

Quantum Control without Quantum States

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We show that combining ideas from the fields of quantum invariants and optimal control can be used to design optimal quantum control solutions without explicit reference to quantum states. The states are specified only implicitly in terms of operators to which they are eigenstates. The scaling in numerical effort of the resultant approach is not given by the typically exponentially growing effort required for the specification of a time-evolved quantum state, but it is given by the effort required for the specification of a time-evolved operator. For certain Hamiltonians, this effort can be polynomial in the system size. We describe how control problems for state preparation and the realization of propagators can be formulated in this approach, and we provide explicit control solutions for a spin chain with an extended Ising Hamiltonian. The states considered for state-preparation protocols include eigenstates of Hamiltonians with more than pairwise interactions and these Hamiltonians are also used for the definition of target propagators. The cost of describing suitable time-evolving operators grows only quadratically with the system size, allowing us to construct explicit control solutions for up to 50 spins. While subexponential scaling is obtained only in special cases, we provide several examples that demonstrate favorable scaling beyond the extended Ising model.

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I. INTRODUCTION

The availability of well-controlled quantum systems offers the prospect of progress toward a broad range of applications [1], including quantum simulation [2,3] and quantum computation [4–6]. The exponential growth of the Hilbert space in such systems suggests that even moderately small quantum systems could be employed to achieve tasks that would be impractical to perform classically [4,7]. While the benefits of this scaling have inspired tremendous efforts toward the development of quantum technological devices [6,8–11], the scaling also has disastrous implications on our abilities to simulate the dynamics of quantum systems [12].

Most attempts to devise control schemes of quantum systems are thus restricted to exact analyses performed on small systems [13,14], with potential extensions to larger system via approximate techniques [15,16] and specific systems that admit efficient descriptions [17,18], or to analyses that are approximate to start with [19]. While this

exponential scaling seems an insurmountable obstacle in general, there are specific instances of quantum states that can be described with an effort that scales more favorably than exponentially [20,21].

A very efficient, even though implicit, way of describing some quantum states is in terms of the operator (or operators) to which a state is an eigenstate [22]. There is, for example, a large variety of quantum many-body Hamiltonians with highly complicated ground states [23–25]. The Hamiltonian itself is specified in terms of the interaction geometry, the type of interaction mechanism, and some parameters specifying quantities such as interaction strengths. For many systems, the number of parameters required for this specification scales polynomially with the number of interacting objects; the description is thus *efficient*. The ground state of many such Hamiltonians, however, often lacks an efficient representation, i.e., a representation specified with a polynomial number of parameters. Implicitly, however, the ground state is specified via the Hamiltonian. This implicit description of states is foundational to the stabilizer formalism [26] and to adiabatic quantum computation [27].

Building on this concept of implicit state characterization, this paper introduces a framework for optimal control that avoids explicit construction of quantum states, while not being limited to adiabatic time scales. Formulating an optimal quantum control formalism in terms of operators, we demonstrate a method that can help to solve control

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problems that are computationally intractable using traditional state-vector-based approaches and that does not require an approximate treatment.

The underlying idea is inspired by the framework of quantum invariants [28–30], i.e., Hermitian operators $\mathcal{I}(t)$ satisfying the equation of motion

$$\frac{\partial \mathcal{I}}{\partial t} + i[H(t), \mathcal{I}(t)] = 0 \quad (1)$$

in the Schrödinger picture.

Each such invariant has instantaneous eigenvectors, i.e., generally time-dependent vectors satisfying the eigenvalue relation

$$\mathcal{I}(t) |\Psi(t)\rangle = \gamma |\Psi(t)\rangle. \quad (2)$$

Due to the unitary dynamics resulting from Eq. (1), any eigenvalue γ of $\mathcal{I}(t)$ is time independent. Since every nondegenerate instantaneous eigenvector specifies a solution of the time-dependent Schrödinger equation with the time-dependent Hamiltonian $H(t)$ [28], invariants are commonly used tools in optimal quantum control [31].

The existing use of quantum invariants in optimal quantum control is based on the identification of analytic time dependencies that make an operator satisfy Eq. (1) for a certain type of Hamiltonian, such as the driven harmonic oscillator Hamiltonian and the Hamiltonian of a single driven spin [32–34]. Once such an analytic form is identified, the resultant invariant provides a very elegant means of engineering a time-dependent Hamiltonian that induces the desired dynamics.

Finding such analytic expressions is practical only for particularly simple cases and it does seem elusive to find an analytic invariant for quantum systems with a large number of interacting subsystems. The goal of this paper is thus to develop an approach that benefits from some aspects of quantum invariants but that does not rely on the existence of an analytic form of an invariant. This approach will combine elements from optimal control based on quantum invariants [31] and from numerical quantum control with state vectors or propagators [1,35]. It relies on iterative numerical refinement of a time-dependent Hamiltonian, but instead of the commonly employed numerical integration of the Schrödinger equation, the present approach is based on numerical integration of the equation of motion of quantum invariants, i.e., Eq. (1). Since such numerical integration does not require the existence of analytic solutions, this approach can indeed be applicable to interacting quantum systems.

Instead of defining a control target for state vectors or propagators, control targets are defined for operators $\mathcal{I}(t)$, satisfying the equation of motion of quantum invariants given in Eq. (1). This avoids reference to quantum states with corresponding exponential effort and, as shown with

explicit examples, there are interacting quantum systems for which the description of the time-dependent operator $\mathcal{I}(t)$ does *not* require an exponential effort.

II. IMPLICIT QUANTUM CONTROL

Instead of numerically propagating the Schrödinger equation explicitly for a time-dependent state vector, the proposed approach relies on numerically propagating Eq. (1) for an operator $\mathcal{I}(t)$. Following the eigenvalue relation given in Eq. (2), this provides all information on the desired state vector, but as long as $\mathcal{I}(t)$ is not diagonalized, this information remains implicit.

In this section, we show how to define a control target $\mathcal{I}_T$ for an operator $\mathcal{I}(t)$ following the dynamics of Eq. (1), such that numerical pulse-shaping techniques can be applied to Eq. (1), and such that the resultant Hamiltonian induces the desired dynamics in the underlying Schrödinger equation.

While translating a control problem from the Schrödinger equation to the corresponding Liouville–von Neumann equation, i.e., Eq. (1), does not, in general, provide any improvement in efficiency, there are indeed instances such as Eqs. (20) and (21), discussed in more detail below, and a series of further examples listed in Sec. V, for which this translation results in an exponential improvement.

A. Operator expansion

The crucial aspect to determine whether the present approach is more efficient than approaches based on state vectors is the dimension of the space in which the dynamics of $\mathcal{I}(t)$ following Eq. (1) take place.

Since there is a multitude of different operators with the same ground state, there is no unique choice for the initial condition $\mathcal{I}(0)$ to represent a given initial state $|\Psi(0)\rangle$ and this freedom can be used to find an initial condition $\mathcal{I}(0)$ that allows for particularly efficient propagation.

Formalization of this statement requires the definition of the system Hamiltonian. In the following, it is considered to be of the form

$$H(t) = \sum_{j=1}^{d_0} h_j(t) \mathfrak{h}_j, \quad (3)$$

spanned by a fixed set of d_0 operators $\mathfrak{h}_j$ with scalar expansion coefficients $h_j(t)$. Some of those can be time independent and fixed (as in a drift Hamiltonian) but some should be time dependent and tunable (as in a control Hamiltonian).

The ansatz

$$\mathcal{I}(t) = \sum_{j=1}^d a_j(t) \mathfrak{a}_j \quad (4)$$

for the operator $\mathcal{I}(t)$ to be propagated with a set of d time-independent operators $\mathfrak{a}_j$ and time-dependent scalar expansion coefficients $a_j(t)$ is sufficient to solve Eq. (1) for any choice of the time-dependent coefficients $h_j(t)$, if the commutation relations

$$[\mathfrak{a}_j, \mathfrak{h}_k] = -i \sum_{l=1}^d \lambda_{lj}^k \mathfrak{a}_l, \quad (5)$$

with real coefficients λ_{lj}^k , are satisfied for all $k \in [1, d_0]$ and $j \in [1, d]$.

An ansatz given by Eq. (4) that does not lead to the closed-commutator relations of Eq. (5) can be salvaged with an increase of the set of operators $\mathfrak{a}_j$, i.e., an increase of d . Given a set of d operators $\mathfrak{a}_j$ with a pair of operators $\mathfrak{a}_{j_0}$ and $\mathfrak{h}_{k_0}$ such that the commutator $[\mathfrak{a}_{j_0}, \mathfrak{h}_{k_0}]$ cannot be expanded in terms of the set of d operators $\mathfrak{a}_j$, one can define $\mathfrak{a}_{d+1} = i[\mathfrak{a}_{j_0}, \mathfrak{h}_{k_0}]$ as an additional element, increasing the value of d by 1. In any finite-dimensional system, this process can be continued until Eq. (5) is satisfied for all pairs $\mathfrak{a}_j, \mathfrak{h}_k$.

In practice, this construction can be initiated with a single element $\mathfrak{a}_1$, i.e., with $d = 1$, and the eventual value of d depends on the choice of initialization. Since the effort to integrate Eq. (1) grows with increasing d , it is desirable to find small sets of operators $\mathfrak{a}_j$ with closed-commutator relationships, but even with suitable choices, d will typically be larger than d_0 .

B. Lie algebra

The construction of the set of operators $\{\mathfrak{a}_j\}$ discussed above is a slight variant of the construction of a Lie algebra, i.e., a set of d operators $\mathfrak{h}_j$ with a closed-commutator relationship $[\mathfrak{h}_j, \mathfrak{h}_k] = -i \sum_{l=1}^d \lambda_{jl}^k \mathfrak{h}_l$ for all $j, k \in [1, d]$. Similarly to the above construction, it can be initiated with a set of d_0 operators with $d_0 < d$ and the construction is completed when all commutation relations are closed.

Crucially, the propagator induced by the time-dependent Hamiltonian $H(t)$ [Eq. (3)] is *not* necessarily of the form $U(t) = \exp\left(-i \sum_{j=1}^{d_0} b_j(t) \mathfrak{h}_j\right)$ with time-dependent scalar functions $b_j(t)$ and the terms $\mathfrak{h}_j$ ($j \in [1, d_0]$) in the system Hamiltonian but, typically, terms with $j > d_0$ of the Lie algebra also contribute. In turn, a propagator of the form $U = \exp(-iK)$ with an operator K that cannot be expanded in terms of the basis elements of the Lie algebra (i.e., $\mathfrak{h}_j$, $j \in [1, d]$) cannot be realized with the dynamics induced by $H(t)$ in Eq. (3) and is thus considered not reachable [36].

In the explicit examples presented in Secs. III and IV, the time-evolving operator will be expanded in terms of the Lie algebra generated by the operators $\mathfrak{h}_j$ with $j \in [1, d_0]$. In order to find small sets of operators $\{\mathfrak{a}_j\}$ it can, however, also be beneficial to consider situations beyond Lie algebras, as exemplified in Sec. V.

C. Equations of motion

With the explicit expansion in terms of the sets of operators $\{\mathfrak{a}_j\}$ and $\{\mathfrak{h}_k\}$, the equation of motion given in Eq. (1) reads [37]

$$\frac{\partial \mathcal{I}}{\partial t} = i \sum_{j,k} a_j(t) h_k(t) [\mathfrak{a}_j, \mathfrak{h}_k] = \sum_{j,k,l} a_j(t) h_k(t) \lambda_{lj}^k \mathfrak{a}_l. \quad (6)$$

Since the set of operators $\mathfrak{a}_j$ is linearly independent, this implies the differential equation

$$\dot{\mathbf{a}}(t) = \sum_{j,k} \lambda_{lj}^k a_j(t) h_k(t), \quad (7)$$

which can be written compactly as

$$\dot{\mathbf{a}}(t) = K(t) \mathbf{a}(t), \quad (8)$$

with the vector $\mathbf{a}$ and a matrix K with elements

$$K_{lj}(t) = \sum_k h_k(t) \lambda_{lj}^k. \quad (9)$$

The Hermitian operators $\mathfrak{a}_j$ can always be chosen to be mutually orthonormal, such that Eq. (5) implies

$$\lambda_{lj}^k = i \text{tr}([\mathfrak{a}_j, \mathfrak{h}_k] \mathfrak{a}_l). \quad (10)$$

Invariance of the trace under cyclic permutation implies that

$$\lambda_{lj}^k = i \text{tr}([\mathfrak{a}_l, \mathfrak{a}_j] \mathfrak{h}_k) = -\lambda_{jl}^k. \quad (11)$$

In this case, the matrix K is real and antisymmetric [33] such that the induced dynamics is orthogonal, i.e., unitary and real.

