Integrability and chaos in the quantum brachistochrone problem

S. Malikis [*] and V. Cheianov
Instituut-Lorentz, Universiteit Leiden, Leiden, The Netherlands

(Received 30 January 2024; revised 24 May 2024; accepted 10 July 2024; published 2 August 2024)

The quantum brachistochrone problem addresses the fundamental challenge of achieving the quantum speed limit in applications aiming to realize a given unitary operation in a quantum system. Specifically, it looks into optimization of the transformation of quantum states through controlled Hamiltonians, which form a small subset in the space of the system's observables. Here we introduce a broad family of completely integrable brachistochrone protocols, which arise from a judicious choice of the control Hamiltonian subset. Furthermore, we demonstrate how the inherent stability of the completely integrable protocols makes them numerically tractable and therefore practicable as opposed to their nonintegrable counterparts.

DOI: 10.1103/PhysRevA.110.022205

I. INTRODUCTION

Determining the optimal time required to achieve a unitary operation in a given quantum system holds fundamental significance, particularly in the context of the quantum dpeed limit [1,2]. It also carries important implications in the context of quantum control [3–5] such as quantum computing [6,7], shortcuts to adiabaticity [8], and quantum state preparation [9,10]. The quantum brachistochrone problem belongs to the class of formal problems aiming to facilitate this task. It was first introduced by Carlini *et al.* [11]. It can also incorporate other optimization approaches, like the quantum Zermelo navigation [12]. Moreover, it has been used to realize experimentally different optimal quantum qubit gates [13–15].

At a conceptual level, the quantum brachistochrone problem stems from the challenge of realizing a specific unitary transformation within a quantum system through a process known as "driving." This process entails a time-dependent manipulation of the system's Hamiltonian within a constrained parameter space defined by the architecture of quantum hardware. While numerous trajectories exist in this Hamiltonian parameter space that yield the same unitary evolution operator, of primary importance is the one that accomplishes the desired outcome with the smallest effort possible. In essence, the quantum brachistochrone is defined as the global minimum of a quantum cost function, which is the dimensionless product of the quantum computation time and the spectral norm of the control Hamiltonian. The mathematical intricacy of the quantum brachistochrone problem arises from the limitation imposed on the space of control Hamiltonians, typically confined to a small subset of all system observables.

The formal statement of the brachistochrone problem consists in specifying the Hilbert space, the choice of the subset of allowed Hamiltonians, and the desired unitary. Given such data one proceeds to solving the optimization problem, which translates into a boundary value problem for a system of nonlinear ordinary differential equations (ODEs). Several cases that can be solved analytically were presented in [16–19]. However, the problem in its generality remains analytically intractable and, in the case of moderately large systems, numerically hard as the common numerical recipes such as the shooting method [20] fail when the initialization of the search starts away from true solution [21,22]. In an attempt to tackle this difficulty, an alternative numerical approach was explored in [23], where the problem was reformulated into searching for geodesics curves in the unitary group. Moreover, in [24], they reformulated the problem by exploiting the additional symmetries of the prolem. Successful as this numerical recipe may be, it is naturally limited to gates of small dimensionality.

It is worth noting that the dimension of the system of quantum brachistochrone ODEs scales exponentially with the size of the quantum system, due to the exponential dependence of the Hilbert space with the number of particles. As the number of dynamical variables increases and the dynamics becomes more unstable solving the problem in full generality eventually becomes a formidable task. In fact, computational complexity endemic to all chaotic nonlinear equations [25] is likely to place the quantum brachistochrone problem into the same category of numerically hard problems as, e.g., the long-term forecast in the Lorenz system [26]. For this reason, it is important to identify special cases, which demonstrate stable dynamics, and which can be scaled to large system sizes. A particularly important subset of such cases is formed of completely integrable systems. Not only do such systems exhibit numerically stable trajectories, but they also (at least in principle) admit for various reductions and solutions by quadratures. Furthermore, by virtue of the phenomenon of Kolmogorov-Arnold-Möser (KAM)-stability [27–31], such systems give access to a much broader class of numerically easy nonintegrable brachistochrone problems achieved through small deformations of the space of allowed Hamiltonians.

