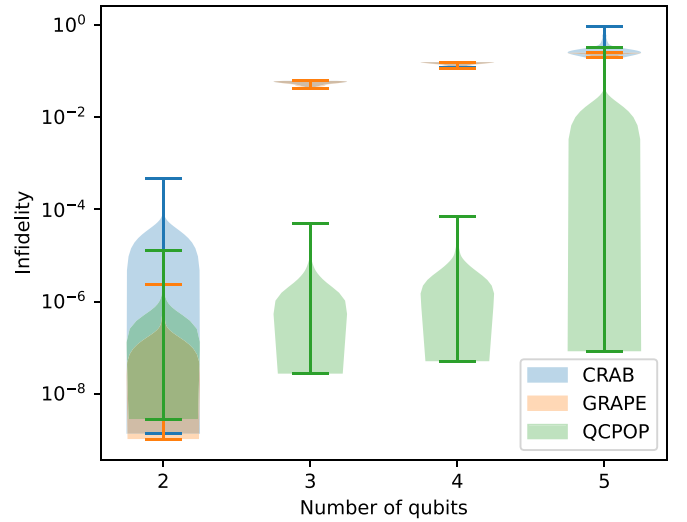


FIG. 6. Infidelity comparison between different quantum optimal control methods for the controlled Ising model with a different number of qubits, for 100 random reachable unitary targets. The color shading is the range of infidelities and the width is the frequency. For three and four qubits, CRAB and GRAPE almost fully intersect, making them hard to distinguish.

compute the polynomial to optimize are linear for the MPO representation and exponential for the dense representation.

Now we compare the error of the QCPOP method with the errors of the currently used methods GRAPE [31] and CRAB [32], with the initial guess as a random control function. The polynomial we obtain from our tensor network approach is the same as the dense matrix method, and the tensor network applications in GRAPE and CRAB are formulated for MPS evolution. Therefore, we do an error comparison without using tensor networks, which will only make the accuracy of GRAPE and CRAB worse, while QCPOP will remain the same.

In particular, we sample from an ensemble of random control parameters $\mathbf{x} = \{x_1, x_2, x_3\}$ for which $x_1, x_2, x_3 \in [-1, 1]$. For each control signal, we simulate the evolution using qutip [43] to obtain the target unitary. Subsequently, we solve the quantum optimal control problem for the target unitary with the first level of the moment-SOS hierarchy and a second-order Magnus expansion. We do this for 100 different control parameters and for different numbers of qubits in the Ising Hamiltonian model. We illustrate the results in Fig. 6.

For very small system size (two qubits), we see that GRAPE performs the best, followed closely by QCPOP and then CRAB. As we increase the system size, all three methods get worse but, while GRAPE and CRAB become unreliable methods with high infidelities, QCPOP generally maintains infidelity below 1%, a major improvement with respect to the other methods.

VI. CONCLUSION

We have presented a method to represent the time evolution of controlled quantum systems using matrix product operators. This allowed for the calculation of the approximate unitary operator solution to the TDSE of large quantum

systems in a scalable manner. We improved the exponential matrix size increase in dense matrix methods by using matrix product operators, which scale linearly in size. These scaling properties could be used to solve quantum optimal control problems for large quantum systems, which would be infeasible to calculate using a dense matrix form. Our use of the MPOs was limited to systems that present specific properties related to localized interactions, which allowed us to represent them efficiently using tensor networks and for short time evolution. Using the MPO representation, there was no direct loss in accuracy, and the quality of the approximation was fully determined by the orders of truncation of the Magnus and Chebyshev approximations. The lack of loss in accuracy of the MPO solution with respect to the dense matrix solution arises from not using bond reduction algorithms. This allowed us to work with unitary operators without considering the state evolution and also using unknown coefficients in the tensor

network, which leads to the formulation of the quantum optimal control problem of gate synthesis, through QCPOP, that we showed improves upon current methods for the example provided.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [46].