D. Formulation of the control problem

If formulated in terms of Eq. (8) instead of the underlying Schrödinger equation, the dimension of the dynamics underlying the control problem is given by the size d of the set of operators $\{\mathfrak{a}_j\}$ and not by the dimension of the underlying Hilbert space.

In general, d can be quadratically larger than the size of the Hilbert space but, as exemplified in the following, there are several instances of practical importance in which d is much smaller. The goal of the following discussion is to benefit from this reduced dimensionality for optimal-control problems.

While, typically, control problems are defined in terms of a target state or a target gate, the present framework requires a control target for the operator $\mathcal{I}$ and defining this requires some care. In the following, we will discuss this for the problems of state preparation and for the realization of propagators.

1. State preparation

The problem of state preparation is a natural application of the present framework, because Hamiltonians can typically be specified efficiently, whereas the explicit specification of their eigenstates is often not efficient.

With a control problem defined in terms of a target state, the target functional is naturally defined in terms of this state. The present approach leaves much more freedom, since there are many operators $\mathcal{I}_T$ that have a given target state as ground state. There are thus many conceivable choices for $\mathcal{I}_T$ and a good choice is a central part of the control problem within the present approach.

For the problem of finding a time-dependent Hamiltonian such that the system evolves from the ground state of an initial operator H_I to the ground state of a final operator H_T , it seems tempting to define the initial condition $\mathcal{I}(0) = H_I$ and the control target $\mathcal{I}_T = H_T$. However, since the spectrum of $\mathcal{I}(t)$ is time independent, this would necessarily imply the restriction that H_I and H_T have the same spectrum.

Moreover, if the operators $\mathfrak{h}_j$ in the system Hamiltonian [Eq. (3)] do not generate the maximal Lie algebra, i.e., an algebra that contains a complete set of operators apart from the identity, then there are unitary propagators that cannot be realized with the system Hamiltonian, as discussed in the penultimate paragraph of Sec. II B. That means that even if H_I and H_T have the same spectrum, it is not necessarily possible to realize the dynamics such that an operator $\mathcal{I}(t)$ with the initial condition $\mathcal{I}(0) = H_I$ evolves toward the final value $\mathcal{I}(T) = H_T$; i.e., the target $\mathcal{I}_T = H_T$ is not reachable (explicit examples demonstrating that specific targets can be reached are discussed in Secs. III B 1 and III B 2).

It is thus necessary to impose all of the following requirements:

- (i) The initial condition $\mathcal{I}(0)$ needs to be specified such that the initial state $|\Psi_I\rangle$ (an eigenvector of H_I) is an eigenstate of $\mathcal{I}(0)$ with a nondegenerate eigenvalue γ .
- (ii) The control target $\mathcal{I}_T$ needs to be specified such that the target state $|\Psi_T\rangle$ (an eigenvector of H_T) is an eigenstate of $\mathcal{I}_T$ with the same eigenvalue γ .
- (iii) The control target needs to be reachable with the dynamics induced by the system Hamiltonian $H(t)$, i.e., the dynamics following Eq. (8).

In attempting to satisfy these requirements, it can be helpful to consider the following aspects.

For (i): In most control problems, the initial operator H_I would be a noninteracting operator, i.e., a sum of single-qubit terms (or, more generally, single-particle terms) without any interactions. As such, the initial condition $\mathcal{I}(0)$ can also be chosen to be noninteracting. As long as the single-qubit parts of $\mathcal{I}(0)$ are nondegenerate, such

an operator has a unique nondegenerate ground state and the associated eigenvalue is given by the sum of all the single-qubit ground-state eigenvalues. In cases in which the initial operator $\mathcal{I}(0)$ is interacting, it might be challenging to verify the nondegeneracy of the ground state. There is certainly no unique recipe to do this, but one option would be to show unitary equivalence of this operator with a nondegenerate noninteracting operator.

For (ii): There is a general approach to numerically constructing a reachable control target that is applicable if the set of operators $\{\mathfrak{a}_j\}$ is taken to coincide with the Lie algebra generated by the operators $\mathfrak{h}_j$ defining the system Hamiltonian in Eq. (3). Given any initial condition $\mathcal{I}(0)$, one can numerically simulate the dynamics of $\mathcal{I}(t)$ under a Hamiltonian that evolves adiabatically from H_I to H_T , as demonstrated in Sec. III B 3. In practice, this implies numerical integration of Eq. (8), with an effort that scales with d and not with the exponentially large dimension of the system Hilbert space. The final operator $\mathcal{I}_T$ obtained in this fashion necessarily has the same spectrum as $\mathcal{I}(0)$ because of unitarity of the dynamics, its ground state coincides with the ground state of H_T because of adiabaticity, and it is reachable with the dynamics induced by the system Hamiltonian.

For (iii): Given Eq. (8), the question of reachability of an operator $\mathcal{I}_T$ starting from an operator $\mathcal{I}(0)$ is equivalent to the question of reachability of a vector $\mathbf{a}^T$ (such that $\mathcal{I}_T = \sum_j a_j^T \mathfrak{a}_j$) starting from a vector $\mathbf{a}(0)$ (such that $\mathcal{I}(0) = \sum_j a_j(0) \mathfrak{a}_j$), given the time-dependent operators $K(t)$ [Eq. (9)]. The question of reachability at hand is thus equivalent to standard reachability of vectors with a linear differential equation, as in the case of state control with the Schrödinger equation [38].

Requirements (i), (ii), and (iii) do not result in a unique choice of initial condition $\mathcal{I}(0)$ and target $\mathcal{I}_T$, and this freedom of choice can be used to select an initial condition $\mathcal{I}(0)$ that can be expanded in a set of operators $\{\mathfrak{a}_j\}$ such that the commutation relations in Eq. (5) are closed even though d is small.

Some of the examples discussed in Sec. III will rely on the numerical construction of control targets with simulated adiabatic dynamics. While such a numerical construction is a generally applicable approach, there are also instances in which suitable control targets can be defined analytically, as exemplified in Secs. III B 1 and III B 2.

2. State fidelity

Given a consistent definition for initial condition $\mathcal{I}(0)$ and control target $\mathcal{I}_T$, a generic choice for objective function is the infidelity

$$\mathcal{J} = 1 - \frac{\text{tr}(\mathcal{I}(T) \mathcal{I}_T)}{\text{tr}(\mathcal{I}_T^2)}, \quad (12)$$

where T is the final time at which the goal of the control problem is intended to be reached. Since the infidelity is readily expressed as

$$\mathcal{J} = 1 - \frac{\mathbf{a}(T) \cdot \mathbf{a}_T}{\|\mathbf{a}_T\|^2}, \quad (13)$$

with the vector $\mathbf{a}_T$ of the control target $\mathcal{I}_T$, the effort to evaluate the infidelity scales with the dimension d and not with the dimension of the system Hilbert space.

If $\mathcal{I}(T)$ coincides exactly with the control target $\mathcal{I}_T$, then it is ensured that the system state coincides with the desired nondegenerate eigenstate of $\mathcal{I}_T$, i.e., with the target state. Since both the state infidelity and the infidelity defined in Eq. (12) are continuous functions, continuity implies that in the limit of vanishing infidelity $\mathcal{J}$ for the nondegenerate operator $\mathcal{I}(T)$, the infidelity of the realized quantum state also approaches its ideal value. In practice, a more quantitative estimate is desirable to assess the quality of an optimal-control solution.

In order to obtain such an estimate, which will depend on the spectrum of H_T , it is helpful to express the final state $|\Psi(T)\rangle$ as

$$|\Psi(T)\rangle = \langle\Psi_T|\Psi(T)|\Psi_T\rangle + P_e|\Psi(T)\rangle, \quad (14)$$

with the target state $|\Psi_T\rangle$, i.e., the ground state of H_T , and the projector P_e onto the space spanned by the excited states of H_T .

The expectation value of H_T with respect to $|\Psi(T)\rangle$ reads

$$\langle\Psi(T)|H_T|\Psi(T)\rangle = |\langle\Psi_T|\Psi(T)\rangle|^2 E_0 + \langle\phi|H_T|\phi\rangle, \quad (15)$$

with $|\phi\rangle = P_e|\Psi(T)\rangle$ and the ground-state energy E_0 of H_T . The norm of the vector $|\phi\rangle$ is given in terms of the state fidelity $F = |\langle\Psi_T|\Psi(T)\rangle|^2$ via the relation

$$\langle\phi|\phi\rangle = 1 - F. \quad (16)$$

With the inequality

$$\frac{\langle\phi|H_T|\phi\rangle}{\langle\phi|\phi\rangle} \geq E_1, \quad (17)$$

in terms of the energy E_1 of the first excited state of H_T , the state fidelity is bounded by

$$1 - F \leq \frac{\langle\Psi(T)|H_T|\Psi(T)\rangle - E_0}{E_1 - E_0}. \quad (18)$$

The state infidelity $1 - F$ can thus be bounded in terms of the ground-state energy E_0 , the first-excited-state energy E_1 of the Hamiltonian H_T , and the expectation value $\langle\Psi(T)|H_T|\Psi(T)\rangle$. At first sight, it might seem that evaluating this expectation value requires explicit construction

of the state vector $|\Psi(T)\rangle$. Since, however, the state vector $|\Psi(t)\rangle = U(t)|\Psi(0)\rangle$ follows the unitary dynamics $U(t)$ induced by the system Hamiltonian, the expectation value can be evaluated in terms of the initial state $|\Psi(0)\rangle$ and a time-evolved operator $U^\dagger(T)H_T U(T)$. The latter can be obtained by backward propagation of Eq. (1) and for any operator H_T expanded in terms of the operators $\{\mathbf{a}_j\}$ ($j \in [1, d]$), this can be done with the same effort as required for propagation of $\mathcal{I}(t)$. As long as expectation values with respect to the initial state $|\Psi(0)\rangle$ can be specified efficiently, as it is typically the case in problems of state preparation, adiabatic quantum computation, or quantum approximate optimization algorithms [27,39,40], the state fidelity F can be bounded efficiently by Eq. (18).

3. Desired unitary

Similar to the problem of state preparation, the task of realizing a specific unitary—the central problem in quantum simulation [41]—can also be addressed using the present approach, though there are some key differences. In the above problem of state preparation, there is not a unique choice of control target $\mathcal{I}_T$ for a given initial condition $\mathcal{I}(0)$. This is different for a control problem with the goal of realizing a given unitary $\mathcal{U}_T$. In this case, the control target corresponding to an initial condition $\mathcal{I}(0)$ must read $\mathcal{I}_T = \mathcal{U}_T \mathcal{I}(0) \mathcal{U}_T^\dagger$.

If there is a unitary V that commutes with $\mathcal{I}_T$, i.e., $[V, \mathcal{I}_T] = 0$, then the relation $\mathcal{I}_T = V \mathcal{I}_T V^\dagger = V \mathcal{U}_T \mathcal{I}(0) \mathcal{U}_T^\dagger V^\dagger$ also holds. Reaching the target $\mathcal{I}_T$ does thus not necessarily verify that the propagator $\mathcal{U}_T$ is realized. Ensuring that one operator $\mathcal{I}(t)$ with an initial condition $\mathcal{I}(0)$ evolves toward the target $\mathcal{I}_T = \mathcal{U}_T \mathcal{I}(0) \mathcal{U}_T^\dagger$ that is consistent with the unitary $\mathcal{U}_T$, therefore, does not necessarily guarantee that the unitary $\mathcal{U}_T$ is indeed realized. Similarly to the definition of a faithful objective function in terms of a set of initial and final states, the present approach also requires a set of initial conditions $\mathcal{I}_j(0)$ and corresponding targets $\mathcal{I}_{Tj} = \mathcal{U}_T \mathcal{I}_j(0) \mathcal{U}_T^\dagger$ for the definition of an objective function that is minimized exactly for the desired unitary $\mathcal{U}_T$. Unlike standard methods for gate characterization, which often require an exponentially large set of initial and final states [42,43], this operator-based approach typically requires only a small number of initial conditions [44].

A possible choice of a faithful objective function is given by

$$\mathcal{J}_{\mathcal{U}_T} = 1 - \frac{1}{N_c} \sum_{j=1}^{N_c} \frac{\text{tr}(\mathcal{I}_j(T) \mathcal{U}_T \mathcal{I}_j(0) \mathcal{U}_T^\dagger)}{\text{tr}(\mathcal{I}_j(0)^2)}, \quad (19)$$

with a sufficiently large number N_c of initial conditions $\mathcal{I}_j(0)$. The initial conditions $\mathcal{I}_j(0)$ can, e.g., always be chosen as a minimal set of operators from $\{\mathbf{a}_j\}$ such that

there is no operator in $SU(2^n)$ that commutes with all the transformed operators $\mathcal{U}_T \mathcal{I}_j(0) \mathcal{U}_T^\dagger$.

Since each summand in Eq. (19) can be evaluated analogously to Eq. (12), the objective function $\mathcal{J}_{\mathcal{U}_T}$ can indeed be evaluated with polynomial effort.