In this paper, we present a class of completely integrable brachistochrone problems. This class, in particular, contains the exactly solved cases discovered in previous literature [16–19]. Complete integrability is achieved through the suitable choice of the space of control Hamiltonians, which are regarded as a generating set of a Lie algebra. Complete

[*]Contact author: malikis@lorentz.leidenuniv.nl

integrability arises from a relationship between the the control Hamiltonian subspace and Cartan decompositions of the associated Lie group [su(n) in our case]. The construction of the integrable cases is inspired by the classical integrable Lie-Poisson Hamiltonian systems [32,33]. After describing the general construction of the class of completely integrable quantum brachistochrone problems, we proceed to the investigation of the numerical stability of quantum brachistochrone equations in systems with a small Hilbert space. We find that the numerical stability of integrable protocols is significantly better than of an arbitrary chaotic protocol. Furthermore, the numerical data hint that, with increasing dimension of the Hilbert space, the boundary value problem in a generic nonintegrable case becomes increasingly hard to solve.

The structure of the paper is as follows. First we give a general overview of the quantum brachistochrone and discuss its general properties. Thereafter we describe the construction of a class of integrable brachistochrone protocols. Then we perform numerical investigation of the stability of integrable and nonintegrable protocols showing the qualitative difference. We, furthermore discuss evidence that the solution of the problem becomes increasingly more difficult with increasing dimension of the Hilbert space.

II. GENERAL OVERVIEW

A. Optimization problem and the cost function

In this paper we only consider quantum systems having a finite-dimensional computational Hilbert space. In practical hardware problems, such a space is usually associated with the soft (low-energy) part of the spectrum of a physical Hamiltonian. The soft spectrum needs to be separated from the rest of the energy eigenvalues by a sufficiently large energy gap to avoid unwanted excitations of the system outside the confines of the computational space. All observables discussed below are restrictions of the experimentally accessible physical observables to the computational Hilbert space.

Imagine that we want to realize a unitary operator $\hat{U}_d \in \mathrm{SU}(n)$ on an n-dimensional computational Hilbert space as an evolution operator generated by a time-dependent control Hamiltonian. More precisely, consider the evolution operator $U(t)$ satisfying the Schrödinger equation

$$i\partial_t \hat{U}(t) = \hat{H}(t)\hat{U}(t), \quad \hat{U}(0) = \mathbb{I}. \tag{1}$$

We are looking for a time-dependent Hamiltonian $H(t)$ such that at the end of computation $t = t_f$, the unitary evolution operator will satisfy $\hat{U}(t_f) = \hat{U}_d$. Generally, for a given U_d there are infinitely many such Hamiltonians. The optimization problem arises from the task of finding the "shortest" trajectory $\hat{H}(t)$, which is crudely the one that minimizes the protocol duration t_f (see below for clarification). The problem becomes nontrivial if we assume that $\hat{H}(t)$ can only be chosen from a subspace of the space of all quantum observables.

Before proceeding to the mathematical specifics we recall some basic facts about the quantum brachistochrone problem. First, we note that trivial multiplication of $H(t)$ by a number λ leads to the rescaling of the computation time $t_f \mapsto t_f/\lambda$. For this reason, the computation time itself is not a good choice of the optimisation functional. Rather, one introduces a dimensionless cost function $t_f \times \max_t ||\hat{H}(t)||$ where $||\ldots||$ stands for the Frobenius norm of an operator. The dimensionless optimisation functional admits for further simplification owing to a gauge symmetry of the original optimisation problem. We note that the Schrödinger equation is invariant under the redefinition $t \mapsto t' = \varphi(t)$ and $\hat{H}(t) \mapsto \hat{H}'(t) = \dot{\varphi}(t)H[\varphi(t)]$, where $\varphi(t)$ is any monotonically increasing function of time satisfying $\varphi(0) = 0$. This implies that one solution $H_*(t)$ to the quantum brachistochrone problem one generates a family of equivalent solutions parameterized by the gauge function $\varphi(t)$. In particular, one can easily see that there exists a gauge choice such that $\dot{\varphi}(t)||\hat{H}_*[\varphi(t)]|| = t_f \max_t ||\hat{H}_*(t)||$, while $\varphi(t_f) = 1$. With this choice of gauge the cost function can be written as

$$S = \int_0^1 dt||\hat{H}(t)|| \tag{2}$$

and the quantum brachistochrone problem becomes a variational problem for the functional S with the boundary conditions $\hat{U}(0) = \mathbb{I},\ \hat{U}(1) = \hat{U}_d$.

