On the practicality of time-optimal two-qubit Hamiltonian simulation

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What is the time-optimal way of using a set of control Hamiltonians to obtain a desired interaction? Vidal, Hammerer and Cirac [Phys. Rev. Lett. 88 (2002) 237902] have obtained a set of powerful results characterizing the time-optimal simulation of a two-qubit quantum gate using a fixed interaction Hamiltonian and fast local control over the individual qubits. How practically useful are these results? We prove that there are two-qubit Hamiltonians such that time-optimal simulation requires infinitely many steps of evolution, each infinitesimally small, and thus is physically impractical. A procedure is given to determine which two-qubit Hamiltonians have this property, and we show that almost all Hamiltonians do. Finally, we determine some bounds on the penalty that must be paid in the simulation time if the number of steps is fixed at a finite number, and show that the cost in simulation time is not too great.

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I. INTRODUCTION

A central question of quantum information science is to determine the minimal time required to perform a quantum computation using a set of physical resources known to be universal for computation. Our understanding of what resources are universal for computation is very well-developed, and it is known [22] that when fast local control is available, any unitary dynamics capable of generating entanglement is universal for computation. However, the question of using these resources in a time-optimal fashion is, by comparison, understood relatively poorly.

This paper considers a particular simplified setting, that of time-optimal simulation of two-qubit unitaries using a fixed interaction Hamiltonian and arbitrary fast local control. Arbitrary fast local control means that the evolution of the interaction Hamiltonian may be interrupted by arbitrary single-qubit operations, and that these operations take no time to perform. This assumption corresponds to certain experimental setups where single-qubit operations are performed on a much faster time scale than joint operations. Hammerer, Vidal and Cirac [1, 2] have given a construction for this simulation, as well as an elegant expression for the minimum achievable simulation time.

The simulation scheme of Hammerer et al. uses, in general, an infinite number of steps to achieve time optimality. That is, the interaction Hamiltonian is, in general, interrupted an infinite number of times by local operations, and the time between each interruption is infinitesimal. A simulation scheme requiring infinitely many time steps is not practical for at least two reasons. First, the original premise that local operations can be performed in zero time is no longer valid if one must perform infinitely many of them. Second, the effects of noise on such a simulation will overwhelm the intended coherent dynamics. The purpose of our paper is to ask, first, whether infinitely many time steps are actually required, in general, for time-optimal simulation? We will find that the answer is yes. Indeed, we will show that the overwhelming majority of two-qubit interaction Hamiltonians have this property. Given this, we then address the question of determining how close to time optimal a simulation can get, given that one demands a simulation using only a finite number of time steps.

The paper is structured as follows. In Sec. II we review results about two-qubit time-optimal simulation in the limit of fast control. In Sec. III we provide a procedure for determining which two-qubit Hamiltonians require infinitesimal time steps when used in this setting. Finally, in Sec. IV we quantify the sacrifice that must be made to time-optimality when one insists on having a simulation using a finite number of time steps. Sec. V concludes the paper.

II. PRELIMINARIES

The purpose of this section is to introduce notation and to review some concepts and results associated with time-optimal two-qubit simulation in the limit of fast local control. We end the section with an introduction to the idea of a “lazy” two-qubit Hamiltonian.
A. Notation

Up to rescaling of the ground state energy, an arbitrary two-qubit Hamiltonian can be parameterised as an equation:

\[ H = I \otimes (\vec{a} \cdot \sigma) + (\vec{b} \cdot \sigma) \otimes I + \sum_{i,j=1}^{3} M_{ij} \sigma_i \otimes \sigma_j, \quad (1) \]

where \( \vec{a} \equiv (a_x, a_y, a_z) \) and \( \vec{b} \equiv (b_x, b_y, b_z) \) are real 3-vectors, \( M \) is a 3 by 3 real matrix, and \( \vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) = (X, Y, Z) \) is the vector of Pauli operators. With respect to the computational basis \( \{|0\rangle, |1\rangle\} \), the Pauli operators are represented by the following matrices:

\[ X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (2) \]

When all the entries \( M_{ij} \) are zero we say that the Hamiltonian is local. Otherwise we say that the Hamiltonian is nonlocal. We say that a unitary \( U \) is local if it can be expressed as a tensor product \( U = A \otimes B \) of single-qubit unitaries. Otherwise we say the unitary is nonlocal. We shall henceforth restrict the single-qubit unitaries to be elements of the special unitary group \( SU(2) \) (i.e., the group of two-by-two unitaries having unit determinant).

B. Time optimal simulation

A simulation scheme to approximate an arbitrary two-qubit unitary, \( U \), using a fixed Hamiltonian, \( H \), and arbitrary local unitaries may, without loss of generality, be written as follows.

\[ U = (A_N \otimes B_N)e^{-iHt_N}(A_{N-1} \otimes B_{N-1})e^{-iHt_{N-1}} \ldots (A_1 \otimes B_1)e^{-iHt_1}(A_0 \otimes B_0), \quad (3) \]

where the parameters \( t_n \) are nonnegative. That is, in order to achieve the desired dynamics we can apply \( H \) as many times as we wish for arbitrary lengths of time, interspersed with arbitrary operations on the individual qubits. We occasionally refer to Eq. (3) as being a circuit for \( U \). It is worth noting that the assumption that \( H \) contains no \( I \otimes I \) term and that single-qubit unitaries are in \( SU(2) \), implies that \( U \) is in \( SU(4) \). These restrictions entail no loss in generality, as they simply take advantage of the fact that the global phase of a unitary operator is irrelevant.