4. Numerical optimization

Once a control target $\mathcal{I}_T$ and an objective function, such as $\mathcal{J}$ [Eq. (12)] or $\mathcal{J}_{\mathcal{U}_T}$ [Eq. (19)], is specified, one can use any numerical pulse-shaping algorithm [1] to design a time-dependent Hamiltonian that realizes dynamics from $\mathcal{I}(0)$ to $\mathcal{I}(T)$, at a final time T , that is close to $\mathcal{I}_T$. Since Eq. (8) with an antisymmetric matrix K induces orthogonal (unitary and real) dynamics, any numerical algorithm that is applicable to the Schrödinger equation (such as KROTOV [45], GRAPE [13], or CRAB [16]) is directly applicable and techniques to construct, e.g., gradients with respect to control parameters also directly apply to Eq. (8) (for more details on the implementation, see Appendix B).

Since any such optimization is based on numerically exact integration of Eq. (8), there is no restriction to adiabaticity and the duration T of the control protocol can be chosen as short as is allowed by the physical constraints of the underlying system.

E. A bird's eye view on the algorithm

Putting everything together, the resultant methodology for state control can be summarized in terms of the following algorithm.

Given a Hamiltonian with tunable time dependence [Eq. (3)] and a set of operators $\{\mathbf{a}_j\}$, such that the closed-commutator relationships [Eq. (5)] are satisfied:

- (1) Choose an initial condition $\mathcal{I}(0) = \sum_j a_j(0) \mathbf{a}_j$, with a nondegenerate ground state.
- (2) Find a control target $\mathcal{I}_T$ that implicitly specifies the target state and that needs to be reachable from initial condition $\mathcal{I}(0)$ with the dynamics induced by the system Hamiltonian.
- (3) Design an optimized time dependence of the system Hamiltonian [Eq. (3)], with the dynamics described by Eq. (8), to minimize an objective function formulated in terms of the expansion coefficients of the control target $\mathcal{I}_T$ in the set of operators $\{\mathbf{a}_j\}$. The design of this time dependence can be pursued with any pulse-shaping algorithm that applies to linear differential equations.

The resultant time-dependent Hamiltonian is such that the system, if initialized in the ground state of $\mathcal{I}(0)$, evolves toward the ground state of $\mathcal{I}_T$.

The algorithm for control of unitary dynamics is largely equivalent but it requires more than one initial condition,

and the target for each initial condition is defined uniquely through the desired unitary.

III. STATE PREPARATION IN A DRIVEN SPIN CHAIN

The approach outlined in Sec. II is applicable to any set of operators satisfying Eq. (5). The benefits of this approach depend on the size d of the resulting set $\{\mathbf{a}_j\}$. There does not seem to be an existing algebraic framework to determine the system Hamiltonians with an associated set of operators $\{\mathbf{a}_j\}$ that is significantly smaller than the size of the system Hilbert space, but the existence of such Hamiltonians can be demonstrated with explicit examples.

Section V provides a list of exemplary spin systems and sets of operators with a size that is polynomial in the number of spins. Since such a list of examples is necessarily a bit technical, the following discussion and the subsequent Sec. IV will illustrate the application of the general control framework outlined in Sec. II with the specific case of a linear spin chain with nearest-neighbor interactions, as depicted in Fig. 1.

In such a configuration, the system dynamics are induced by the system Hamiltonian

$$H(t) = g \sum_{j=1}^{n-1} X_j X_{j+1} + \sum_{j=1}^n f_j(t) Z_j + \sum_{j \in \{1, n\}} w_j(t) X_j, \quad (20)$$

which consists of a constant interaction term and single-qubit control terms. The constant term contains nearest-neighbor interactions in terms of the Pauli X operators, while the single-qubit control terms, with tunable time-dependent functions $f_j(t)$ and $w_j(t)$, contain the Pauli Z operators and the Pauli X operators on the end spins of the chain (see Fig. 1).

Without the single-qubit X terms, the Hamiltonian would correspond to the regular Ising model. The parity conservation of the Ising model imposes limits on the achievable control and the Ising model admits a treatment in terms of free fermions [46] that helps to overcome the exponential effort required to simulate the system dynamics.



FIG. 1. A linear spin chain of n qubits with nearest-neighbor XX interactions. Single-qubit Z driving and X driving on the end qubits enables efficient preparation of various quantum states, including Greenberger-Horne-Zeilinger (GHZ) and cluster states, and the realization of effective dynamics with multiqubit interactions.

The Hamiltonian $H(t)$ in Eq. (20), on the other hand, has no conserved quantities for $g \neq 0$ and general time-dependent functions $f_j(t)$ and $w_j(t)$; i.e., there is no operator A (apart from multiples of the identity) that commutes with all operators Z_j , X_1 , X_n , and $\sum_{j=1}^{n-1} X_j X_{j+1}$ (as discussed in more detail in Appendix A).

The Lie algebra generated by nested commutators of the individual terms in the Hamiltonian [Eq. (20)] contains $d = 2n^2 + 3n + 1$ terms as discussed in Sec. V A and they are given by

$$Z_i, \quad (21a)$$

with $i \in [1, n]$,

$$X_j Z_{jk} X_{j+k+1}, \quad (21b)$$

$$Y_j Z_{jk} Y_{j+k+1}, \quad (21c)$$

$$X_j Z_{jk} Y_{j+k+1}, \quad (21d)$$

$$Y_j Z_{jk} X_{j+k+1}, \quad (21e)$$

with $j \in [1, n - k - 1]$, $k \in [0, n - 2]$, and the shorthand notation $Z_{jk} = \prod_{i=1}^k Z_{i+j}$,

$$Z_{0j} X_{j+1}, \quad (21f)$$

$$Z_{0j} Y_{j+1}, \quad (21g)$$

$$X_{n-j} Z_{(n-j)j}, \quad (21h)$$

$$Y_{n-j} Z_{(n-j)j}, \quad (21i)$$

with $j \in [0, n - 1]$, and, finally,

$$\prod_{i=1}^n Z_i. \quad (21j)$$

While the system Hamiltonian [Eq. (20)] contains only the terms Z_j , $X_j X_{j+1}$, X_1 , and X_n , the operator $\mathcal{I}(t)$ needs to be expanded in terms of the full set of Eq. (21) so that Eq. (5) is satisfied and the ansatz in Eq. (4) is sufficiently general to allow for integration of Eq. (1).

Since Eq. (21) contains a quadratic number of terms, the present framework reduces a control problem in an exponentially large Hilbert space to a problem in a vector space of quadratic growth. Due to this quadratic scaling, it is possible to design optimal-control protocols for spin chains

of lengths that are inaccessible for approaches based on quantum states.

The following examples are motivated by typical problems of quantum simulation and state preparation or stabilization. They exploit the fact that the Lie algebra given in Eq. (21) contains three-body interactions such as $X_j Z_{j+1} X_{j+2}$ or even n -body interactions that cannot be realized by static means. The goal of the following two sections, Secs. III A and IV A, will thus be to find time-dependent functions $f_j(t)$ and $w_j(t)$ in the system Hamiltonian $H(t)$ [Eq. (20)] that ensure that the system dynamics with only the two-body interaction in Eq. (20) are helpful for preparation of states or realization of propagators that are characterized by three-body interactions or interactions between more than three spins.

A. Target Hamiltonians

Following the discussion of Sec. II D 1, one can seek to find time-dependent functions $f_j(t)$ and $w_j(t)$ in the system Hamiltonian $H(t)$ [Eq. (20)], such that the system evolves from an initial state to a desired final state. Typical choices for an initial state are given by separable states that can be specified efficiently but final states of interest are often highly entangled states. The following discussion will thus avoid the explicit specification of a state vector, but both the initial state and the final state to be realized will be specified in terms of a Hamiltonian to which they are the ground state.

A natural choice of noninteracting Hamiltonian based on Eq. (20) is given by the initial conditions $f_j(0) = f_k(0)$ for all j, k , $f_j(0) \gg g$, and $w_j(0) = 0$ for all j , i.e., noninteracting spins with a single-spin- Z Hamiltonian.

Crucially, the Hamiltonians defining the final state to be realized do not need to be of the form of the system Hamiltonian in Eq. (20) but any Hamiltonian comprised of the operators given in Eq. (21), including three-spin interactions or interactions between more than three spins, is a viable choice.

As interacting Hamiltonians defining target states, the subsequent discussion encompasses the Hamiltonian

$$H_G = - \sum_{j=1}^{n-1} X_j X_{j+1} - \prod_{i=1}^n Z_i, \quad (22)$$

the ground state of which is a Greenberger-Horne-Zeilinger (GHZ) state, which holds significant importance in the fields of quantum sensing [47], quantum communication [48,49], and macroscopic quantum mechanics [50], attracting great experimental interest [51,52].

Another interesting example is the Hamiltonian

$$H_C = Z_1 X_2 + \sum_{j=1}^{n-2} X_j Z_{j+1} X_{j+2} + X_{n-1} Z_n, \quad (23)$$

the ground state of which is the one-dimensional n -qubit cluster state for measurement-based quantum computation [53].

Since the Hamiltonians H_G and H_C admit an analytic construction of a target invariant, the following discussion also includes the example

$$H_D = H_C + \sum_{j=1}^{n-1} X_j X_{j+1}, \quad (24)$$

to demonstrate that no analytic solutions are necessary preconditions for the present approach. In particular, this Hamiltonian has a vanishing gap in the limit $n \rightarrow \infty$, which rules out optimal-control techniques based on matrix-product states (MPSs) [16] as practical alternatives.

B. Control targets

As discussed in Sec. II D 1, for the present problem, a natural choice for the initial condition $\mathcal{I}(0)$ is given by

$$\mathcal{I}_0 = \sum_j Z_j. \quad (25)$$

The definition of the corresponding control target, however, requires some care, and it needs to be done separately for the three different control problems defined in terms of the three Hamiltonians H_G , H_C , and H_D .

1. Control target for GHZ-state Hamiltonian

Even though it is generally not possible to define the control target $\mathcal{I}_T$ in terms of the Hamiltonian the ground state of which is supposed to be realized, this is possible in the case of H_G . Since H_G can be expressed as

$$H_G = W_G^\dagger \mathcal{I}_0 W_G, \quad (26)$$

with

$$W_G = \left(\prod_{k=1}^{n-1} e^{-i\frac{\pi}{4}(X_k Y_{k+1})} \right) e^{i\frac{\pi}{4}(X_1 - X_n)}, \quad (27)$$

where the factors in the product are in increasing order in the index k , the two operators H_G and $\mathcal{I}_0$ have the same spectrum; and since every factor in W_G is induced by elements of the Lie algebra [Eq. (21)], the unitary W_G can indeed be realized with the Hamiltonian $H(t)$ in Eq. (20). The control target $\mathcal{I}_G = H_G$ is thus a valid choice for the task of realizing the ground state of H_G .

2. Control target for cluster-state Hamiltonian

The construction of control target $\mathcal{I}_C$ for the task of realizing the ground state of H_C is very similar to the case of H_G above.

H_C can be expressed as

$$H_C = W_C^\dagger \mathcal{I}_0 W_C, \quad (28)$$

with

$$W_C = \left(\prod_{k=1}^{n-1} e^{(-1)^k i\frac{\pi}{4}(X_k X_{k+1})} \right) e^{i\frac{\pi}{4}(X_1 + X_n)}. \quad (29)$$

Also here, all the terms in W_C are induced by elements of the Lie algebra [Eq. (21)]. Since W_C is unitary, the control target $\mathcal{I}_C = H_C$ is thus a valid choice for the task of realizing the ground state of H_C starting with the ground state of $\mathcal{I}_0$.

3. Control target for H_D

While control targets could be defined analytically for the control problem of realizing the ground state of H_G and H_C , the case of H_D seems to require a numerical construction. The target $\mathcal{I}_D = H_D$ is unreachable from $\mathcal{I}(0)$ with unitary dynamics, so a numerical target $\mathcal{I}_D$ with the same ground state as H_D must be constructed.

Propagating $\mathcal{I}(t)$ according to Eq. (1) yields operators that are naturally reachable with the available dynamics and choosing a Hamiltonian $H_a(t)$ with an adiabatically slow time dependence can help to find an operator $\mathcal{I}_a(T_a)$ the ground state of which is also the ground state of $H_a(T_a)$ at the end of the adiabatic dynamics.

The following example is based on the choice

$$H_a(t) = \left(1 - \frac{t}{T_a}\right) H_I + \frac{t}{T_a} H_D + \frac{t}{T_a} \left(1 - \frac{t}{T_a}\right) H_B, \quad (30)$$

where the last term with

$$H_B = \sum_j Z_j + \sum_{j=1}^{n-1} X_j X_{j+1} + X_1 + X_n \quad (31)$$

vanishes at the initial and final points in time ($t = 0$ and $t = T_a$) but turns some level crossings into avoided crossings, so that the adiabatic dynamics do indeed ensure transfer from the ground state of H_I to the ground state of H_D .