B. AB decomposition

The space of all physical observables constrained to the n-dimensional computational Hilbert space coincides with the space of all Hermitian endomorphisms of that space. In a given basis, the nontrivial endomorphisms are represented by traceless Hermitian $n \times n$ matrices, which form a vector space naturally endowed with a structure of the Lie algebra su(n). Let $\hat{\gamma}_k$ be some basis in the vector space of $n \times n$ traceless Hermitian matrices, for instance, the generalized Gell-Mann matrices [34], then $\{\hat{e}_k\}$, where $\hat{e}_k = -i\hat{\gamma}_k$, will form a basis in the defining representation of su(n). In the following we will assume the trace-form orthonormality condition $\mathrm{Tr}(\hat{\gamma}_i\hat{\gamma}_j) = \delta_{ij}$. In a given basis, the time-dependent Hamiltonian can be represented by a trajectory in a $n^2 - 1$-dimensional Euclidean coordinate space

$$\hat{H}(t) = \sum_{j=1}^{n^2-1} a_j(t)\hat{\gamma}_j. \tag{3}$$

If one had access to the entire Lie algebra, the extremals of the functional (2) would be delivered by the time-independent Hamiltonians of the form $\hat{H}_0 = i\log(\hat{U}_d)$, labeled by the choice of the branch of the logarithm function. In practice, however, the space of available Hamiltonians may be restricted, in which case time-independent solutions to the optimization problem do not generally exist. In such as situation, the optimization problem for the functional (2) may still admit for a solution, albeit with a time-dependent trajectory $a_j(t)$ lying within the permitted component of the operator space. Obviously, in order for the optimization problem to have a solution for any $\hat{U}_d \in \mathrm{SU}(n)$, the permitted subspace of the operator space should generate the entire space of observables su(n) in the Lie-algebraic sense. To formalize the constrained optimization problem we introduce the following definition.

Definition 1. The AB decomposition: Let $\mathbb{G}$ be the vector space of all observables (that is traceless Hermitian operators) on the computational space and let $\mathbb{A} \subset \mathbb{G}$ be the subspace of physically accessible Hamiltonians, that is any $\hat{H}(t)$ has to satisfy $\hat{H}(t) \in \mathbb{A}$ at all t. Then the following orthogonal decomposition will be called the *AB* decomposition of $\mathbb{G}$:

$$\mathbb{G} = \mathbb{A} \oplus \mathbb{B}. \tag{4}$$

Here the $\mathbb{A}$ and $\mathbb{B}$ subspaces are assumed to be orthogonal relative to the trace form.

We note, that the *AB* decomposition of the space of observables directly translates into a decomposition of the corresponding Lie algebra. Let $\mathfrak{g}$ be the defining representation of su(n). Then the decomposition (4) induces the following decomposition of $\mathfrak{g}$:

$$\mathfrak{g} = \mathfrak{a} + \mathfrak{b}, \tag{5}$$

where $\mathfrak{a} = \{-i\hat{A}|\hat{A} \in \mathbb{A}\}$, and $\mathfrak{b} = \{-i\hat{B}|\hat{B} \in \mathbb{B}\}$.

Given an *AB* decomposition, we can choose the orthonormal basis of $\mathbb{G}$ in the form $\{\hat{\gamma}_i\} = \{\hat{A}_i\} \cup \{\hat{B}_j\}$, where $\{\hat{A}_i\}$ and $\{\hat{B}_j\}$ are the orthonormal bases of $\mathbb{A}$ and $\mathbb{B}$, respectively. The constraint on the control Hamiltonian can then be stated as

$$\mathrm{Tr}(\hat{H}(t)\hat{B}_j) = 0, \quad j = 1, \dots, \dim \mathbb{B} \tag{6}$$

with an explicit solution in the form

$$\hat{H} = \sum_i \alpha_i \hat{A}_i. \tag{7}$$

Definition 2. Operator controllable AB decomposition: An *AB* decomposition is called operator controllable if for every $\hat{U}_d \in \mathrm{SU}(n)$, there exists a continuous trajectory $\hat{H} : [0, 1] \to \mathbb{A}$ that generates $\hat{U}_d$ in the sense of the boundary value problem (1).

Obviously, for the *AB* decomposition to be operator-controllable the Lie algebra $\mathfrak{g} = \mathrm{su}(n)$ must not have any proper subalgebras containing $\mathfrak{a}$. In other words, $\mathfrak{a}$ has to be a generating set of $\mathfrak{g}$ [35]. It is worth noting that operator controllability, which we focus on here, is a stronger requirement than the (pure) state controllability [4].