Correspondingly to the simulation Eq. (3) is the interaction time, which we define to be the total time \( t_1 + \ldots + t_N \) for which the interaction Hamiltonian is applied. For a given \( U \) and \( H \), there are many possible circuits each giving rise to a simulation of \( U \). Over this range of possible circuits for \( U \), there is a corresponding range of values for the interaction time. A circuit which achieves the minimum interaction time for a given \( U \) and \( H \) is said to be time-optimal. We define \( C_H(U) \) to be the minimum achievable interaction time for simulating \( U \) using

\( H \). Reference [1] gives a simple expression for \( C_H(U) \), in the two-qubit scenario. To discuss this result, we first briefly review the canonical form of a two-qubit unitary and two-qubit Hamiltonian operator.

C. The canonical form of \( U \) and \( H \)

For any unitary \( U \in SU(4) \) there exists a canonical decomposition [2, 3].

\[ U = (C_1 \otimes D_1)e^{-i(\theta_1 X \otimes X + \theta_2 Y \otimes Y + \theta_3 Z \otimes Z)}(C_2 \otimes D_2), \quad (4) \]

where \( C_1, D_1, C_2, \) and \( D_2 \) are single-qubit special unitaries, and \( \theta_1, \theta_2, \) and \( \theta_3 \) are unique real numbers satisfying

\[ \pi/4 \geq \theta_1 \geq \theta_2 \geq |\theta_3| \geq 0. \quad (5) \]

Although 15 parameters are needed in order to completely specify an arbitrary two-qubit unitary \( U \in SU(4) \), the canonical decomposition shows us that the nonlocal behaviour of \( U \) can be characterised in terms of only three parameters, \( \theta_1, \theta_2, \) and \( \theta_3 \). We call these three parameters the canonical-form parameters of \( U \) and the operator \( U_{\theta} \equiv e^{-i(\theta_1 X \otimes X + \theta_2 Y \otimes Y + \theta_3 Z \otimes Z)} \) the canonical form of \( U \).

The local parts \( C_1, D_1, C_2, \) and \( D_2 \) of the canonical decomposition do not affect the interaction time, as they can be trivially included in the first and last steps, \( A_0 \otimes B_0 \) and \( A_N \otimes B_N \), of a simulation. Therefore the canonical-form parameters are all we need to know about \( U \) in order to calculate the minimum required interaction time for Eq. (3).

How does one calculate the canonical-form parameters? For completeness, we review the method given in Appendix A of [1].

In the following it will be helpful to take advantage of properties of the so-called magic basis [2],

\[ |1\rangle = \frac{i}{\sqrt{2}}(|01\rangle + |10\rangle) \]
\[ |2\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \]
\[ |3\rangle = \frac{i}{\sqrt{2}}(|00\rangle - |11\rangle) \]
\[ |4\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \]

It is known [2] that, when expressed in the magic basis, local two-qubit special unitaries are real, and canonical-form unitaries are diagonal. This means that in the magic basis the canonical decomposition looks like \( U = RDS \), where \( R \) and \( S \) are real orthogonal matrices, and \( D \) is diagonal. The diagonal elements of \( D \) can be easily written in terms of the canonical-form parameters of \( U \): if
we define
\[
\varphi_1 = \theta_1 + \theta_2 - \theta_3,
\]
\[
\varphi_2 = \theta_1 - \theta_2 + \theta_3,
\]
\[
\varphi_3 = -\theta_1 + \theta_2 + \theta_3,
\]
\[
\varphi_4 = -\theta_1 - \theta_2 - \theta_3,
\]
then the diagonal elements of \( D \) are \( e^{-i\varphi_1} \), \( e^{-i\varphi_2} \), \( e^{-i\varphi_3} \), and \( e^{-i\varphi_4} \). Note that Eq. 6 together with Eq. 5 implies that
\[
\frac{3\pi}{4} \geq \varphi_1 \geq \varphi_2 \geq \varphi_3 \geq \varphi_4 \geq -\frac{3\pi}{4}.
\] (7)

We have that \( U^T U = S^T D R^T R D S = S^T D^2 S \), so the eigenvalues of \( U^T U \) are just the squares of the diagonal elements of \( D \). That is,
\[
\text{eig}(U^T U) = \{e^{-2i\varphi_1}, e^{-2i\varphi_2}, e^{-2i\varphi_3}, e^{-2i\varphi_4}\}.
\] (8)

To determine the canonical-form parameters for a particular \( U \), we first calculate the eigenvalues of \( U^T U \) (where the transpose is taken in the magic basis), then derive the \( \varphi_j \) via Eq. 8, and finally solve Eqs. 6. A word of caution: the task of deriving the \( \varphi_j \) from the \( e^{-2i\varphi_j} \) is not as trivial as it may first seem. The problem is that, in general, there is no guarantee that the values \(-2\varphi_j\) will lie in any particular branch of the logarithm function. So, naively taking the argument of \( e^{-2i\varphi_j} \) will not necessarily give you \(-2i\varphi_j\). A relatively simple procedure exists to correct for this problem 8. However in the context of Sec. III we will see later that taking the logarithm of \( e^{-2i\varphi_j} \) along the standard branch of the logarithm function will suffice to evaluate \(-2\varphi_j\).