A control target $\mathcal{I}_D = \mathcal{I}_a(T_a)$ can be constructed numerically with the adiabaticity parameter T_a sufficiently large. Since any numerical propagation is based on Eq. (8), the numerical effort follows the quadratic scaling of the Lie algebra [Eq. (21)] and not the exponential scaling of the Hilbert space.

Once the control target is defined, it can be used to construct a time-dependent Hamiltonian that achieves the state transfer in a diabatic fashion.

C. Results: State transfer

In Fig. 2(a), we depict the infidelity $\mathcal{J}$ [Eq. (12)] obtained with numerically optimized time-dependent Hamiltonians as a function of the number n of spins in a chain, with n ranging from 5 to 50. The different solid symbols correspond to the three different target operators discussed in Sec. III A, namely, H_G [Eq. (22)] (red diamonds), H_C [Eq. (23)] (blue squares), and H_D [Eq. (24)] (black triangles). The optimizations for H_G and H_C are intentionally stopped when the infidelities fall below 10^{-6} . The optimization for H_D , however, requires a longer running time and is therefore terminated once a maximum number of iterations, around 10^3 , is reached.

The empty red diamonds and blue squares depict the bound of Eq. (18) on the state fidelity for the ground states of H_G and H_C . The gap between the infidelities for the operators and the bounds on the state infidelity grows approximately linearly with the number of qubits (for more details, see Appendix C). For practical implementations, this growing gap does not seem to pose a relevant limitation, since state infidelities on the order of 10^{-5} are below what is currently achievable or verifiable even from few-qubit states [54].

The Hamiltonian H_D is gapless, i.e., the gap between the ground state and the first excited state vanishes in the thermodynamic limit. For finite-size chains, this gap gets progressively smaller with increasing system size, making the bound of Eq. (18) unsuited for H_D . The state fidelity in this case is thus estimated from numerical propagations with MPSs [55,56] for qubit numbers $n \leq 30$, as depicted

by the empty triangles in Fig. 2(a). Despite the efficient matrix-product representation of the initial and final states, the states at in-between times created by the controlled dynamics for $n \geq 35$ require bond dimensions exceeding 500, rendering numerical propagation impractical. Both the operator infidelities [Eq. (12)] and the state infidelities are larger than for H_G and H_C . This is mostly due to the closing gap of H_D , which results in increasing errors in the adiabatic evolution used to obtain the target $\mathcal{I}_D$. The optimization of the control pulses is made consistent with the estimated error of $\mathcal{I}_D$, i.e., the optimization algorithm is terminated when infidelities of the order of the accuracy of $\mathcal{I}_D$ are reached. For any finite system, this error can be reduced further if needed and the present accuracy is chosen in accordance with the practical limitations of existing quantum devices [54].

In all three cases shown in Fig. 2(a), the achieved state fidelities confirm successful optimal control for system sizes far outside the regime accessible to explicit state control. All deviations from perfect vanishing infidelity are due to finite numerical accuracy. In Fig. 2, the accuracy is chosen to not exceed the limits imposed by system imperfections of current or foreseeable quantum devices too excessively, but higher accuracies can be reached if technological advances require more accurate solutions.

Interestingly, because of the constant interaction term in the system Hamiltonian [Eq. (20)], there is a minimal time required for the state transfer, also referred to as the quantum speed limit [57]. In order to obtain infidelities as low as in Fig. 2, the duration of the controlled dynamics needs

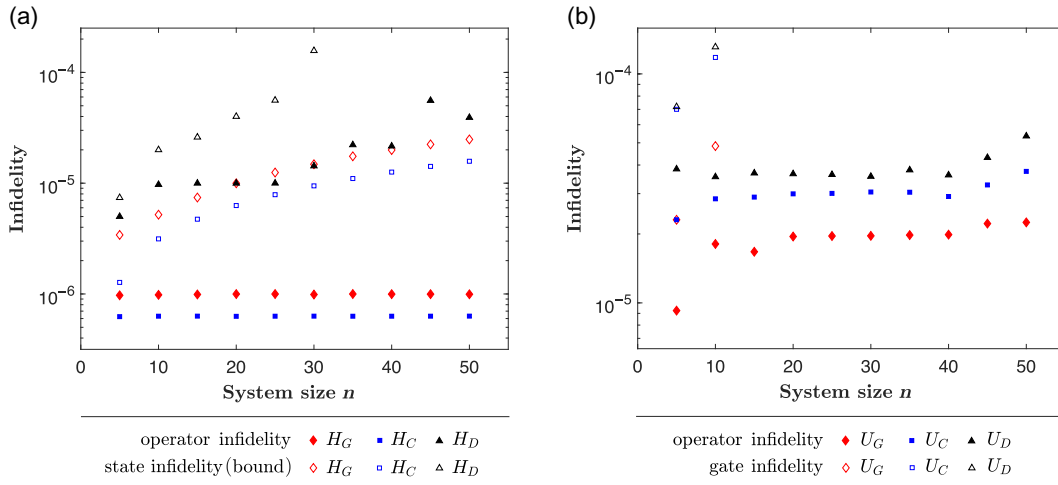


FIG. 2. The infidelity for the dynamics for a spin chain [Eq. (20)] with optimized single-qubit driving, as a function of the system size n : (a) ground state; (b) propagator. The solid shapes depict (a) operator infidelities $\mathcal{J}$ [Eq. (12)] in log scale for state transfer and (b) operator infidelities $\mathcal{J}_{U_T}$ [Eq. (19)] for quantum gates. The empty diamonds and squares (a) depict bounds [Eq. (18)] on state infidelities, while the empty triangles (a) represent state infidelities based on matrix-product-state (MPS) representations and the empty shapes (b) depict gate infidelities. As result of the optimization, the values of the infidelities $\mathcal{J}$ and $\mathcal{J}_{U_T}$ are largely independent of the system size n . Actual state and gate infidelities do grow with increasing system size but they remain well below what can be achieved given the experimental imperfections of actual quantum devices.

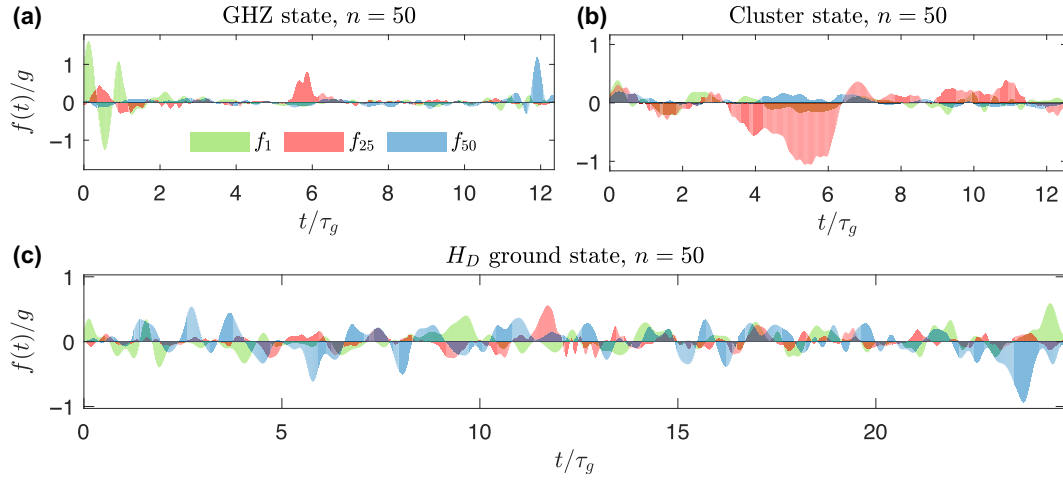


FIG. 3. The optimized pulses, f_1 , f_{25} , and f_{50} , for state transfer in a chain with 50 spins as function of time t in multiples of the interaction time $\tau_g = 2\pi/g$: (a) GHZ state, $n = 50$; (b) cluster state, $n = 50$; (c) H_D ground state, $n = 50$. The operator infidelities obtained with these pulses are (a) approximately 10^{-5} for the GHZ state, (b) approximately 10^{-5} for the cluster state, and (c) approximately 2×10^{-5} for the ground state of H_D . The duration of the controlled dynamics is longer for H_D in (c) than in the other cases. This is likely due to the difficulty in realizing the ground state of a gapless model.

to increase with the system size, but a modest approximately linear increase of approximately $n\tau_g/4$ for H_G and H_C , and approximately $n\tau_g/2$ for H_D , with the qubit number n and the time scale $\tau_g = 2\pi/g$ given by the interaction constant g in Eq. (20), is sufficient for the ground-state transfer. The time dependence in the system Hamiltonian is parametrized in terms of piecewise constant pulses that are suitable for numerical-optimization algorithms. To ensure the linear increase in gate time while maintaining a constant control duration per time bin across all system sizes, the number of time bins in the pulse must also increase linearly with the system size. The results in Fig. 2 are obtained with pulses of $10n$ bins, except for U_G with $20n$ bins, but the exact number can be adjusted depending on the desired infidelity.

Despite the challenging goal of realizing eigenstates of Hamiltonians beyond pairwise interactions, the necessary control pulses do not exhibit undesired characteristics such as excessively high amplitudes or frequencies. Even optimizations without penalty for high amplitudes do not yield amplitudes exceeding the coupling strength g by a factor of 2. The spectral width obtained with a standard optimization (see Appendix B 3) is not excessive but it is broader than necessary. It is thus possible to smooth pulses with only a moderate increase in infidelity and to use these smoothed pulses as initial conditions for further optimization.

In Fig. 3, we depict pulse shapes obtained in such a fashion for $f_1(t)$, $f_{25}(t)$, and $f_{50}(t)$ in a chain with $n = 50$ spins, i.e., driving patterns for the spins at the edges and center of the chain. In addition to the smooth temporal shape, the highest amplitudes are of the order of g and even this moderately strong driving arises only in short intervals.

For the GHZ state, the optimized pulses hint at a pattern of sequential driving of the spins from left to right along the chain, as the pulses for the spins on the left peak first. This is shown in Fig. 3(a) for the first, 25th, and 50th spins, and this sequential pattern does indeed occur for the pulses of the other spins in the chain.

The pulse shapes for smaller chains have qualitatively similar shapes but both the duration and the number of time bins are approximately proportional to the system size. The pulse data for all spins and system sizes ranging from 5 to 50 are provided in Ref. [58].

IV. REALIZATION OF PROPAGATORS

Preparing an eigenstate of a Hamiltonian with specific interactions has applications in computational problems [59,60]. In quantum simulation [41], on the other hand, it is of interest to explore the dynamics induced by a given Hamiltonian. Such applications require—in addition to an initial-state preparation—the realization of propagators. These propagators, characterized by Hamiltonians beyond pairwise interactions, such as H_G , H_C , and H_D discussed in Sec. III A, cannot be realized by static means, and the present approach can be used to find time-dependent functions $f_j(t)$, $w_1(t)$, and $w_n(t)$ in the system Hamiltonian $H(t)$ [Eq. (20)], such that the resultant propagator is of the form $\exp(-iH_T T)$, with a Hamiltonian including more-than-pairwise interactions at a given time T .

The realization of such effective Hamiltonians is commonly pursued based on Floquet theory [61] and the present approach allows us to go beyond the common perturbative treatment that is typically required [62].

The realization of the desired propagators is exemplified here in more detail for $\exp(-i\pi/8 H_G)$, $\exp(-i\pi/8 H_C)$, and $\exp(-i\pi/8 H_D)$, given by the three Hamiltonians H_G [Eq. (22)], H_C [Eq. (23)], and H_D [Eq. (24)], and system dynamics in terms of the Hamiltonian $H(t)$ in Eq. (20).

A. Objective function

The crucial question that will ultimately determine the required numerical effort is how many (and which) initial conditions $\mathcal{I}_j(0)$ for the infidelity $\mathcal{J}_{U_T}$ in Eq. (19) need to be considered in order to obtain a faithful objective function.

With the initial conditions

$$\mathcal{I}_j(0) = Z_j, \quad (32a)$$

for $j \in [1, n]$,

$$\mathcal{I}_{j+n}(0) = X_j X_{j+1}, \quad (32b)$$

for $j \in [1, n-1]$, and

$$\mathcal{I}_{2n}(0) = X_1 + X_n, \quad (32c)$$

the infidelity $\mathcal{J}_{U_T}$ in Eq. (19) vanishes exactly for the target gate U_T , for any target that is reachable with $H(t)$ in Eq. (20). That is, the relation $U\mathcal{I}_j(0)U^\dagger = U_T\mathcal{I}_j(0)U_T^\dagger$ can be simultaneously satisfied for all these choices $\mathcal{I}_j(0)$ only if $U = U_T \exp(i\varphi)$, where $\exp(i\varphi)$ is a global phase factor.