To construct $\hat{U}_d$, we have to perform a constrained optimisation of the functional (2). It is advantageous to state such an optimization problem in terms of the Lagrangian calculus of variations on the Lagrangian manifold SU(n). To this end, we note that

$$\hat{H}(t) = i\partial_t \hat{U}(t)\hat{U}^\dagger(t) \tag{8}$$

is an element of the tangent space, which has the meaning of the velocity, and that the condition (6) is a set of $m = \dim \mathbb{B}$ nonholonomic constraints, which can be imposed with the help of m Lagrange multipliers. The corresponding Lagrange functional takes the local form

$$S = \int_0^1 dt \left[\sqrt{\mathrm{Tr}(\partial_t \hat{U} \partial_t \hat{U}^\dagger)} + i \sum_{j=1}^{\dim \mathbb{B}} \lambda_j Tr(\hat{B}_j \partial_t \hat{U} \hat{U}^\dagger) \right]. \tag{9}$$

The Lagrange functional (9) can be viewed as an action describing constrained motion of a point particle on a group manifold.

The Euler-Lagrange equations for the functional (9) (see the Appendix for details) consist of Eqs. (6), due to variation with respect to the Lagrange multipliers λ_i, and the quantum brachistochrone equation

$$\frac{d}{dt}(\hat{H} + \hat{D}) + i[\hat{H}, \hat{D}] = 0, \tag{10}$$

where we introduce the operator

$$\hat{D} = \sum_i \lambda_i \hat{B}_i. \tag{11}$$

Equation (10) was first derived in [11,36] using a slightly different approach. In a given orthonormal basis $\{\hat{\gamma}_i\}$ Eq. (10) is equivalent to a system of nonlinear differential equations for the coordinates α_i, λ_i on the tangent bundle of the unitary group [23]

$$\begin{aligned} \dot{a}_i(t) &= i \sum_j \lambda_j \mathrm{Tr}(\hat{H}[\hat{A}_i, \hat{B}_j]), \\ \dot{\lambda}_i(t) &= i \sum_j \lambda_j \mathrm{Tr}(\hat{H}[\hat{B}_i, \hat{B}_j]). \end{aligned} \tag{12}$$

The Euler-Lagrange equations are supplemented by the initial condition $\hat{U}(0) = \mathbb{I}$ and the condition that $\hat{U}(1) = \hat{U}_d$. One can see that the brachistochrone problem turns into the boundary value problem for a set of nonlinear ODEs. The form of these equations is completely determined by the choice of the *AB* decomposition.

Generally, Eqs. (12) do not admit for an analytic solution. TIn order to solve the boundary value problem, one typically employs numerical methods, such as the shooting method or gradient descent routines [20–22]. However, as the number of dynamical variables (α_i, λ_j) increases quadratically with the rank of the group, chaos kicks in making the numerical routines increasingly inefficient. Still, even for large n one can identify particularly serendipitous *AB* decompositions, for which numerical convergence remains very good within either the entire phase space or, at least, a sufficiently large basin of stability. A natural class of such good *AB* decompositions is the one associated with *completely integrable* quantum brachistochrone equations. It is worth noting, that, apart from being well behaved in terms of the Lyapunov stability, completely integrable cases admit, at least, in principle, for solutions in terms of purely algebraic equations. Furthermore, small nonintegrable deformations of such integrable cases will give rise to equations with large stability islands. These observations prompt a natural task of identification and classification of all completely integrable *AB* decompositions.

In the following sections, we present a Lie-algebraic construction of a large class of *AB* decompositions leading to completely integrable brachistochrone equations. However, before delving into these details, we shall conclude the present section with discussion of some general properties of the brachistochrone problem.

C. Properties of the quantum Brachistochrone equations

First, we derive two useful conservation laws associated with Eqs. (12). By multiplying Eqs. (12) to a_i and λ_i, respectively, performing summations over all i and utilizing the cyclicity of trace, we find

$$\frac{d||\hat{H}(t)||_F^2}{dt} = 0, \quad \frac{d||\hat{D}(t)||_F^2}{dt} = 0. \tag{13}$$

This implies that the initial conditions, both on $\hat{H}(t)$ and $\hat{D}(t)$, determine the cost function of the protocol. Actually this stems from a wider symmetry. Equation (10) is essentially

$$\frac{d(\hat{H}+\hat{D})}{dt} = \frac{i}{2}[\hat{H}+\hat{D}, \hat{H}-\hat{D}]. \tag{14}$$

Therefore the operators $\hat{H}+\hat{D}$, $\hat{H}-\hat{D}$ form a Lax pair. This means that quantities $F_k = \mathrm{Tr}[(\hat{H}+\hat{D})^k]$ for $k \in \mathbb{N}$ are conserved, even though not all F_k's are algebraically independent.