Closely related to the canonical form for a two-qubit unitary is the canonical form for a two-qubit Hamiltonian. It is discussed in section V.A of 2, where it is referred to as the normal form. Given the purely nonlocal part
\[
H_I = \sum_{i,j=1}^{3} M_{ij} \sigma_i \otimes \sigma_j
\] (9)
of a Hamiltonian \( H \), when it is expressed in the form Eq. 11, the canonical form of \( H \) is defined to be the unique Hermitian operator
\[
H_\sigma = \alpha_1 X \otimes X + \alpha_2 Y \otimes Y + \alpha_3 Z \otimes Z
\] (10)
that satisfies
\[
H_I = (A \otimes B) H_\sigma (A^\dagger \otimes B^\dagger)
\] (11)
for some local unitary \( A \otimes B \), where \(|\alpha_1| \geq |\alpha_2| \geq |\alpha_3|\). The existence and uniqueness of this canonical form is established in 2, where it is shown that \( \alpha_1, \alpha_2 \) and \( |\alpha_3| \) are the singular values of the matrix \( M \), and \( \text{sgn}(\alpha_3) = \text{sgn}(\det M) \).

The canonical form of a Hamiltonian \( H \) encapsulates the nonlocal behaviour of the evolution of \( H \) for very small time steps. This can be seen as follows. From sections III.B and V.A of 2 we can write
\[
e^{-iHt} = (A \otimes B) e^{-iH_\sigma t} (C \otimes D) + O(t^2)
\]
\[
= (A \otimes B) e^{-i(\alpha_1 X \otimes X + \alpha_2 Y \otimes Y + \alpha_3 Z \otimes Z)} (C \otimes D) + O(t^2)
\] (12)
for some local unitaries \( A, B, C, \) and \( D \). To order \( t \), the evolution of \( H \) is given by a unitary having canonical-form parameters \( t\alpha_1, t\alpha_2 \) and \( t\alpha_3 \).

D. Expression for \( C_H(U) \)

We are almost ready to review the expression for \( C_H(U) \) given in 12. Before we do so we review the concept of special-majorization. Special-majorization describes a particular type of partial ordering of three-vectors. Its use in 2 allows certain results to be described very succinctly. To define special-majorization, it is necessary to first introduce the idea of a special-ordered three-vector. Given a real vector \( \vec{\beta} = (\beta_1, \beta_2, \beta_3) \), the corresponding special-ordered vector \( \vec{\beta}^* \) is defined as follows. The absolute value of the components of \( \vec{\beta}^* \) are given by the absolute value of the components of \( \vec{\beta} \) rearranged in nonincreasing order. That is, \( |\vec{\beta}_1^*| = |\vec{\beta}_{\pi(1)}| \) for the permutation \( \pi(j) \) that gives \( |\beta_1^*| \geq |\beta_2^*| \geq |\beta_3^*| \).

The definition is completed by specifying that \( \beta_1^* \) and \( \beta_2^* \) are nonnegative, and that \( \beta_3^* \) has the same sign as the product \( \beta_1 \beta_2 \beta_3 \). Then, \( \vec{\beta} \) is said to be special-majorized by \( \vec{\gamma}^* \) (denoted \( \vec{\beta} \prec_s \vec{\gamma}^* \)) if
\[
\beta_1^* \leq \gamma_1^* \leq \gamma_2^* \leq \gamma_3^*
\]
\[
\beta_1^* + \beta_2^* - \beta_3^* \leq \gamma_1^* + \gamma_2^* - \gamma_3^*
\] (13)
\[
\beta_1^* + \beta_2^* + \beta_3^* \leq \gamma_1^* + \gamma_2^* + \gamma_3^*,
\] (14)
where \( \vec{\beta}^* \) and \( \vec{\gamma}^* \) are the special-ordered versions of \( \vec{\beta} \) and \( \vec{\gamma} \).

Let \( H \) be a two-qubit Hamiltonian having canonical form \( H_\sigma \) and let \( U \) be a two-qubit unitary having canonical form \( U_\sigma \). Then \( C_H(U) \), the minimum time required to simulate \( U \) using \( H \), is given by the minimum value of \( t_S \geq 0 \) such that either
\[
\vec{\beta} \prec_s \vec{\alpha} t_S \quad \text{or} \quad \vec{\beta} + (-\frac{\pi}{2}, 0, 0) \prec_s \vec{\alpha} t_S
\] (15)
holds.