To see that this is indeed the case, it is helpful to note that the set of relations $U\mathcal{I}_j(0)U^\dagger = U_T\mathcal{I}_j(0)U_T^\dagger$ is equivalent to the set of commutation relations

$$[U_T^\dagger U, \mathcal{I}_j(0)] = 0. \quad (33)$$

As shown in Appendix A, the only operators that commute with each of the operators in Eq. (32) are multiples of the identity, which leaves $U_T^\dagger U = \exp(i\varphi)\mathbb{1}$ as the only solution.

While this provides a faithful objective function, its use in an optimization implies the evaluation of $2n$ summands in Eq. (19) at any step in the optimization. For the sake of efficiency, it can be preferable to use the objective functional $\mathcal{J}_{U_T}$ with only five initial conditions:

$$\mathcal{I}_1(0) = \sum_k Z_{2k+1}, \quad (34a)$$

$$\mathcal{I}_2(0) = \sum_k Z_{2k}, \quad (34b)$$

$$\mathcal{I}_3(0) = \sum_k X_{2k+1} X_{2k+2}, \quad (34c)$$

$$\mathcal{I}_4(0) = \sum_k X_{2k} X_{2k+1}, \quad (34d)$$

$$\mathcal{I}_5(0) = X_1 + X_n. \quad (34e)$$

Even though the optimal value can be obtained for propagators different than U_T , the optimizations do not seem to converge to such a solution in practice. Since verification requires only a single propagation, it is numerically advantageous to use this objective function [with Eqs. (34) as initial conditions] for the optimization and eventually use the faithful objective function [with Eqs. (32) as initial conditions] only for verification of the final solution.

B. Results: Propagators

In Fig. 2(b), we depict the infidelities $\mathcal{J}_{U_T}$, defined in Eq. (19) together with Eq. (32), as a function of the system size n . The solid red diamonds, blue squares, and black triangles correspond to the target unitaries $U_G = \exp(-i\pi/8 H_G)$, $U_C = \exp(-i\pi/8 H_C)$, and $U_D = \exp(-i\pi/8 H_D)$, respectively. This is based on optimized piecewise constant pulses with a duration of approximately $n\tau_g$ and $20n$ bins for U_G , and approximately τ_g and $10n$ bins for U_C and U_D .

The empty shapes in the figure show actual gate infidelities, $1 - |\text{tr}(U^\dagger(T)U_T)|^2 / 2^{2n}$, obtained with numerically exact integration of the Schrödinger equation. Since this type of verification is limited by the exponential scaling of the Hilbert space, actual gate infidelities are shown for up to $n = 10$ only. Within what is numerically achievable, the gate infidelities do confirm the success of the control protocols designed with the present framework and, similarly to the task of state preparation, the realization of desired propagators is achieved with infidelities far below what could be experimentally resolved with existing technology [5,6].

Also, the duration of the controlled dynamics required for the realization of a desired propagator has a fundamental limit given by the time scale $\tau_g = 2\pi/g$. The numerically observed minimal time required to implement the unitaries induced by H_C and H_D is independent of the system size but the minimal time required to implement the unitary induced by H_G scales linearly in the number of qubits. Given that H_C and H_D contain at most three-body interactions, whereas H_G contains an n -body interaction, i.e., an interaction the type of which changes with increasing system size n , the numerically observed dependence of minimal durations of controlled dynamics seem consistent with the underlying problem, which generates some confidence that the obtained solutions are close to the actual global solution of the control problem.

In Fig. 4, we depict the optimized driving patterns f_1 , f_{25} , and f_{50} obtained with the same procedure of smoothing and reoptimization as in Fig. 3. Given the fundamental difficulty of quantum simulating the n -body interaction $\prod_{i=1}^n Z_i$ in U_G with a system Hamiltonian including only pairwise interactions, the required duration of the controlled dynamics is substantially longer than in the cases

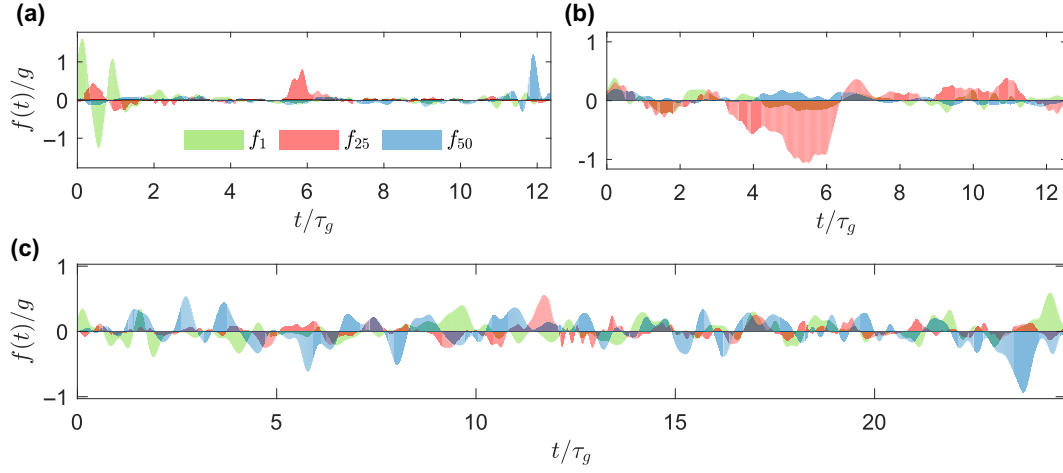


FIG. 4. The optimized pulses, f_1 , f_{25} , and f_{50} , for the realization of propagators in a chain with 50 spins as a function of time t , in units of τ_g : (a) U_C propagator, $n = 50$; (b) U_D propagator, $n = 50$; (c) U_G propagator, $n = 50$. The resultant operator infidelities are (a) approximately 4×10^{-5} for U_C , (b) approximately 9×10^{-5} for U_D , and (c) approximately 10^{-4} for U_G . For U_G , $f_{50} = f_1$ and hence is not shown. The pulses for U_G in (c) are longer due to the difficulty in quantum simulating an n -body interaction with a pairwise controlled Hamiltonian.

of U_C and U_D . Quite surprisingly, the second half of the time period shown in Fig. 4(c) is essentially uncontrolled dynamics. Nevertheless, the full duration of $50\tau_g$ seems to be necessary in order to reach high fidelities, but the controlled dynamics during the first half seems to drive the system to a state that evolves mostly under the influence of the XX interactions toward the target state in the interval $[25\tau_g, 50\tau_g]$. The pulse data for smaller system sizes are provided in Ref. [58].

V. MORE SETS OF OPERATORS WITH POLYNOMIAL SCALING

While the discussion in Secs. III and IV is meant to exemplify the use of the current approach for actual control problems, a similarly detailed discussion for further examples would be repetitive. The goal of this section is thus to provide further insight into sets of operators for which the present approach provides an advantage over treatments in terms of state vectors. In the following, a few exemplary algebras with polynomial scaling are provided for different interaction geometries. The corresponding commutation relations are available at Ref. [58].

A. Spin chain

The Lie algebra specified in Eq. (21) is generated by the terms

$$\mathfrak{h}_j = Z_j, \quad (35a)$$

with $j \in [1, n]$,

$$\mathfrak{h}_{j+n} = X_j X_{j+1}, \quad (35b)$$

with $j \in [1, n-1]$, and

$$\mathfrak{h}_{2n} = X_1, \quad (35c)$$

$$\mathfrak{h}_{2n+1} = X_n. \quad (35d)$$

The commutators between terms in Eq. (35a) and terms in Eq. (35b) yield operators of the form $X_j Y_{j+1}$ and $Y_j X_{j+1}$, and the commutators between those and terms in Eq. (35a) yields operators of the form $Y_j Y_{j+1}$. The Lie algebra thus contains the terms

$$X_j X_{j+1}, \quad X_j Y_{j+1}, \quad Y_j X_{j+1}, \quad Y_j Y_{j+1}. \quad (36)$$

The commutators between such terms yield operators of the form $A_j Z_{j+1} B_{j+2}$ (with A and $B \in \{X, Y\}$), and nested commutators with several terms of Eq. (36) yield operators of the form

$$A_j Z_{j+1} \dots Z_{j+k} B_{j+k+1}. \quad (37)$$

The commutators between these $(k+2)$ -body interactions and the terms X_1 and X_n [Eqs. (35c) and (35d)] yield the terms

$$Z_1 \dots Z_l A_{l+1}, \quad (38a)$$

$$A_{n-l} Z_{n-l+1} \dots Z_n, \quad (38b)$$

and

$$Z_1 \dots Z_n. \quad (38c)$$

These are exactly the terms specified in Eq. (21) and they do indeed form a closed Lie algebra.

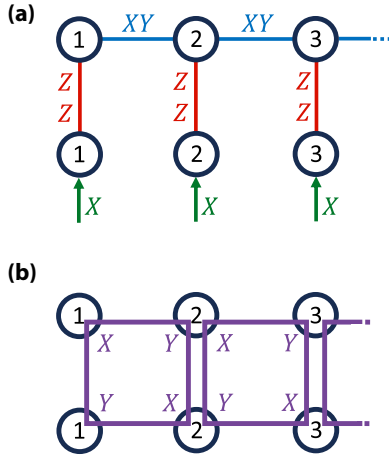


FIG. 5. (a) A spin comb with nearest-neighbor XY interactions in the top chain and ZZ interactions between spins of different chains. (b) The single-spin X driving in (a) enables the realization of effective dynamics with four-spin interactions matching the toric code plaquette operators given in Eq. (42).

With n terms in Eq. (35a), $2n(n-1)$ terms in Eq. (37) [that include Eqs. (35b) and (36) as special cases], $2n-1$ terms from Eqs. (38a) and (38b) each, as well as one term in Eqs. (35c), (35d) and (38c), respectively, the total number of elements in the Lie algebra is $d = 2n^2 + 3n + 1$.

B. Driven spin comb

In Fig. 5(a), we depict an interaction geometry that results in a Lie algebra of quadratic size in the qubit number n that can be used to realize elementary building blocks of topologically protected quantum information processing [63]. It is a comb structure with a linear chain of $m = n/2$ qubits with nearest-neighbor interactions and a second chain of another m qubits interacting only with qubits on the first chain.

Because of this geometry, each Pauli operator carries two indices. The first (lower) index specifies the position of the qubit within its chain and the second (upper) index identifies the chain itself (1 for the top chain and 2 for the bottom chain).

The elementary Hamiltonian terms $\mathfrak{h}_i$ (for the definition of a system Hamiltonian in Eq. (3)) are given by

$$\mathfrak{h}_j = Z_j^1 Z_j^2, \quad (39a)$$

with $j \in [1, m]$,

$$\mathfrak{h}_{j+m} = X_j^2, \quad (39b)$$

with $j \in [1, m]$, and

$$\mathfrak{h}_{j+2m} = X_j^1 Y_{j+1}^1, \quad (39c)$$

with $j \in [1, m-1]$. In order to understand the Lie algebra generated by Eq. (34)—and, in particular, its scaling with m —it is instructive to start with the Lie algebra generated by the terms in Eq. (39c) only. The terms in Eq. (39c) form a subset of the terms in Eq. (36) and, similarly to the discussion in Sec. V A, the resultant Lie algebra is comprised of the terms

$$X_j^1 Z_{jk} Y_{j+k+1}^1, \quad (40)$$

with $j+k+1 \leq m$ and the shorthand notation $Z_{jk} = \prod_{i=1}^k Z_{i+j}^1$.

Commutation between the terms in Eq. (40) and the terms in Eq. (39a) yields the terms

$$Y_j^1 Z_{jk} Y_{j+k+1}^1 Z_j^2, \quad (41a)$$

$$X_j^1 Z_{jk} X_{j+k+1}^1 Z_{j+k+1}^2, \quad (41b)$$

$$Y_j^1 Z_{jk} X_{j+k+1}^1 Z_j^2 Z_{j+k+1}^2. \quad (41c)$$

With $m(m-1)/2$ terms in Eq. (40) [that includes the elements in Eq. (39c)], three terms in Eq. (41), and m elements in Eq. (39a), the Lie algebra generated by the terms in Eqs. (39a) and (39c) thus contains $2m^2 - m$ terms.

Commutation with the terms in Eq. (39b) yields terms of similar structure to the terms in Eq. (41), but with operators Z_j^2 and/or Z_{j+k+1}^2 replaced by the corresponding operator of X or Y type. The number of operators of the type in Eqs. (41a) and (41b) is thus increased by a factor of 3 and the number of operators of the type in Eq. (41c) is increased by a factor of 9. The Lie algebra generated by all the terms in Eq. (39) thus has $3m(3m-1)/2$ terms.