Next, we remark that the Lagrange functional (9) is invariant under global right shifts $U \mapsto Ug$, where $g \in \mathrm{SU(N)}$. By virtue of Noether's theorem, this symmetry results in the conservation of the generalized angular momentum

$$\partial_t[\hat{U}^\dagger(\hat{H}+\hat{D})\hat{U}] = 0. \tag{15}$$

This equation can help determining the evolution of the optimal $\hat{H}(t)$, $\hat{D}(t)$. If one knows the initial state at $t=0$ and the unitary at $t=t_f$ (and not the path from $[0, t_f]$) one can find the final state. This conservation law is useful in our problem since it creates a relationship between the initial, final configuration of $\hat{H}(t)+\hat{D}(t)$ and the final unitary operator $\hat{U}_d$. Note that a similar property holds for the operator $\hat{U}_{-D}$ the operator that is generated through the $-D$ operator: $i\partial\hat{U}_{-D} = -\hat{D}\hat{U}_{-D}$,

$$\hat{U}^\dagger_{-D}(t)(\hat{H}(t)+\hat{D}(t))\hat{U}_{-D}(t) = \hat{H}(0)+\hat{D}(0). \tag{16}$$

Combining these we can get the commutation relation

$$[\hat{U}^\dagger_{-D}\hat{U}, \hat{H}(0)+\hat{D}(0)] = 0. \tag{17}$$

Moreover, by expressing the conservation law (15) and using Eq. (1)

$$i\partial_t\hat{U}(t) = \hat{U}(t)[\hat{H}(0)+\hat{D}(0)] - \hat{D}(t)\hat{U}(t), \tag{18}$$

we can rewrite the evolution operator in the following form [considering $\hat{U}(0) = \hat{U}_{-D}(0) = \mathbb{I}$]:

$$\hat{U}(t) = \hat{U}_{-D}(t)\exp\{-i[\hat{H}(0)+\hat{D}(0)]t\}. \tag{19}$$

We shall use this equation later in our discussion of a special case of completely integrable brachistochrone equation.

Conservation laws and related equations following from the general symmetries of the problem are useful, however, they are not sufficient to make the problem completely solvable. In the next section we show how to narrow down the set of brachistochrone problems to those, which are completely integrable in the Arnold-Liouville sense.

III. INTEGRABLE SU(N) BRACHISTOCHRONE EQUATION

Various definitions of integrability exist. Historically, integrability emerged as the property of equations of motion to admit for an analytic solution, achieved through techniques like separation of variables. Subsequently, a mathematical framework evolved, wherein integrability is construed as the commutativity of a sufficient number of independent Hamiltonian flows within a system's phase space. Both manifestations of integrability engender a stable and predictable behavior in a system. Both perspectives will be used in the present section.

We begin with examining the special case of time-independent Lagrange multipliers. The AB decomposition resulting in this integrable system was introduced in [19].

A. Complete integrability with time-independent Lagrange multipliers

Consider a class of trajectories such that Lagrange multipliers λ_i are constants of motion, i.e.,

$$\dot{\lambda}_i = 0, \quad \text{for all} \quad i = 1, \dots, \dim\mathbb{B}. \tag{20}$$

For such trajectories the corresponding differential equations for α_i's in Eqs. (12) can be solved explicitly

$$\mathbf{a}(t) = \exp(\hat{C}t)\mathbf{a}(0), \quad \hat{C}_{ab} = \sum_i f_{aib}\lambda_i. \tag{21}$$

In this expression f is the structure constant of the Lie algebra of observables, i.e., $[\hat{e}_i, \hat{e}_j] = \sum_k f_{ijk}\hat{e}_k$, the index i runs through the basis of the $\mathbb{B}$ subspace, while the indices a and b run through the elements of the subspace $\mathbb{A}$. Also we denote the set of all a_i's in a vector $\mathbf{a}(t) = (a_1(t)\cdots \quad a_N(t) \quad)^T$.