E. The lazy Hamiltonian

We now introduce the the central concept of a “lazy” Hamiltonian. For a given two-qubit Hamiltonian \( H \), we define a function \( \tau(t) \) as follows:
\[
\tau(t) = C_H(e^{-iHt}).
\] (17)
That is, $\tau(t)$ is the minimum total time for which the Hamiltonian $H$ must be applied, when it is being used together with arbitrary local unitaries, to simulate its own action $e^{-iHt}$. Such a simulation would be of the form

$$e^{-iHt} = (A_N \otimes B_N)e^{-iH_{NN}(A_{N-1} \otimes B_{N-1})}e^{-iH_{N-1}} \ldots (A_1 \otimes B_1)e^{-iH_1}(A_0 \otimes B_0).$$

(18)

The trivial “simulation” having the single step $e^{-iHt}$ has an interaction time of $t$. Thus the minimum achievable interaction time will be no greater than $t$:

$$\tau(t) \leq t.$$  

(19)

Under what circumstances will $\tau(t)$ be less than $t$? It turns out that this question is very closely linked to our main question: what are the circumstances under which a time-optimal simulation will require infinitesimal time steps?

Consider the class of two-qubit Hamiltonians having the following property:

$$\tau(t) < t \quad \forall t > 0.$$  

(20)

We shall say that a Hamiltonian is “lazy” if it is nonlocal and satisfies Eq. (20).

**Proposition 1** If a Hamiltonian is lazy, then the time-optimal simulation of any two-qubit nonlocal unitary $U$ using $H$ requires infinitely many time steps.

**Proof:** Suppose there exists a time-optimal simulation scheme, of the form of Eq. (8), for a nonlocal $U$ using a lazy Hamiltonian $H$, where the number of time steps $N$ is finite. At least one of the $t_n$ must be nonzero, otherwise the simulation would be unable to produce nonlocal dynamics. For such a nonzero $t_n$, consider the corresponding factor $e^{-iHtn}$ in the simulation. Since $H$ is lazy, there exists a simulation for $e^{-iHtn}$ having an interaction time less than $t_n$. If we substitute such a simulation for $e^{-iHtn}$ back into the simulation for $U$, then the new simulation for $U$ now has a lesser interaction time than it did before. However this contradicts the assumption that the original simulation was time optimal. Hence the premise that the original simulation had finite time steps is false. Thus we conclude that any lazy Hamiltonian will require infinitesimal time steps when used for the time-optimal simulation of any nonlocal two-qubit unitary $U$.  

To show that a particular $H$ is lazy, it is sufficient to show that $\tau(t) < t$ for all $t$ in some interval $(0, \epsilon)$ for any positive $\epsilon$. To see this, note that if there is a simulation for $e^{-iHt}$ with interaction time $t_n < t$, then clearly there exists a simulation for $e^{-iHnt}$ with interaction time $t_n^n$, for any positive integer $n$. Thus, $\tau(t) < t$ implies that $\tau(nt) < nt$ for all positive integers $n$. So, if $\tau(t) < t$ for all $t \in (0, \epsilon)$, then $\tau(t) < t$ for all $t > 0$.

**III. GENERAL PROCEDURE**

Which two-qubit Hamiltonians are lazy? We have seen in the previous section (proposition 1) that lazy two-qubit Hamiltonians require infinitely many time steps if they are to be used for time-optimal control, and thus are impractical. In this section we provide a simple set of sufficient conditions for a Hamiltonian to be lazy, expressed in terms of the parameters of the Hamiltonian.

The parameterisation in Eq. (1) is more general than $H_{NN}$ and only if $(A \otimes B)H(A^\dagger \otimes B^\dagger)$ is lazy, where $A$ and $B$ are any single-qubit unitaries. This is a consequence of the fact that $e^{-iHt}$ has the same canonical form as $e^{-i(A \otimes B)(A^\dagger \otimes B^\dagger)t}$. Thus, without loss of generality we choose to only consider Hamiltonians where the purely nonlocal part is in canonical form, that is

$$H = I \otimes (\vec{a} \cdot \vec{\sigma}) + (\vec{b} \cdot \vec{\sigma}) \otimes I + \sum_{j=1}^{3} \alpha_j \sigma_j \otimes \sigma_j,$$  

(21)

where $\alpha_1 \geq \alpha_2 \geq |\alpha_3|$.