Within this Lie algebra are terms of the form

$$\mathcal{Q}_j = X_j^1 Y_{j+1}^1 Y_j^2 X_{j+1}^2, \quad (42)$$

corresponding to a four-body interaction on four spins, forming a square as depicted in Fig. 5(b). The operators $\mathcal{Q}_j$ and $\mathcal{Q}_{j+1}$ act on two different quartets of spins with an overlap on two spins (with index $j+1$). The factor of $\mathcal{Q}_j$ on these spins is given by $Y_{j+1}^1 X_{j+1}^2$ and the factor of $\mathcal{Q}_{j+1}$ on these spins is given by $X_{j+1}^1 Y_{j+1}^2$. All the operators $\mathcal{Q}_j$ are thus mutually commuting, even though their single-spin factors on overlapping spins are not mutually commuting. The present example is thus suitable for the realization of a ribbon of plaquette operators of the toric code [25].

C. Hexagonal spin ladder

In Fig. 6, we depict a spin ladder with hexagonal structures, similar the Kitaev honeycomb model [25] but with the two interactions of the spin at the bottom of each hexagon commuting with each other. This interaction geometry results in a Lie algebra of dimension

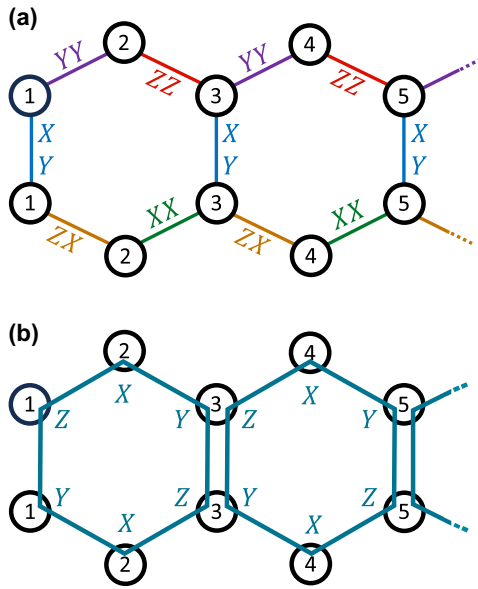


FIG. 6. (a) A spin ladder with hexagonal structures. Each spin interacts with its nearest neighbors but—in contrast to the Kitaev honeycomb model, which includes only mutually noncommuting interactions for any spin—there is one spin (at the bottom of each hexagon) that has two commuting interactions. (b) The interaction geometry in (a) results in a Lie algebra of quadratic size, with elements including the plaquette operators given in Eq. (44), which are crucial in the field of topological stabilizer codes.

$(25n^2 - 40n + 12)/32$ with $n = 4n_h + 2$ spins, where n_h is the number of hexagons. In contrast, the interaction geometry of the original Kitaev honeycomb model scales exponentially $(2^{n_h} n(n-1)/2)$.

The individual operators $\mathfrak{h}_j$ entering the system Hamiltonian read

$$\mathfrak{h}_j = Y_{2j-1}^1 Y_{2j}^1, \quad (43a)$$

$$\mathfrak{h}_{j+(m-1)/2} = Z_{2j}^1 Z_{2j+1}^1, \quad (43b)$$

$$\mathfrak{h}_{j+m-1} = X_{2j}^2 X_{2j+1}^2, \quad (43c)$$

$$\mathfrak{h}_{j+(3m-3)/2} = Z_{2j-1}^2 X_{2j}^2, \quad (43d)$$

$$\mathfrak{h}_{l+2m-2} = X_{2l-1}^1 Y_{2l-1}^2, \quad (43e)$$

with $m = n/2$, $j \in [1, (m-1)/2]$, $l \in [1, (m+1)/2]$. The resultant Lie algebra can be constructed systematically similarly to the discussion in Sec. V A; because of the more intricate interaction geometry, the exact form of the individual elements is a bit bulkier and it is deferred to Appendix D.

Crucially, the Lie algebra contains the six-body plaquette operators

$$P_j = Z_{2j-1}^1 X_{2j}^1 Y_{2j+1}^1 Y_{2j-1}^2 X_{2j}^2 Z_{2j+1}^2, \quad (44)$$

as depicted schematically in Fig. 6(b). These operators, which commute with the Kitaev honeycomb Hamiltonian [25], form a central part in the realization of error-correcting surface codes on hexagonal lattices [64,65]. In particular, plaquette operators together with two-body operators such as $X_{2l-1}^1 Y_{2l-1}^2$, can form the basis for stabilizer operators, as exemplified by the XYZ^2 topological stabilizer code [66]. The present framework can thus be used to aid the realization of quantum error correction.

VI. DISCUSSION AND OUTLOOK

The techniques discussed in this paper integrate into, and form a part of, the spectrum of quantum optimal-control techniques. They are inspired by control techniques that are based on analytic forms $\mathcal{I}_a(t)$ of dynamical quantum invariants. For the explicit system Hamiltonian $H(t)$ [Eq. (20)] discussed in this paper, such an analytic form $\mathcal{I}_a(t)$ would need to be formulated so that, a Hamiltonian that satisfies Eq. (1) together with $\mathcal{I}_a(t)$ contains only the terms Z_j ($j \in [1, n]$), X_1 , and X_n and the interaction term $\sum_{j=1}^n X_j X_{j+1}$, but none of the additional terms listed in Eq. (21). Finding such an analytic expression seems to be an insurmountable task and the main goal of this paper is to avoid the dependence on such analytic expressions.

Notable existing approaches with goals similar to those pursued in this paper include counterdiabatic driving [67–70], which requires additional terms in the system Hamiltonian to ensure that the system dynamics follow adiabatic evolution, even beyond the regime in which the adiabatic approximation holds. For the system Hamiltonian $H(t)$ [Eq. (20)], counterdiabatic terms would typically include terms listed in Eq. (21) but that are not contained in the system Hamiltonian in Eq. (20). Such terms can typically not be realized exactly but they can be approximated as the result of higher-order processes in a time-dependent Hamiltonian [67]. The present approach aims at avoiding such approximations and the existence of a closed commutation relation [Eq. (5)] enables doing this in a numerically exact fashion.

The realization of propagators defined by Hamiltonians that cannot be implemented in practice by the static means discussed in Sec. IV is commonly pursued in the context of Floquet engineering [71,72]. While Floquet theory guarantees the existence of such propagators at periodically occurring points in time for periodically time-dependent Hamiltonians, it does not provide us with the ability to construct such propagators exactly. Existing approaches are thus typically based on perturbative constructions. Also in this context, the present approach can be helpful in overcoming the restriction to perturbative regimes and in finding numerically exact solutions.

The construction of explicit control solutions in this work makes use of the popular algorithm for computing the gradients with respect to control parameters utilized

in GRAPE [13,73] but the structural equivalence between the Schrödinger equation and Eq. (8) implies that the full range of optimal quantum control algorithms is applicable to the present approach. For example, more recent methods to construct gradients [74], alternative parametrizations of the control functions (e.g., in terms of Gaussian pulses [16]), or formulations that do not require back-propagation during optimization [75] could be employed to achieve smoother solutions and potentially enhance the convergence of the optimal-control algorithms.

While the exponential scaling of composite quantum systems poses fundamental constraints that cannot be overcome in general, the fact that there are sets of operators with favorable scaling does allow us to overcome them in specific cases. With control over interaction geometries in various platforms such as superconducting qubits [76], trapped ions, and Rydberg atoms [77], the present approach can help to fully exploit the qubit count in current devices (ranging up to 256 [77]) without the need of long gate sequences that are conflicting with decoherence and the accumulation of individual gate errors. While verification of the functionality of a quantum device is a challenging problem [78], the description of quantum dynamics in terms of invariants can also be used to make predictions for the targeted dynamics that can be experimentally tested.

With three- and four-body interactions naturally arising in the dynamics induced by the spin Hamiltonian given in Eq. (20), the present approach can also support the realization of error-correcting codes [79,80] and topologically protected quantum information processing [63]. With the advent of highly controllable systems that pose control problems beyond the limitations of classical simulations [77], there is a growing need for control techniques with good scaling behavior. Optimizations with the present framework can help to avoid or support costly experimental optimizations [51,81]. The resulting ability to create quantum states that allow for sensing at the Heisenberg limit makes the present approach a valuable tool for the community's effort toward the development of quantum technological applications.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The optimized pulse and computer code for this work are available without restriction [58].

APPENDIX A: ABSENCE OF SYMMETRIES IN THE SYSTEM HAMILTONIAN

We will show here that there is no symmetry in the Hamiltonian

$$H(t) = \sum_{j=1}^n f_j(t) Z_j + g \sum_{j=1}^{n-1} X_j X_{j+1} + \sum_{j \in \{1,n\}} w_j(t) X_j \quad (\text{A1})$$

for $g \neq 0$ and general time-dependent functions $f_j(t)$ and $w_j(t)$, i.e.,

there is no n -qubit operator A^n (besides multiples of the identity) that commutes with each of the operators $Z_1, Z_2, \dots, Z_n, X_1, X_n$ and $\sum_{j=1}^n X_j X_{j+1}$.

The requirement to commute with each of the operators $Z_1, Z_2, \dots, Z_n$ implies that A^n can be expanded in terms of tensor products of $\mathbb{1}$ and Z terms only.

The requirement to also commute with X_1 and X_n then implies that A^n is of the form

$$A^n = \mathbb{1} \otimes D^n \otimes \mathbb{1}, \quad (\text{A2})$$

with an $(n-2)$ -qubit operator D^n that can be expanded in terms of tensor products of $\mathbb{1}$ and Z terms or, more explicitly, as

$$A^n = \mathbb{1}_1 \otimes F^n \otimes \mathbb{1}_{n-1} \otimes \mathbb{1}_n + \mathbb{1}_1 \otimes G^n \otimes Z_{n-1} \otimes \mathbb{1}_n, \quad (\text{A3})$$

with $(n-3)$ -qubit operators F_n and G_n , that can be expanded in terms of tensor products of $\mathbb{1}$ and Z terms.

In order to address commutativity with

$$\sum_{j=1}^{n-1} X_j X_{j+1} = H_x^n, \quad (\text{A4})$$

it is instructive to express H_x^n as

$$H_x^n = H_x^{n-1} \otimes \mathbb{1}_n + \mathbb{1}_{1\dots n-1} \otimes X_{n-1} \otimes X_n. \quad (\text{A5})$$

The commutator $[A^n, H_x^n]$ thus reads

$$[A^n, H_x^n] = [\mathbb{1}_1 \otimes G^n \otimes Z_{n-1}, H_x^{n-1}] \otimes \mathbb{1}_n \quad (\text{A6})$$

$$+ 2i\mathbb{1}_1 \otimes G^n \otimes Y_{n-1} \otimes X_n \quad (\text{A7})$$

$$+ [\mathbb{1}_1 \otimes F^n \otimes \mathbb{1}_{n-1}, H_x^{n-1}] \otimes \mathbb{1}_n. \quad (\text{A8})$$

Since the term in Eq. (A7) is the only term with a factor X_n , the commutator can vanish only if G^n vanishes. If this is the case, however, then the right-hand side in Eq. (A6)

also vanishes, such that the commutator reduces to

$$[A^n, H_x^n] = [\mathbb{1}_1 \otimes F^n \otimes \mathbb{1}_{n-1}, H_x^{n-1}] \otimes \mathbb{1}_n, \quad (\text{A9})$$

with an operator

$$A^{n-1} = \mathbb{1}_1 \otimes F^n \otimes \mathbb{1}_{n-1}, \quad (\text{A10})$$

which is exactly of the form of Eq. (A2) but for $n - 1$ instead of n qubits.

The result to be proven thus holds for an n -qubit system, provided that it holds for an $(n - 1)$ -qubit system, and since one can readily verify it explicitly for a two-qubit system, the proof is completed by induction.

APPENDIX B: NUMERICAL SIMULATION AND OPTIMIZATION

This appendix describes the numerical techniques used to find the optimal-control strategies for the problems of state transfer and realization of propagators, as detailed in Secs. III and IV. The optimal solutions minimize a fidelity measure [defined in Eq. (12) for state transfer and in Eq. (19) for propagator realization] by finding a suitable time dependence of the system Hamiltonian in Eq. (20).

The operator is propagated with the equation of motion in Eq. (8), where the matrix $K(t)$ is given by the structure constants [Eq. (9)]. We provide the structure constants for the Lie algebra of Eq. 21 in a computer-readable format in Ref. [58]. One can obtain these structure constants by computing the commutator relation between the basis elements either analytically, or numerically with the help of the PAULI ALGEBRA package in *Mathematica* [82].