The explicit solution (21) of the reduced system (12), is a significant step forward, however, it does not automatically guarantee the existence of an algebraic solution for the evolution law of the group element given in Eq. (1). Next we demonstrate that in the case of time-independent Lagrange multipliers such an algebraic solution does indeed exist. We note that if Lagrange multipliers are constants of motion then the operator $\hat{D}$ is also time independent. This simplifies Eq. (19)

$$\hat{U}(t) = \exp[i\hat{D}(0)t]\exp\{-i[\hat{H}(0)+\hat{D}(0)]t\}. \tag{22}$$

For $t=1$ this becomes an algebraic equation defining the initial values $a_i(0)$ and λ_i in terms of the desired operator $\hat{U}_d$. In combination with Eq. (21) it provides a complete algebraic solution for the brachistochrone problem. It is worth noting that, despite a tremendous reduction in the complexity of the original problem, Eq. (22) remains nontrivial due to its nonlinearity and multivaluedness of its solutions.

A comprehensive exploration of the conditions leading to trajectories (20) presents an intriguing task, one that remains far from being exhaustively addressed. Nonetheless, a distinctive case stands out, in which these trajectories emerge directly from the structure of the AB decomposition, enveloping the entirety of the phase space. One general way to achieve this is by choosing the $\mathfrak{b}$ to be a subalgebra of $\mathfrak{g}$. In such a case, Eq. (20) follows from Eqs. (12) and the fact that $i[\hat{B}_i, \hat{B}_j] \in \mathbb{B}$, which is orthogonal to $\hat{H} \in \mathbb{A}$ with respect to trace inner product. This class of brachistochrone equations, along with Eq. (22) were first found in [19].

We conclude the recap of the exactly solvable case of constant Lagrange multipliers with a discussion of a special case of the AB decomposition having a pseudo-Cartan form. In such a case, the algebraic equations arising from the boundary value problem admit for some further simplifications. Consider a Lie algebra $\mathfrak{g}$. Then a decomposition $\mathfrak{g} = \mathfrak{l} + \mathfrak{p}$ is pseudo-Cartan if

$$[\mathfrak{l}, \mathfrak{l}] \subseteq \mathfrak{l}, \quad [\mathfrak{p}, \mathfrak{p}] \subseteq \mathfrak{l}, \quad [\mathfrak{p}, \mathfrak{l}] \subseteq \mathfrak{p}. \tag{23}$$

It is easy to confirm that if in the decomposition (5) one chooses $\mathfrak{a} = \mathfrak{p}$ and $\mathfrak{b} = \mathfrak{l}$ then a brachistochrone protocol is generated with time-independent Lagrange multipliers. Moreover, when $\mathfrak{l} = \mathrm{su}(N-1)$, its orthogonal compliment $\mathfrak{p}$ is the smallest generating set in $\mathrm{su}(N)$, that is, the smallest set of controlled Hamiltonians giving access to the computation on the whole unitary group. We note that to the best of our knowledge the pseudo-Cartan decomposition was first employed in the context of optimal quantum control in [37].

For *AB* decompositions having a pseudo-Cartan form it is possible to get some further insights into the structure of Eq. (22).

Proposition 1. Let a brachistochrone problem with an AB decomposition a pseudo-Cartan decomposition. Given two different $\hat{U}_d, \hat{U}_d'$, where $\hat{U}_d' = \exp(i\hat{X})\hat{U}_d \exp(-i\hat{X})$ and $\hat{X} \in \mathbb{B}$. The two unitary operators have the same cost function.

Proof. Take Eq. (22) at $t = 1$ for $\hat{U}_d$. We assume that its solution is $\hat{H}_0, \hat{D}_0$. By multiplying both sides with $\exp(i\hat{X}), \exp(-i\hat{X})$ from left and right, respectively, we get $\hat{U}_d'$ in the left-hand side (lhs). By considering the defining properties (23) we know that

$$\hat{H}_0' = e^{i\hat{X}}\hat{H}_0 e^{-i\hat{X}}, \quad \hat{D}_0' = e^{i\hat{X}}\hat{D}_0 e^{-i\hat{X}} \tag{24}$$

belong in $\mathbb{A}$, $\mathbb{B}$, respectively. This means that this is the solution for the $\hat{U}_d'$. Therefore the cost function, i.e., the Frobenius norm of $\hat{H}_0'$ is the same with $\hat{H}_0$. ■

B. Liouville-integrable brachistochrone equations

In the previous section, the integrability of the protocol stemmed directly from the conservation of the Lagrange multipliers. Here we introduce a more general *AB* decomposition that does not require conservation of λ_i and thus generates a wider class integrable brachistochrone protocols. The construction will exploit the Lax representation of the equations of motion for the generalized Euler-Arnold top [32,33]. To streamline discussion, we will not distinguish between su(n) and its defining matrix representation. Furthermore, will not distinguish between su(n) and its dual space, making use of the isomorphism between the two due to the trace-form inner product.