Recall from subsection II C that we define a Hamiltonian to be lazy if $\tau(t) < t$ over some interval $(0, \epsilon)$. Suppose we could find a Taylor series expansion

$$\tau(t) = \tau(0) + \tau(1)t + \tau(2)t^2 + \ldots$$  

(22)

for $\tau(t)$ in the variable $t$. Thus,

$$\tau(t) - t = \tau(0) + (\tau(1) - 1)t + \tau(2)t^2 + \ldots$$  

(23)

Then, because we can assume $t$ is small, the corresponding Hamiltonian is lazy if and only if the first nonzero item in the list $\tau(0)$, $(\tau(1) - 1)$, $\tau(2)$, $\tau(3)$, ... is negative. Our procedure involves finding expressions for the first few items in that list, in terms of the parameters $\vec{a}$, $\vec{b}$ and $\vec{\sigma}$ of the Hamiltonian. We then find the conditions under which each expression will be negative. We find that in fact $\tau(0) = \tau(1) - 1 = \tau(2) = 0$ always, and so $\tau(3)$ is the first term that may be negative. Accordingly, in the analysis that follows we consider the behaviour of $\tau(t)$ up to order $t^3$, so as to arrive at some nontrivial conditions for a Hamiltonian being lazy.

**A. Procedure to find the Taylor coefficients of $\tau(t)$**

We seek expressions for the Taylor coefficients of $\tau(t)$, namely, $\tau(0)$, $\tau(1)$, $\tau(2)$, and $\tau(3)$. The expression for $C_H(U)$ involves the canonical-form parameters $\theta_1$, $\theta_2$ and $\theta_3$ of the unitary $U$. So we first try to find expressions for the canonical-form parameters $\theta_1(t)$, $\theta_2(t)$ and $\theta_3(t)$ of the unitary $e^{-iHt}$. From subsection II C the canonical-form parameters can be expressed in terms of parameters $\varphi_1, \ldots, \varphi_4$, where

$$\text{eig}(e^{-iH(t)} e^{-iHt}) = \{e^{-i2\varphi_1}, \ldots, e^{-i2\varphi_4}\},$$  

(24)
Define $\tilde{K}(t)$ to be the first three terms in the expansion of $K(t)$ in Eq. (25). That is,

$$
\tilde{K}(t) = -it(H^T + H) + \frac{1}{2}(-it^2)[H^T, H] + \frac{1}{12}(-it^3)[[H^T, [H^T, H]] + [H, [H, H^T]]].
$$

Then, if we define

$$
\tilde{\lambda}(t) = -\frac{1}{2t}\text{eig}(\tilde{K}(t))
$$

we have

$$
\tilde{\varphi}(t) = \left(\tilde{\lambda}(t)\right)^\dagger + O(t^4).
$$

We can find the first four Taylor coefficients of each component of $\tilde{\lambda}(t)$ in the following way. Each component of $\tilde{\lambda}(t)$ satisfies the characteristic equation

$$
f(t) = \text{det}(\tilde{K}(t) + 2i\lambda(t)) = 0.
$$

We can substitute a Taylor series for $\lambda(t)$:

$$
f(t) = \text{det}(\tilde{K}(t) + 2i(\lambda^{(0)} + \lambda^{(1)}t + \ldots)) = 0.
$$

Since Eq. (31) must be true for a range of values of $t$, then all coefficients in a Taylor series for $f(t)$ must be zero. Finding expressions for the coefficients $f^{(j)}$, and solving the equations $f^{(j)} = 0$, will give us the coefficients $\lambda^{(0)}$, $\lambda^{(1)}$, etc. Note that when we wish to find a particular term $f^{(j)}$, we need only include terms in the expansion of $\lambda(t)$ in Eq. (31) to order $t^j$.

How can we use the Taylor coefficients of $\tilde{\lambda}(t)$ to find the Taylor coefficients of $\tilde{\varphi}(t)$? Does the ordering operation in Eq. (35) present a difficulty? Not really. Say that we knew the Taylor series for each of the four functions $\lambda_1(t), \ldots, \lambda_4(t)$. We would simply order these vector components with respect to the zero-order Taylor coefficients:

$$
\lambda_1^{(0)} \geq \lambda_2^{(0)} \geq \lambda_3^{(0)} \geq \lambda_4^{(0)}.
$$

If it happened that none of the $\lambda^{(0)}$ were equal, that is $\lambda_1^{(0)} > \lambda_2^{(0)} > \lambda_3^{(0)} > \lambda_4^{(0)}$, then Eq. (35) would immediately imply that

$$
\tilde{\varphi}(t) = \tilde{\lambda}(t) + O(t^4)
$$

for $t$ in some interval $[0, \epsilon]$. That is, for small $t$, $\tilde{\varphi}(t)$ is equal to $\tilde{\lambda}(t)$ up to order $t^3$, where the components of $\tilde{\lambda}(t)$ are arranged so the zeroth Taylor coefficients are in decreasing order. In the special case where some of the zero-order coefficients $\lambda_1^{(0)}, \lambda_2^{(0)}, \lambda_3^{(0)}, \lambda_4^{(0)}$ are equal, then we break the tie by considering the first-order coefficients, and if those are equal we consider the next highest order and so on. In what follows, we will use the ordering scheme as described in this paragraph, so that we may use Eq. (35) instead of Eq. (34).
B. Procedure to find the Taylor coefficients of the components of \( \tilde{\lambda}(t) \).

In this subsection we describe the calculation of the Taylor coefficients of the components of \( \tilde{\lambda}(t) \).