APPENDIX A: OPERATIONS TO SOLVE THE TDSE

We want to show how the only necessary operations to compute $U(T)$ are scalar products, sums, and products of MPOs. For this, let us write the terms of the Magnus expansion

$$\Omega_1 = -i \int_0^T H(t) dt = -i \int_0^T H_0 + u(t)H_c dt = \left(-i \int_0^T dt\right)H_0 + \left(-i \int_0^T u(t)dt\right)H_c = aH_0 + bH_c \quad (A1)$$

for scalars a and b . From now on we use the notation $H(t_i) = H_i$ and $u(t_i) = u_i$. Similarly, the second term will be

$$\Omega_2 = -\frac{1}{2} \int_0^T dt_1 \int_0^{t_1} [H_1, H_2] dt_2 = \left(-\frac{1}{2} \int_0^T dt_1 \int_0^{t_1} (u_2 - u_1) dt_2\right) [H_0, H_c] = c[H_0, H_c] \quad (A2)$$

for scalar c . For the third term we have

$$\begin{aligned} \Omega_3(T) &= \frac{i}{6} \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} ([H_1, [H_2, H_3]] + [[H_1, H_2], H_3]) dt_3 \\ &= \left(\frac{i}{6} \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} (u_3 - 2u_2 + u_1) dt_3\right) [H_0, [H_0, H_c]] \\ &\quad + \left(\frac{i}{6} \int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} (2u_1 u_3 - u_1 u_2 - u_2 u_3) dt_3\right) [[H_c, H_0], H_c] \\ &= d[H_0, [H_0, H_c]] + e[[H_c, H_0], H_c] \end{aligned} \quad (A3)$$

for scalars d and e . The rest of the terms follow similarly.

For the Chebyshev approximation, we have

$$\begin{aligned} U(T) &\approx J_0(1)\mathbb{I} + 2 \sum_{i=1}^p J_i(1)T_i = [J_0(1) + 2J_2(1)]\mathbb{I} + 2J_1(1)\Omega^{(n)} + 4J_2(1)(\Omega^{(n)})^2 + \dots \\ &= s\mathbb{I} + l\Omega^{(n)} + q(\Omega^{(n)})^2 + \dots \end{aligned} \quad (A4)$$

for scalars s , l , and q . Thus, we can obtain $U(T)$ only with the three MPO operations defined in the paper.

APPENDIX B: TROTTERIZATION CONTROLLED ISING MODEL

We consider a controlled Ising Hamiltonian

$$H(t) = H_Z + H_X(t) \quad (B1)$$

$$= \sum_{i=1}^{N-1} J \sigma_i^z \sigma_{i+1}^z + u(t) \sum_{i=1}^N \sigma_i^x \quad (B2)$$

and we write the total time evolution of the unitary operator via time discretization as $U(T) = U_K U_{K-1} \dots U_2 U_1$, where $U_j = e^{-i\Delta t H(\Delta t j)}$.

Now we let $U_j \approx e^{-i\Delta t H_X(\Delta t j)} e^{-i\Delta t H_Z}$, with an error of $O(\Delta t^2)$, where each term can be factorized as

$$U_X = e^{-i\Delta t H_X(\Delta t j)} = \prod_i^N e^{-i\Delta t u(\Delta t j) \sigma_i^x}, \quad (\text{B3})$$

$$U_Z = e^{-i\Delta t H_Z} = \prod_i^{N-1} e^{-i\Delta t J \sigma_i^z \sigma_{i+1}^z}. \quad (\text{B4})$$

We can efficiently write these two exponentials as MPOs. For U_X we have $2 \times 2 \times 1 \times 1$ tensor cores

$$W_X^{[i]} = G(\phi), \quad G(\phi) = \begin{pmatrix} \cos(\phi) & -i \sin(\phi) \\ -i \sin(\phi) & \cos(\phi) \end{pmatrix}, \quad (\text{B5})$$

where $\phi = u(\Delta t j)\Delta t$ for $i = 1, \dots, N$, so this MPO has bond dimension 1. For U_Z we first define $\theta = \Delta t J$ and we let the tensor cores be

$$W_Z^{[1]} = \begin{pmatrix} c^{N-1} I \\ c^{N-1} \sqrt{t} \sigma^z \end{pmatrix}^T, \quad W_Z^{[N]} = \begin{pmatrix} I \\ \sqrt{t} \sigma^z \end{pmatrix}, \quad (\text{B6})$$

$$W_Z^{[i]} = \begin{pmatrix} I & \sqrt{t} \sigma^z \\ \sqrt{t} \sigma^z & t I \end{pmatrix} \forall i \in \{2, \dots, N-1\}, \quad (\text{B7})$$

where $c = \cos(\theta)$ and $t = \tan(\theta)$. The MPO representing the time step U_j will have a bond dimension of 2. The bond dimension for the MPO representing the total time evolution for a time interval discretized into K steps will be 2^K .