We begin by introducing the time-dependent element $\hat{t} = -i(\hat{H} + \hat{D})$, and writing its expansion in a given orthonormal basis su(n), as

$$\hat{t} = \sum_j x_j(t)\hat{e}_j. \tag{25}$$

Here $x_i(t)$ is either a dynamical variable or a Lagrange multiplier, depending on which subspace, $\mathbb{A}$ or $\mathbb{B}$, the corresponding $\hat{e}_j$ lies in. The brachistochrone equation can then be written in the form

$$\frac{d}{dt}\hat{t} = [\hat{t}, \mathcal{P}_B\hat{t}]. \tag{26}$$

In this equation $\mathcal{P}_B \in \mathrm{End}(\mathfrak{g})$ is the projector onto the B subspace, which implies $\mathcal{P}_B\hat{t} = -i\hat{D}$. Our goal is to demonstrate that, given an appropriate choice of the projector $\mathcal{P}_B$, Eq. (26) can be viewed as a certain limit of a known completely integrable dynamical system. To this end we recall the general construction of the Lax representation of the Euler-Arnold top.

Let $\mathfrak{g} = \mathfrak{l} + \mathfrak{p}$ be a pseudo-Cartan decomposition of su(n) [38]. We can then write the element $\hat{t}$ in the form $\hat{t} = \hat{l} + \hat{s}$ where l and s lie in $\mathfrak{l}$, $\mathfrak{p}$, respectively,

$$\hat{l} = \sum_{\mathfrak{l}} x_i(t)\hat{e}_i, \quad \hat{s} = \sum_{\mathfrak{p}} x_i(t)\hat{e}_i. \tag{27}$$

Now, let us fix some element $\hat{a} \in \mathfrak{p}$ and introduce the following Lax matrix:

$$\hat{L} = \hat{a}\lambda + \hat{l} + \frac{\hat{s}}{\lambda}, \quad \lambda \in \mathbb{C}, \tag{28}$$

where $\lambda \in \mathbb{C}$ is the spectral parameter. This matrix will be used to construct the brachistrochrone equation in the Lax form.

To obtain the second matrix in the Lax pair, we introduce a scalar function

$$\phi(\hat{x}) = \mathrm{Tr}\,\varphi(\hat{x}), \tag{29}$$

where

$$\varphi(z) = \sum_{k=0}^{K} c_k z^k \tag{30}$$

is a degree K polynomial. Note that according to Eq. (14), $\phi(\hat{t})$ is a constant of motion under the brachistochrone evolution. For a given set of coefficients $\{c_k\}$, we define the element

$$\hat{b} = \nabla\phi(\hat{x})|_{\hat{x}=\hat{a}} = \varphi'(\hat{a}), \tag{31}$$

which is the gradient of the function ϕ at $\hat{x} = \hat{a}$. One can easily see that $[\hat{a}, \hat{b}] = 0$ holds for any choice of $\hat{a}$ and $\{c_k\}$.

Within the subgroup of $\mathfrak{l}$ we perform a further decomposition $\mathfrak{l} = \mathfrak{l}_a + \mathfrak{l}^{\perp}$, where $\mathfrak{l}_a$ is the centraliser of $\hat{a}$

$$\mathfrak{l}_a : \{\hat{x} \in \mathfrak{l}, \quad [\hat{x}, \hat{a}] = 0\}, \tag{32}$$

which is a subalgebra of $\mathfrak{l}$.