In the magic basis, the Hamiltonian, \( H \), in Eq. (21) reads

\[
H = \begin{pmatrix}
\alpha_1 - \alpha_2 + \alpha_3 & -ia_3 - ib_3 & -ia_2 + ib_2 & -ia_1 - ib_1 \\
-ia_3 + ib_3 & -\alpha_1 + \alpha_2 + \alpha_3 & ia_1 - ib_1 & -ia_2 - ib_2 \\
-ia_2 - ib_2 & ia_1 + ib_1 & \alpha_1 - \alpha_2 - \alpha_3 & ia_3 - ib_3 \\
-ia_1 + ib_1 & ia_2 + ib_2 & -ia_3 + ib_3 & \alpha_1 + \alpha_2 - \alpha_3
\end{pmatrix}.
\]

(39)

The components of \( \tilde{K}(t) \) in the magic basis are found with the aid of the computer algebra system Maple. This is straightforward in any of the standard computer algebra systems, and the specific form is both complex and not particularly illuminating, so we will not reproduce the components of \( \tilde{K}(t) \) here. Note that each component is a third-order polynomial in \( t \).

Next, we find expressions for \( f^{(0)}, \ldots, f^{(6)} \). To find \( f^{(n)} \), we evaluate the expression \( f(t) \) in Eq. (37) using Maple, including terms in the series \( \lambda^{(0)} + \lambda(1)t + \ldots \) up to at least order \( t^n \). Then, \( f^{(n)} \) is given by the coefficient of the \( t^n \) term in this expression. Explicit expressions for \( f^{(n)} \) will not be given here as they are rather lengthy and not illuminating. They are polynomials in the parameters of the Hamiltonian.

The next step is to solve the equations \( f^{(n)} = 0, n = 0, \ldots, 6 \), via Maple. The results are as follows.

- Solving \( f^{(0)} = 0 \) yields \( \lambda^{(0)} = 0 \). That is, the zero-order Taylor coefficients of each component of \( \tilde{\lambda}(t) \) are zero. Thus, from Eq. (35) and Eq. (6) we have \( \bar{\theta}^{(0)} = 0 \).

- Solving \( f^{(1)} = 0, f^{(2)} = 0, \) and \( f^{(3)} = 0 \) provides no new information about the \( \lambda^{(n)} \).

- Solving \( f^{(4)} = 0 \) yields four solutions, one for each component in \( \tilde{\lambda}(t) \). We write them in nonincreasing order as follows:

\[
\begin{align*}
\lambda_1^{(1)} &= \alpha_1 + \alpha_2 - \alpha_3 \\
\lambda_2^{(1)} &= \alpha_1 - \alpha_2 + \alpha_3 \\
\lambda_3^{(1)} &= -\alpha_1 + \alpha_2 + \alpha_3 \\
\lambda_4^{(1)} &= -\alpha_1 - \alpha_2 - \alpha_3 
\end{align*}
\]

This gives \( \bar{\theta}^{(1)} = (\alpha_1, \alpha_2, \alpha_3) \).

- Solving \( f^{(5)} = 0 \) gives \( \lambda^{(2)} = 0 \). Thus, \( \bar{\theta}^{(2)} = 0 \).

- Solving \( f^{(6)} = 0 \) gives four solutions to \( \lambda^{(3)} \), so long as we assume \( \alpha_1 > \alpha_2 > \alpha_3 \). Each of the four solutions for \( \lambda^{(3)} \) correspond to one of the four solutions to \( \lambda^{(1)} \) (which were substituted in turn).

Thus, we are able to correctly associate each of the four solutions to a particular component of the ordered vector \( \tilde{\lambda}(t) \). For the sake of brevity we will not reproduce the expressions for \( \lambda^{(3)} \). Rather, we just provide the resulting expressions for \( \theta_j^{(3)} \):

\[
\begin{align*}
\theta_1^{(3)} &= \frac{1}{6} (-\alpha_1 (a_1^2 + a_2^2 + b_1^2 + b_3^2) + 2\alpha_2 a_3 b_3 + 2\alpha_3 a_2 b_2) \\
\theta_2^{(3)} &= \frac{1}{6} (-\alpha_2 (a_1^2 + a_3^2 + b_1^2 + b_3^2) + 2\alpha_1 a_3 b_3 + 2\alpha_3 a_1 b_1) \\
\theta_3^{(3)} &= \frac{1}{6} (-\alpha_3 (a_1^2 + a_2^2 + b_1^2 + b_2^2) + 2\alpha_1 a_2 b_2 + 2\alpha_2 a_1 b_1). \\
\end{align*}
\]

(41)

The special cases \( \alpha_1 = \alpha_2 = \alpha_3, \alpha_1 = \alpha_2 > \alpha_3 \) and \( \alpha_1 > \alpha_2 = \alpha_3 \) provide different (and rather more complicated) solutions for the \( \lambda^{(3)} \) compared with above. Arriving at the solution in these cases requires solving up to \( f^{(10)} = 0 \). We will not write out these results explicitly.