1. Coefficient vectors of the initial and target operators

In our method, numerical propagation and optimization are done entirely with the coefficients in a basis expansion of the operators, i.e., the coefficients a_j in the expansion

$$\mathcal{I} = \sum_j a_j \mathfrak{a}_j, \quad (\text{B1})$$

where $\mathfrak{a}_j$ are the basis elements listed in Eq. (21). In this section, we describe how to find these coefficient vectors for the initial and target operators discussed in the paper.

a. State preparation

The initial operator $\mathcal{I}_0$ [Eq. (25)] and the targets $\mathcal{I}_G \equiv H_G$ [Eq. (22)] and $\mathcal{I}_C \equiv H_C$ [Eq. (23)] are already written as explicit expansions of the basis elements, so the coefficients can be readily read off.

The control target $\mathcal{I}_D$ with the same ground state as H_D is obtained by evolving the initial operator $\mathcal{I}_0$ under the

adiabatic Hamiltonian

$$H_a(t) = (1 - t/T_a) \sum_j Z_j + (t/T_a) H_D + (t/T_a)(1 - t/T_a) \times \left(\sum_j Z_j + \sum_{j=1}^{n-1} X_j X_{j+1} + X_1 + X_n \right), \quad (\text{B2})$$

where T_a is a sufficiently long duration. In the d -dimensional space of the Lie algebra, $H_a(t)$ corresponds to

$$K_a(t) = (1 - t/T_a) \sum_j K_j^z + (t/T_a) K_D + (t/T_a)(1 - t/T_a) \times \left(\sum_j K_j^z + \sum_{j=1}^{n-1} K_j^{xx} + K_1^x + K_n^x \right), \quad (\text{B3})$$

where K_j^z, K_D, K_j^{xx} , and K_j^x are the $d \times d$ adjoint representation matrices of $Z_j, H_D, X_j X_{j+1}$, and X_j , respectively (see Eq. (9)). Starting with the initial coefficient vector $\mathbf{a}_0$ of $\mathcal{I}_0$, one propagates with

$$\dot{\mathbf{a}}(t) = K_a(t) \mathbf{a}(t), \quad (\text{B4})$$

for the duration T_a to obtain the coefficient vector $\mathbf{a}_D$ of $\mathcal{I}_D$.

b. Propagators

Realizing a propagator U_T requires more than a single pair of initial and target operators $\{\mathcal{I}(0), U_T \mathcal{I}(0) U_T^\dagger\}$. Instead, $2n$ pairs of initial and final operators, $\{\mathcal{I}_j(0), \mathcal{I}_{Tj} \equiv U_T \mathcal{I}_j(0) U_T^\dagger\}$, are sufficient, with the initial operators $\mathcal{I}_j(0)$ selected from Eq. (32). Obtaining the coefficient vectors of $\mathcal{I}_j(0)$ is straightforward, as they are already expressed in terms of the basis elements of the Lie algebra in Eq. (21).

The propagators U_G, U_C , and U_D considered in our work are of the common form

$$U_T = e^{-i\theta \mathcal{H}}, \quad (\text{B5})$$

where θ is a phase and $\mathcal{H}$ a linear combination of the basis elements of the Lie algebra. The final condition $\mathcal{I}_{Tj} \equiv U_T \mathcal{I}_j(0) U_T^\dagger$ corresponds to propagating $\mathcal{I}_j(0)$ with the Hamiltonian $H(t)$ [Eq. (20)] for a duration θ . Starting with the coefficient vector $\mathbf{a}(0)$ of $\mathcal{I}_j(0)$, one propagates the equation

$$\dot{\mathbf{a}}(t) = K \mathbf{a}(t), \quad (\text{B6})$$

where K is the adjoint representation matrix of $H(t)$, for the duration $T_P = \theta$. Then, $\mathbf{a}(T_P)$ is the coefficient vector of the target $\mathcal{I}_{Tj}$.

2. Computing infidelity and gradient

Piecewise control is used for the individual X_j and Z_j drivings of the system Hamiltonian [Eq. (20)], while the coupling strength g in the interaction term $X_j X_{j+1}$ is assumed to be constant. The pulse duration T is divided into M intervals, each with a fixed driving amplitude. The optimization process aims to minimize the infidelity [Eq. (12) or Eq. (19)] by optimizing the set of control amplitudes $\{\{f_j^l, w_j^l, w_n^l\} : 1 \leq l \leq M, 1 \leq j \leq n\}$ and the total duration T . To efficiently evaluate the infidelity during optimization, the operator basis elements $\{a_j\}$ are normalized, i.e., they satisfy $\text{tr}(a_j a_k) = \delta_{jk}$. This normalization simplifies the propagation of operators according to Eq. (8) and the subsequent calculation of the overlap between the target coefficient vector $\mathbf{a}_T$ and the final coefficient vector $\mathbf{a}(T)$ obtained from an initial condition $\mathbf{a}(0)$.

The control problem is formulated within the Lie algebra as finding the final coefficient vector $\mathbf{a}(T)$ to minimize the invariant infidelity $\mathcal{J} = 1 - \mathbf{a}_T \cdot \mathbf{a}(T)$, where $\mathbf{a}_T$ is the target coefficient vector, starting from an initial condition $\mathbf{a}(0)$. The evolution of $\mathbf{a}(t)$ is governed by the adjoint representation matrix $K(t)$ of the system Hamiltonian $H(t)$. If one expresses $H(t) = H_0 + \sum_k c_k(t) H_k^c$, where $c_k(t)$ is the amplitude of the control operator H_k^c , then $K(t) = K_0 + \sum_k c_k(t) K_k^c$, where K_0 and K_k^c are the adjoint representations of H_0 and H_k^c , respectively (see Eq. (9)). For the piecewise control defined above, the solution of $\dot{\mathbf{a}}(t) = K(t)\mathbf{a}(t)$ is

$$\mathbf{a}(T) = \prod_{l=M}^1 \mathcal{U}_l \mathbf{a}(0), \quad (\text{B7})$$

where

$$\mathcal{U}_l = e^{\Delta t (K_0 + \sum_k c_k^l K_k^c)}. \quad (\text{B8})$$

Note that $\mathcal{U}_l$ is unitary, as $K(t)$ is anti-Hermitian. One first computes and stores the set of forward- and backward-propagated vectors, defined by

$$\mathbf{a}_m = \mathcal{U}_m \mathcal{U}_{m-1} \dots \mathcal{U}_1 \mathbf{a}(0),$$

$$\mathbf{b}_m^\dagger = \mathbf{a}_T^\dagger \mathcal{U}_M \mathcal{U}_{M-1} \dots \mathcal{U}_m,$$

using the recursive relations $\mathbf{a}_m = \mathcal{U}_m \mathbf{a}_{m-1}$ and $\mathbf{b}_m^\dagger = \mathbf{b}_{m+1}^\dagger \mathcal{U}_m$, and then the gradient of $\mathcal{J}$ with respect to c_k^l is

$$\frac{\partial \mathcal{J}}{\partial c_k^l} = \frac{\partial}{\partial c_k^l} \left(1 - \mathbf{b}_{l+1}^\dagger \mathcal{U}_l \mathbf{a}_{l-1} \right) = -\mathbf{b}_{l+1}^\dagger \frac{\partial \mathcal{U}_l}{\partial c_k^l} \mathbf{a}_{l-1}. \quad (\text{B9})$$

The derivative of $\mathcal{U}_l$ is approximated by a second-order method [83]

$$\frac{\partial \mathcal{U}_l}{\partial c_k^l} = \left\{ \Delta t K_k^c - \frac{\Delta t^2}{2} [K_l, K_k^c] \right\} \mathcal{U}_l + O(\Delta t^3), \quad (\text{B10})$$

where $K_l = K_0 + \sum_k c_k^l K_k^c$; thus

$$\frac{\partial \mathcal{J}}{\partial c_k^l} = -\mathbf{b}_{l+1}^\dagger \left\{ \Delta t K_k^c - \frac{\Delta t^2}{2} [K_l, K_k^c] \right\} \mathbf{a}_l, \quad (\text{B11})$$

which is computed by matrix-vector multiplication. The most computationally expensive part is the multiplication of a matrix exponential with a vector for obtaining $\mathbf{a}_m$ and $\mathbf{b}_m^\dagger$ but it can be done efficiently with the Krylov-subspace method owing to the sparsity of $K(t)$.

For calculating the derivative of $\mathcal{J}$ with respect to the duration T , one simply calculates $\mathcal{J}$ again for a perturbed duration $T + dT$ while keeping the amplitudes c_k^l the same, so that

$$\frac{\partial \mathcal{J}}{\partial T} \approx \frac{\mathcal{J}(T + dT) - \mathcal{J}(T)}{dT}. \quad (\text{B12})$$

In our calculation, we choose $g dT = 10^{-10}$.

3. Optimization

We feed the infidelity and its gradient with respect to the control variables to a gradient-based optimization algorithm. The interior-point method is employed and the Hessian is approximated using the limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) method. This algorithm is implemented in the FMINCON function in MATLAB.

For large n , there are many shallow local minima and plateaus in the control landscape for U_G , due to the difficulty of reaching the n -body interaction term. To systematically address these challenges, a three-step procedure is employed. Initially, the symmetry of the control problem is imposed on the control variables, followed by the relaxation of this symmetry. Specifically, we begin with

$$\begin{aligned} H_1^c(t) = & g \sum_{j=1}^{n-1} X_j X_{j+1} + f_1(t) \sum_{j=1}^n Z_j + f_2(t) (Z_1 + Z_n) \\ & + w(t) (X_1 + X_n), \end{aligned} \quad (\text{B13})$$

which is a translationally invariant control, except at the two ends, i.e., it has the same symmetry as the control targets. The optimization is done sequentially from $n = 5$ to $n = 50$ in steps of 5, where the optimal control for $n - 5$ is used as the initial guess for n .

We then lower the infidelity for each n by optimizing with a system Hamiltonian with inversion symmetry

$$\begin{aligned} H_2^c(t) = & g \sum_{j=1}^{n-1} X_j X_{j+1} + \sum_{j=1}^{\lfloor (n+1)/2 \rfloor} f_j(t) (Z_j + Z_{n+1-j}) \\ & + w(t) (X_1 + X_n), \end{aligned} \quad (\text{B14})$$

using the final control in the previous step as the initial guess. Finally, we refine the solution further by optimizing

with a system Hamiltonian that lacks any symmetry:

$$H_3^c(t) = g \sum_{j=1}^{n-1} X_j X_{j+1} + \sum_{j=1}^n f_j(t) Z_j + \sum_{j \in \{1,n\}} w_j(t) X_j. \quad (\text{B15})$$

Each optimization step is done with a maximum of 1000 function-and-gradient evaluations. At every step, small random perturbations are applied to the initial guess to explore 12 nearby solutions in parallel, facilitating escape from traps. In many cases, the threshold infidelity is already reached with $H_1^c(t)$ or $H_2^c(t)$.

$T \approx n\pi/2g$ for the optimizations of H_G , H_C , and $T \approx n\pi/g$ for H_D , and the number of time bins in the piecewise control pulse is $M = 10n$ for all three cases. For U_C and U_D , $T \approx 2\pi g$ and $M = 10n$. For U_G , $T \approx 2n\pi/g$ and $M = 20n$.

4. Adiabatic error estimate

The control target $\mathcal{I}_D$ for H_D is defined as the operator $\mathcal{I}(T_a)$ resulting from simulated adiabatic evolution with a very long duration ($T_a = 2500\tau_g$) from the initial operator $\mathcal{I}(0)$, as described in Sec. B 1 a. In a perfect adiabatic evolution, each eigenstate of $\mathcal{I}(0)$ would evolve to a corresponding eigenstate of H_T and, thus, $\mathcal{I}(T_a)$ would commute with H_T . To verify this commutativity, one can propagate $\mathcal{I}(t)$ with H_T for an additional time T_b randomly chosen from the interval $[50\tau_g, 100\tau_g]$. In the ideal adiabatic limit, since $\mathcal{I}(T_a)$ commutes with H_T , further evolution would not change the system, resulting in $\mathcal{I}(T_a + T_b) = \mathcal{I}(T_a)$. Any deviation from this equality is a measure of adiabatic error and the infidelity $1 - \text{tr}(\mathcal{I}(T_a)\mathcal{I}(T_a + T_b))/\text{tr}(\mathcal{I}(T_a)^2)$ can be used as an estimate of this error.

5. MPS verification

The state infidelity for H_D in Fig. 2 is obtained using MPSs. The ground state of H_D is computed using the density matrix renormalization group (DMRG) algorithm and the final state is obtained by evolving the initial state $|\Psi_0\rangle$ with the matrix-product operator (MPO) W^H method [56], where each time bin is further divided into 20 smaller steps to reduce error. All MPS calculations are done using the TeNPy software package [55].