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- [1] P. J. Ollitrault, A. Miessen, and I. Tavernelli, Molecular quantum dynamics: A quantum computing perspective, *Acc. Chem. Res.* **54**, 4229 (2021).
- [2] D. B. Williams-Young, S. H. Yuwono, A. E. DePrince, III, and C. Yang, Approximate exponential integrators for time-dependent equation-of-motion coupled cluster theory, *J. Chem. Theory Comput.* **19**, 9177 (2023).
- [3] C. P. Koch, U. Boscain, T. Calarco, G. Dirr, S. Filipp, S. J. Glaser, R. Kosloff, S. Montangero, T. Schulte-Herbrüggen, D. Sugny, and F. K. Wilhelm, Quantum optimal control in quantum technologies. Strategic report on current status, visions and goals for research in europe, *EPJ Quantum Technol.* **9**, 19 (2022).
- [4] J. Nys, G. Pescia, A. Sinibaldi, and G. Carleo, *Ab-initio* variational wave functions for the time-dependent many-electron Schrödinger equation, *Nat. Commun.* **15**, 9404 (2024).
- [5] R. Hamazaki, Exceptional dynamical quantum phase transitions in periodically driven systems, *Nat. Commun.* **12**, 5108 (2021).
- [6] G. K.-L. Chan, A. Keselman, N. Nakatani, Z. Li, and S. R. White, Matrix product operators, matrix product states, and *ab initio* density matrix renormalization group algorithms, *J. Chem. Phys.* **145**, 014102 (2016).
- [7] D. E. Parker, X. Cao, and M. P. Zaletel, Local matrix product operators: Canonical form, compression, and control theory, *Phys. Rev. B* **102**, 035147 (2020).
- [8] C. Hubig, I. P. McCulloch, and U. Schollwöck, Generic construction of efficient matrix product operators, *Phys. Rev. B* **95**, 035129 (2017).
- [9] M. C. Bañuls, Tensor network algorithms: A route map, *Annu. Rev. Condens. Matter Phys.* **14**, 173 (2023).
- [10] R. Orús, A practical introduction to tensor networks: Matrix product states and projected entangled pair states, *Ann. Phys. (NY)* **349**, 117 (2014).
- [11] B. Pirvu, V. Murg, J. I. Cirac, and F. Verstraete, Matrix product operator representations, *New J. Phys.* **12**, 025012 (2010).
- [12] F. Fröwis, V. Nebendahl, and W. Dür, Tensor operators: Constructions and applications for long-range interaction systems, *Phys. Rev. A* **81**, 062337 (2010).
- [13] G. M. Crosswhite, A. C. Doherty, and G. Vidal, Applying matrix product operators to model systems with long-range interactions, *Phys. Rev. B* **78**, 035116 (2008).
- [14] S. Keller, M. Dolfi, M. Troyer, and M. Reiher, An efficient matrix product operator representation of the quantum chemical Hamiltonian, *J. Chem. Phys.* **143**, 244118 (2015).
- [15] J. Haegeman, J. I. Cirac, T. J. Osborne, and F. Verstraete, Calculus of continuous matrix product states, *Phys. Rev. B* **88**, 085118 (2013).
- [16] M. Ganahl, P. Thunström, F. Verstraete, K. Held, and H. G. Evertz, Chebyshev expansion for impurity models using matrix product states, *Phys. Rev. B* **90**, 045144 (2014).
- [17] F. A. Wolf, I. P. McCulloch, O. Parcollet, and U. Schollwöck, Chebyshev matrix product state impurity solver for dynamical mean-field theory, *Phys. Rev. B* **90**, 115124 (2014).
- [18] R. Hong, Y.-X. Xiao, J. Hu, A.-C. Ji, and S.-J. Ran, Functional tensor network solving many-body Schrödinger equation, *Phys. Rev. B* **105**, 165116 (2022).
- [19] S. R. Manmana, A. Muramatsu, and R. M. Noack, Time evolution of one-dimensional quantum many body systems, *AIP Conf. Proc.* **789**, 269 (2005).
- [20] S. Szalay, M. Pfeffer, V. Murg, G. Barcza, F. Verstraete, R. Schneider, and O. Legeza, Tensor product methods and entanglement optimization for *ab initio* quantum chemistry, *Int. J. Quantum Chem.* **115**, 1342 (2015).
- [21] C. Mc Keever and M. Lubasch, Towards adiabatic quantum computing using compressed quantum circuits, *PRX Quantum* **5**, 020362 (2024).
- [22] C. Mc Keever and M. Lubasch, Classically optimized Hamiltonian simulation, *Phys. Rev. Res.* **5**, 023146 (2023).
- [23] J. J. García-Ripoll, Time evolution of matrix product states, *New J. Phys.* **8**, 305 (2006).