Thus we have

\[
\bar{\theta}(t) = \bar{\alpha} t + \bar{\theta}^{(3)} t^3 + O(t^4)
\]

(42)

for \( t \) in some interval \([0, \epsilon]\). \( \bar{\theta}^{(3)} \) is given in Eq. (31), except in the special cases noted above.

C. Conditions for laziness

From section II.C of [1], the expression for \( C_H(U) \) takes a simpler form when we have \( \theta_1 + |\theta_3| \leq \pi \). In this special case, \( C_H(U) \) is given by the minimum value of \( t_s \) such that

\[
\bar{\theta} \prec_s \bar{\alpha} t_s,
\]

(43)

where again \( \bar{\theta} \) is the vector of canonical-form parameters of \( U \) and \( \bar{\alpha} \) is the vector of canonical-form parameters of \( H \). This special case certainly holds for the canonical-form parameters of \( e^{-iHt} \) when \( t \) is sufficiently small. In this case Eq. (13) is equivalent to

\[
\begin{align*}
\theta_1 &\leq \alpha_1 t_s \\
\theta_1 + \theta_2 - \theta_3 &\leq (\alpha_1 - \alpha_2 - \alpha_3) t_s \\
\theta_1 + \theta_2 + \theta_3 &\leq (\alpha_1 + \alpha_2 + \alpha_3) t_s,
\end{align*}
\]

(44)

which is equivalent to

\[
\theta_1 \leq \alpha_1 t_s, \quad \frac{\theta_1}{\alpha_1} \leq t_s, \quad \frac{\theta_1 + \theta_2 - \theta_3}{\alpha_1 + \alpha_2 - \alpha_3} \leq t_s, \quad \frac{\theta_1 + \theta_2 + \theta_3}{\alpha_1 + \alpha_2 + \alpha_3} \leq t_s.
\]

(45)

Thus,

\[
C_H(U) = \max \left\{ \frac{\theta_1}{\alpha_1}, \frac{\theta_1 + \theta_2 - \theta_3}{\alpha_1 + \alpha_2 - \alpha_3}, \frac{\theta_1 + \theta_2 + \theta_3}{\alpha_1 + \alpha_2 + \alpha_3} \right\}.
\]

(46)
Given Eq. (42), we have
\[ \tau(t) = t + \tau^{(3)}t^3 + O(t^4) \] (47)
for small \( t \), where \( \tau^{(3)} \) is given by
\[ \tau^{(3)} = \max \left\{ \frac{\theta_1^{(3)}}{\alpha_1}, \frac{\theta_2^{(3)} + \theta_1^{(3)} - \theta_3^{(3)}}{\alpha_1 + \alpha_2 - \alpha_3}, \frac{\theta_2^{(3)} + \theta_3^{(3)} + \theta_1^{(3)}}{\alpha_1 + \alpha_2 + \alpha_3} \right\}. \] (48)

It is clear that whenever \( \tau^{(3)} < 0 \), the Hamiltonian is lazy. It is also clear that \( \tau^{(3)} \) is never greater than zero, because that would imply \( \tau(t) > t \), a contradiction. We find below the solutions (in terms of the parameters of the Hamiltonian) for \( \tau^{(3)} = 0 \); all Hamiltonians which do not belong to this solution set are guaranteed to be lazy. Note, however, that the complement of this solution set does not entirely characterise the class of lazy Hamiltonians, since there may be Hamiltonians in this set that are lazy due to higher-order Taylor coefficients that are negative. So our results may not fully characterise the set of all lazy Hamiltonians.

Let
\[ B_1 = \theta_1^{(3)}, \]
\[ B_2 = \theta_1^{(3)} + \theta_2^{(3)} - \theta_3^{(3)}, \] (50)
\[ B_3 = \theta_1^{(3)} + \theta_2^{(3)} + \theta_3^{(3)}. \] (51)

The coefficient \( \tau^{(3)} \) is zero if and only if at least one of \( B_j \) are zero. It is straightforward to show that for \( \alpha_1 > \alpha_2 > \alpha_3, \)
\[ B_1 = 0 \iff a_2 = a_3 = b_2 = b_3 = 0 \] (52)
\[ B_2 = 0 \iff a_1 = -b_1; a_2 = -b_2; a_3 = b_3 \] (53)
\[ B_3 = 0 \iff a_1 = b_1; a_2 = b_2; a_3 = b_3. \] (54)

We have arrived at the main result of this paper:

**Result 1** Any Hamiltonian of the form of Eq. (24) for which \( \alpha_1 > \alpha_2 > \alpha_3 \) and for which none of the three conditions

1. \( a_2 = a_3 = b_2 = b_3 = 0 \)
2. \( a_1 = -b_1; a_2 = -b_2; a_3 = b_3 \)
3. \( a_1 = b_1; a_2 = b_2; a_3 = b_3 \)

hold, is lazy. Such Hamiltonians will therefore need to be applied infinitely many times when used in a time-optimal simulation of a nonlocal two-qubit unitary.