APPENDIX C: RELATION BETWEEN THE STATE INFIDELITY BOUND AND THE OPERATOR INFIDELITY

Given the system Hamiltonian $H(t)$ [Eq. (20)], the initial condition $\mathcal{I}(0) = \sum_j Z_j$ and a control target $\mathcal{I}_T$ that coincides with the target Hamiltonian H_T (which includes

the cases of H_G and H_C defined in Sec. III A), the bound

$$\mathcal{B} = \frac{\langle \Psi(T) | H_T | \Psi(T) \rangle - E_0}{E_1 - E_0} \quad (\text{C1})$$

in the state infidelity defined in Eq. (18) depends on the operator infidelity $\mathcal{J}$ via the linear relation

$$\mathcal{B} = \frac{n\mathcal{J} - s}{E_1 - E_0}, \quad (\text{C2})$$

with a term s that, under assumptions on typicality, becomes vanishingly small in the limit $n \rightarrow \infty$.

This is proven in the following.

Given the requirement that $\mathcal{I}_T = H_T$, the expectation value in Eq. (C1) satisfies the equality

$$\langle \Psi(T) | H_T | \Psi(T) \rangle = \langle \Psi(0) | \tilde{\mathcal{I}}(T) | \Psi(0) \rangle, \quad (\text{C3})$$

where $\tilde{\mathcal{I}}(T) = U^\dagger(T)\mathcal{I}_T U(T)$, $|\Psi(0)\rangle$ is the ground state of $\mathcal{I}(0)$, and E_0 the ground-state energy of both H_T and $\mathcal{I}(0)$. Using the relations

$$\text{tr}(\mathcal{I}(T)\mathcal{I}_T) = \text{tr}(U(T)\mathcal{I}(0)U^\dagger(T)\mathcal{I}_T) = \text{tr}(\mathcal{I}(0)\tilde{\mathcal{I}}(T)) \quad (\text{C4})$$

and $\text{tr}(\mathcal{I}_T^2) = \text{tr}(\mathcal{I}^2(0))$, the operator infidelity in Eq. (12) can be expressed as

$$\mathcal{J} = 1 - \frac{\text{tr}(\mathcal{I}(0)\tilde{\mathcal{I}}(T))}{\text{tr}(\mathcal{I}^2(0))}. \quad (\text{C5})$$

If the control target is reached exactly, the identity $\tilde{\mathcal{I}}(T) = \mathcal{I}(0)$ holds and any imperfection of the optimal-control solution can be captured by the deviation

$$\Delta\mathcal{I} = \mathcal{I}(0) - \tilde{\mathcal{I}}(T). \quad (\text{C6})$$

The deviation $\Delta\mathcal{I}$ can be expanded in terms of the operators $\mathfrak{a}_j$ [Eqs. (21)] as $\Delta\mathcal{I} = \sum_j c(\mathfrak{a}_j)\mathfrak{a}_j$, with expansion coefficients

$$c(\mathfrak{a}_j) = \frac{\text{tr}(\mathfrak{a}_j \Delta\mathcal{I})}{\text{tr}(\mathfrak{a}_j^2)}. \quad (\text{C7})$$

The operator infidelity can be expressed as

$$\mathcal{J} = \frac{\text{tr}(\mathcal{I}(0)\Delta\mathcal{I})}{\text{tr}(\mathcal{I}^2(0))}. \quad (\text{C8})$$

With $\mathcal{I}(0) = \sum_j Z_j$, $\text{tr}(\mathcal{I}^2(0)) = n2^n$ and the overlaps $\text{tr}(\mathcal{I}(0)Z_j) = 2^n$ and $\text{tr}(\mathcal{I}(0)\mathfrak{a}_j) = 0$ for all operators $\mathfrak{a}_j$

that are not single-spin Z operators [i.e., Eqs. (21b)–(21j)], the operator infidelity reduces to

$$\mathcal{J} = \frac{\sum_j c(Z_j)}{n}, \quad (\text{C9})$$

in terms of the expansion coefficients $c(Z_j)$ defined in Eq. (C7).

Given the ground-state energy $\langle \Psi(0) | \mathcal{I}(0) | \Psi(0) \rangle = E_0$, the bound $\mathcal{B}$ can be expressed as

$$\mathcal{B} = -\frac{\langle \Psi(0) | \Delta \mathcal{I} | \Psi(0) \rangle}{E_1 - E_0}. \quad (\text{C10})$$

With $\Delta \mathcal{I}$ expanded in terms of the operators α_j [Eqs. (21)] and the expectation values $\langle \Psi(0) | Z_j | \Psi(0) \rangle = -1$, $\langle \Psi(0) | \prod_j Z_j | \Psi(0) \rangle = (-1)^n$ and $\langle \Psi(0) | \alpha_j | \Psi(0) \rangle = 0$ for all other cases [i.e., Eqs. (21b)–(21i)], this yields

$$\mathcal{B} = \frac{\sum_j c(Z_j) - s}{E_1 - E_0}, \quad (\text{C11})$$

where $s = (-1)^n c(\prod_j Z_j)$ and the expansion coefficient $c(\prod_j Z_j)$ is defined in Eq. (C7). Together with Eq. (C9), this results in Eq. (C2).

While it is conceivable that $\Delta \mathcal{I}$ is proportional to the operator $\prod_j Z_j$, one would expect that, typically, $\Delta \mathcal{I}$ would have contributions from all operators α_j in Eq. (21). In estimating the magnitude of s , we will thus assume the expansion coefficients $c(\alpha_j)$ to be random, with each coefficient resulting from a distribution with zero mean and standard deviation δ . The typical magnitude of the term

$$n\mathcal{J} = \sum_{j=1}^n c(Z_j) \quad (\text{C12})$$

is then given by its standard deviation, i.e., by $\sqrt{n}\delta$. The typical magnitude of $c(\prod_j Z_j)$, on the other hand, is given by δ . The term s thus becomes negligible as compared to the term $n\mathcal{J}$ for large systems.

In Fig. 7, we depict the deviation of the actual results of Fig. 2(a) from the linear dependence $\mathcal{B} = n\mathcal{J}/(E_1 - E_0)$ as a function of the system size n . The figure shows that the deviation decays rapidly with n . The actual results thus follow the linear dependence to a good approximation.

APPENDIX D: LIE ALGEBRA OF THE HEXAGONAL SPIN LADDER

As shown in the following, the Lie algebra generated by the operators in Eq. (43) for the spin ladder depicted in Fig. 6 scales as $(25n^2 - 40n + 12)/32$ in the number of spins $n = 4n_h + 2$ with n_h hexagons.

In order to arrive at this scaling, it is convenient to start with two noninteracting chains.

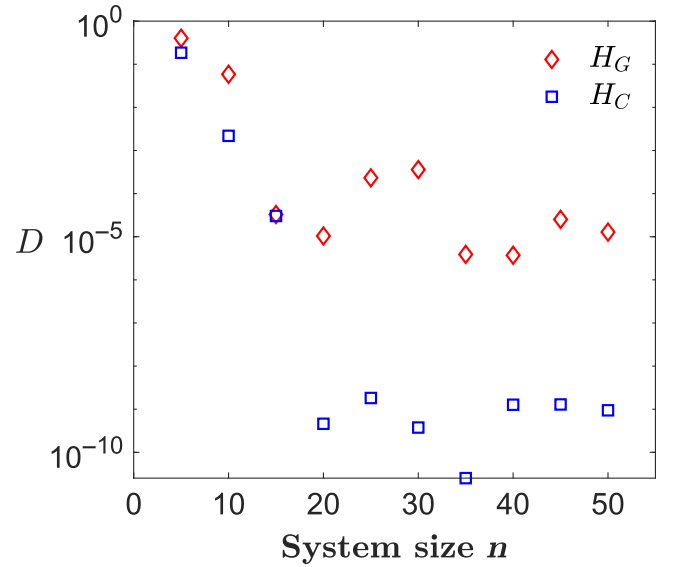


FIG. 7. The deviation $D = |1 - (E_1 - E_0)\mathcal{B}/n\mathcal{J}| = |s|/n\mathcal{J}$, in log scale, from the linear relation between the bound $\mathcal{B}$ on the state infidelity and the operator infidelity $\mathcal{J}$ that is expected to hold in the limit $n \rightarrow \infty$ following Eq. (C2). The deviation obtained from the data shown in Fig. 2(a) decays rapidly with n , consistently with Eq. (C2).

The Lie algebra for the top chain is generated by Eqs. (43a) and (43b). With the shorthand notation $X_{jk} = \prod_{i=1}^k X_{i+j}^1$ and

$$\overline{Y}Z_{jk} = Y_j^1 X_{jk} Z_{j+k+1}^1, \quad (\text{D1a})$$

$$\overline{Z}Y_{jk} = Z_j^1 X_{jk} Y_{j+k+1}^1, \quad (\text{D1b})$$

$$\overline{Y}Y_{jk} = Y_j^1 X_{jk} Y_{j+k+1}^1, \quad (\text{D1c})$$

$$\overline{Z}Z_{jk} = Z_j^1 X_{jk} Z_{j+k+1}^1, \quad (\text{D1d})$$

it is given by the operators γ_{jk} with $j \in [1, m-1]$ and $k \in [0, m-j-1]$, where

$$\gamma_{jk} = \begin{cases} \overline{Y}Z_{jk}, & \text{for odd } j \text{ and odd } k, \\ \overline{Y}Y_{jk}, & \text{for odd } j \text{ and even } k, \\ \overline{Z}Y_{jk}, & \text{for even } j \text{ and odd } k, \\ \overline{Z}Z_{jk}, & \text{for even } j \text{ and even } k. \end{cases} \quad (\text{D2})$$

The Lie algebra for the bottom chain is generated by Eqs. (43c) and (43d) and it includes [besides Eqs. (43c) and (43d)]

$$X_{2j}^2 Y_{2j+1}^2 X_{2j+2}^2, \quad (\text{D3})$$

with $j \in [1, (m-3)/2]$.

With $s \in \{-1, 1\}$, $j \in [1, (m-1)/2]$, and $k \in [0, m-j-1]$, and with Γ_{2j} adopting the four different values

$$\Gamma_{2j} = \begin{cases} X_{2j-1}^2 X_{2j}^2, \\ Y_{2j-1}^2 \mathbb{1}_{2j}^2, \end{cases} \quad (\text{D4})$$

for $s = -1$, and

$$\Gamma_{2j} = \begin{cases} X_{2j}^2 Z_{2j+1}^2, \\ \mathbb{1}_{2j}^2 Y_{2j+1}^2, \end{cases} \quad (\text{D5})$$

for $s = 1$, the Lie algebra generated by the full set of operators in Eq. (43) contains the additional terms

$$X_{2j+s}^1 \Gamma_{2j}, \quad (\text{D6a})$$

$$\bar{Z}Y_{2j+s,k} \Gamma_{2j}, \quad (\text{D6b})$$

$$\bar{Z}Y_{2j-1-k+s,k} \Gamma_{2j}, \quad (\text{D6c})$$

for even k , and

$$\bar{Z}\bar{Z}_{2j+s,k} \Gamma_{2j}, \quad (\text{D6d})$$

$$\bar{Z}Y_{2j+s,k} \Gamma_{2j} Y_{2j+k+s+1}^2, \quad (\text{D6e})$$

$$\bar{Z}Y_{2j+s,k} \Gamma_{2j} X_{2j+k+s}^2 Z_{2j+k+s+1}^2, \quad (\text{D6f})$$

$$\bar{Z}Y_{2j+s,k} \Gamma_{2j} X_{2j+k+s+1}^2 Z_{2j+k+s+2}^2, \quad (\text{D6g})$$

$$\bar{Y}Y_{2j-1-k+s,k} \Gamma_{2j}, \quad (\text{D6h})$$

$$\bar{Z}Y_{2j-1-k+s,k} Y_{2j-1-k+s}^2 \Gamma_{2j}, \quad (\text{D6i})$$

$$\bar{Z}Y_{2j-1-k+s,k} X_{2j-2-k+s}^2 Z_{2j-1-k+s}^2 \Gamma_{2j}, \quad (\text{D6j})$$

$$\bar{Z}Y_{2j-1-k+s,k} X_{2j-1-k+s}^2 X_{2j-k+s}^2 \Gamma_{2j}, \quad (\text{D6k})$$

for odd k . Given that Eqs. (43c)–(43d) contain $(n-2)/2$ elements, Eq. (D2) includes $(n^2/8 - n/4)$ elements [encompassing Eqs. (43a) and (43b)], Eq. (D3) contributes with $(n-6)/4$ elements, and Eq. (D6) adds $(21n^2 - 56n + 92)/32$ operators, the size of the Lie algebra grows as $(25n^2 - 40n + 12)/32$ with the number of qubits $n = 2 + 4n_h$ defined in terms of the number of hexagons n_h .

For $k = 1$, $s = 1$, and $\Gamma_{2j} = X_{2j}^2 Z_{2j+1}^2$, the operator in Eq. (D6i) reduces to the six-body plaquette operators $P_j = Z_{2j-1}^1 X_{2j}^1 Y_{2j+1}^1 Y_{2j-1}^2 X_{2j}^2 Z_{2j+1}^2$ in Eq. (44).

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