- [24] T. Li, P. Venkatesh, N. Shitara, and A. Montoya-Castillo, Numerically exact quantum dynamics with tensor networks: Predicting the decoherence of interacting spin systems, [arXiv:2509.20604](#).
- [25] S. Paeckel, T. Köhler, A. Swoboda, S. R. Manmana, U. Schollwöck, and C. Hubig, Time-evolution methods for matrix-product states, *Ann. Phys. (NY)* **411**, 167998 (2019).
- [26] M. V. Damme, J. Haegeman, I. McCulloch, and L. Vanderstraeten, Efficient higher-order matrix product operators for time evolution, *SciPost Phys.* **17**, 135 (2024).
- [27] A. Miessen, P. J. Ollitrault, and I. Tavernelli, Quantum algorithms for quantum dynamics: A performance study on the spin-boson model, *Phys. Rev. Res.* **3**, 043212 (2021).
- [28] N. F. Robertson, B. Pokharel, B. Fuller, E. Switzer, O. Shtanko, M. Amico, A. Byrne, A. D'Urbano, S. Hayes-Shuptar, A. Akhriev, N. Keenan, S. Bravyi, and S. Zhuk, Tensor network enhanced dynamic multiproduct formulas, *PRX Quantum* **6**, 020360 (2025).
- [29] T. Chanda, P. Sierant, and J. Zakrzewski, Time dynamics with matrix product states: Many-body localization transition of large systems revisited, *Phys. Rev. B* **101**, 035148 (2020).
- [30] M. L. Wall and L. D. Carr, Out-of-equilibrium dynamics with matrix product states, *New J. Phys.* **14**, 125015 (2012).
- [31] N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen, and S. J. Glaser, Optimal control of coupled spin dynamics: Design of NMR pulse sequences by gradient ascent algorithms, *J. Magn. Reson.* **172**, 296 (2005).
- [32] P. Doria, T. Calarco, and S. Montangero, Optimal control technique for many-body quantum dynamics, *Phys. Rev. Lett.* **106**, 190501 (2011).
- [33] M. M. Müller, A. Kölle, R. Löw, T. Pfau, T. Calarco, and S. Montangero, Room-temperature Rydberg single-photon source, *Phys. Rev. A* **87**, 053412 (2013).
- [34] S. van Frank, M. Bonneau, J. Schmiedmayer, S. Hild, C. Gross, M. Cheneau, I. Bloch, T. Pichler, A. Negretti, T. Calarco, and S. Montangero, Optimal control of complex atomic quantum systems, *Sci. Rep.* **6**, 34187 (2016).
- [35] T. Caneva, T. Calarco, R. Fazio, G. E. Santoro, and S. Montangero, Speeding up critical system dynamics through optimized evolution, *Phys. Rev. A* **84**, 012312 (2011).
- [36] J. H. M. Jensen, F. S. Møller, J. J. Sørensen, and J. F. Sherson, Approximate dynamics lead to more optimal control: Efficient exact derivatives *Phys. Rev. A* **103**, 062612 (2021).
- [37] D. I. Bondar, L. B. Gaggioli, G. Korpas, J. Mareček, J. Vala, and K. Jacobs, Globally optimal control of quantum dynamics, *Phys. Rev. Res.* **7**, 043202 (2025).
- [38] L. B. Gaggioli, D. I. Bondar, J. Vala, R. Ovsiannikov, and J. Mareček, Unitary gate synthesis via polynomial optimization, [arXiv:2508.01356](#).
- [39] W. Magnus, On the exponential solution of differential equations for a linear operator, *Commun. Pure Appl. Math.* **7**, 649 (1954).
- [40] D. Fang, D. Liu, and S. Zhu, High-order magnus expansion for Hamiltonian simulation, [arXiv:2509.06054](#).
- [41] S. Blanes, F. Casas, J. Oteo, and J. Ros, The Magnus expansion and some of its applications, *Phys. Rep.* **470**, 151 (2009).
- [42] H. Tal-Ezer and R. Kosloff, An accurate and efficient scheme for propagating the time dependent Schrödinger equation, *J. Chem. Phys.* **81**, 3967 (1984).
- [43] J. Johansson, P. Nation, and F. Nori, QuTiP: An open-source Python framework for the dynamics of open quantum systems, *Comput. Phys. Commun.* **183**, 1760 (2012).
- [44] J. B. Lasserre, Global optimization with polynomials and the problem of moments, *SIAM J. Optim.* **11**, 796 (2001).
- [45] J. Wang, V. Magron, and J.-B. Lasserre, TSSOS: A moment-SOS hierarchy that exploits term sparsity, *SIAM J. Optim.* **31**, 30 (2021).
- [46] <https://github.com/llorebaga/QCMPO>.