These conditions obviously make it very easy to generate examples of lazy Hamiltonians, and imply that almost all two-qubit Hamiltonians are lazy. Note that the special cases \( \alpha_3 = \alpha_2 > \alpha_3, \alpha_1 > \alpha_2 = \alpha_3 \) and \( \alpha_1 = \alpha_2 = \alpha_3 \) yield somewhat more complicated conditions for a Hamiltonian to be lazy. These conditions are complex and not very illuminating, but can be obtained using techniques similar to those described above, so we will not reproduce them here.

### IV. Using Lazy Hamiltonian in Finite Time Steps

The results of the previous section show that almost all two-qubit Hamiltonians are lazy. This means that, in a simulation circuit, infinitesimal time steps must be employed to achieve time-optimality. We now show that, despite this requirement, if finite time steps are used then the corresponding sacrifice of interaction time is not very large — only a small relaxation from strict time-optimality is required in order to reduce the number of time steps to something practical.

To make our results concrete, we consider the case where the unitary being simulated is the controlled-not (CNOT) gate. Similar conclusions can be reached in the general case by following a similar argument to that below, and making use of the results of [10]. It can be shown [1] that the minimum time for simulating a CNOT is \( C_H(CNOT) = \frac{\pi}{\alpha_1} \), where \( \alpha_1 \) is the largest canonical-form parameter of the interaction Hamiltonian. When \( H \) is lazy, can we construct a simulation using a finite number of time steps such that the total interaction time is not much larger than the optimum \( C_H(CNOT) \)? Such a scheme is given in [11], whereby an arbitrary nonlocal two-qubit unitary \( U \) is applied a finite number of times together with local unitaries to simulate a CNOT. Using the scheme in [11], if \( U \) has largest canonical-form parameter \( \theta_1 \) such that
\[ n = \frac{\pi}{4\theta_1}, \] (55)
is an integer greater than one, then the scheme can be used to simulate a CNOT by applying \( U \) exactly \( n \) times. Of course, we are interested in the case when \( U = e^{-iH\Delta} \), that is \( U \) is given by the evolution of an interaction Hamiltonian over a time \( \Delta \). The total interaction time would then be
\[ t_s = n\Delta = \frac{\pi\Delta}{4\theta_1(\Delta)}. \] (56)

From the previous section, the function \( \theta_1(\Delta) \) can be written, for small \( \Delta \), as
\[ \theta_1(\Delta) = \alpha_1\Delta + \theta^{(3)}\Delta^3 + O(\Delta^4). \] (57)

Thus, for small \( \Delta \),
\[ t_s = \frac{\pi}{4\alpha_1 + \theta^{(3)}\Delta^2 + O(\Delta^3)} = C_H(CNOT) - \frac{\pi\theta^{(3)}\Delta^2}{16\alpha_1} + O(\Delta^2). \] (59)

This shows that to simulate a CNOT gate by applying a lazy interaction Hamiltonian in a (finite) number of small time-steps, then the penalty in the total interaction time, as compared with the optimum, is only of order \( \Delta^2 \).

As an example, consider a specific interaction Hamiltonian \( H = 0.1X \otimes X + I \otimes Z \). Using the results of the
FIG. 1: Canonical-form parameter $\theta_1(\Delta)$ of the unitary $e^{-iH\Delta}$, where $H = 0.1X \otimes X + I \otimes Z$.

FIG. 2: Total interaction time as a function of the number of simulation steps, for the simulation of CNOT using the Hamiltonian $H = 0.1X \otimes X + I \otimes Z$.

previous section it can easily be verified that $H$ is lazy. The graph of $\theta_1(\Delta)$ as a function of $\Delta$ is shown in Fig. 1. We choose a range of positive integer values of $n$, and for each $n$ we calculate how long the corresponding time step ($\Delta$) is by numerically solving

$$\theta_1(\Delta) = \frac{\pi}{4n}. \quad (60)$$

No solution to Eq. (60) exists for $n < 8$. This can be seen from the fact that $\pi/(4 \times 7) = 0.112\ldots$, which is greater than the maximum value that $\theta_1(\Delta)$ takes. For $n$ equal to 8 or greater, a corresponding $\Delta$ can be found. Finally, the interaction time $t_s$ required to simulate the CNOT is calculated via Eq. (60). The results are shown in Fig. 2. The dashed line is the optimal time, $C_H(\text{CNOT}) = 5\pi/2$. The results clearly show a near-optimal simulation with relatively small numbers of time steps. For 20 time steps, the total interaction time is just 2.8 percent greater than the optimal.

V. CONCLUSIONS

We have defined a class of “lazy” two-qubit Hamiltonians, those which can simulate themselves faster with the aid of fast local control than with uninterrupted evolution. When a lazy Hamiltonian is used in the time-optimal simulation of any nonlocal two-qubit unitary, we have shown that the simulation will require an infinite number of steps, and thus will be impractical. We have derived a simple set of sufficient conditions enabling us to prove that a given Hamiltonian is lazy. This set of conditions implies that almost all two-qubit Hamiltonians are lazy. Finally, we have shown that only a rather small sacrifice in the simulation time needs to be made in order to use a lazy Hamiltonian in a finite-step simulation.

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