The structure of the subalgebra $\mathfrak{l}_a$ depends on the order of su(n), the choice of the pseudo-Cartan decomposition and the choice of the element $\hat{a}$. We now define the function $\phi_a : \mathfrak{l}_a \to \mathbb{R}$,

$$\phi_a(\hat{x}) = \phi(\hat{a} + \hat{x}), \quad \hat{x} \in \mathfrak{l}_a,$$

and introduce its Hessian tensor at the point $l = 0$:

$$\phi_a'' := \sum_{i,j\in\mathfrak{l}_a} \hat{e}_i \otimes \hat{e}_j \frac{\partial^2\phi_a}{\partial x_i \partial x_j}\bigg|_{\hat{x}=0}. \tag{33}$$

With the help of the Hessian, we define a linear map $\hat{\omega}$ from $\hat{l}$ to itself by

$$\hat{\omega}(\hat{l}) = \begin{cases} \phi_a''\hat{l}, & \text{if } \hat{l} \in \mathfrak{l}_a, \\ \mathrm{ad}_b(\mathrm{ad}_a)^{-1}\hat{l}, & \text{if } \hat{l} \in \mathfrak{l}^{\perp}. \end{cases} \tag{34}$$

With these ingredients we complete the Lax pair with the matrix $\hat{M}$:

$$\hat{M} = \hat{b}\lambda + \hat{\omega}(\hat{l}), \quad \forall\lambda \in \mathbb{C}. \tag{35}$$

The following Lax equation

$$\frac{d\hat{L}}{dt} = [\hat{L}, \hat{M}] \tag{36}$$

describes a class of completely integrable systems known as generalized Euler-Arnold tops [32,33].

We are ready to provide the following theorem.

Theorem 1. For a given element $\hat{p} \in \mathfrak{p}$, define $\hat{a} = \epsilon \hat{p}$, where $\epsilon \in \mathbb{R}$. Let

$$\mathfrak{l}_a = \mathfrak{l}_a^{(A)} + \mathfrak{l}_a^{(B)} \tag{37}$$

be some, possibly trivial, decomposition of the centralizer of $\hat{a}$ into a direct sum of semi-simple subalgebras of $\mathfrak{g}$. Then with an appropriate choice of the polynomial $\varphi(z)$, Eq. (30), the $\varepsilon \to 0$ limit of the Lax equation (36) coincides with the brachistochrone equation (26) where the AB decomposition takes the form

$$\mathfrak{a} = \mathfrak{p} + \mathfrak{l}_a^{(A)}, \quad \mathfrak{b} = \mathfrak{l}^{\perp} + \mathfrak{l}_a^{(B)}. \tag{38}$$

Proof. Let $\mathrm{Spec}(\hat{a}) = \{a_1, a_2, \dots, \}$, be the eigenvalue spectrum of $\hat{a}$ in the defining representation of $\mathfrak{g} = \mathrm{su}(n)$ on the complex vector space $v = \mathbb{C}^n$. To each eigenvalue a_i there corresponds an eigenspace $v_i \in v$ and a simple subalgebra $\mathfrak{l}_a^{(i)} \subseteq \mathfrak{l}_a$, which is the largest subalgebra of $\mathfrak{l}_a$ preserving v_i and acting trivially on its orthogonal complement $v_i^{\perp}$. The centralizer of $\hat{a}$ has the semi-simple decomposition

$$\mathfrak{l}_a = \mathfrak{l}_a^{(1)} + \dots + \mathfrak{l}_a^{(Q)}, \tag{39}$$

where $Q \leqslant n$. Without loss of generality, we may assume a numbering such that

$$\mathfrak{l}_a^{(A)} = \mathfrak{l}_a^{(1)} + \dots + \mathfrak{l}_a^{(q)}, \quad \mathfrak{l}_a^{(B)} = \mathfrak{l}_a^{(q+1)} + \dots + \mathfrak{l}_a^{(Q)}. \tag{40}$$

Consider now the following choice of the polynomial φ :

$$\varphi(z) = \frac{z^2}{2} + \frac{1}{2}\psi(z)\prod_{i=1}^{Q}(z - a_i)^2, \tag{41}$$

where

$$\psi(z) = -\sum_{k=q+1}^{Q}\prod_{\substack{s=1\\ s\neq k}}^{Q}\frac{z - a_s}{(a_k - a_s)^3}. \tag{42}$$

One can easily see that with this choice of φ, the eigenvalues of $\hat{b}$ coincide with the eigenvalues of $\hat{a}$ therefore $\hat{b} = \hat{a}$. It follows immediately that the restriction of $\hat{\omega}(\hat{l})$, as defined in Eq. (34), to the space $\mathfrak{l}^{\perp}$ acts as the identity.

For the restriction of $\hat{\omega}(\hat{l})$ to the subspace $\mathfrak{l}_a$ we have

$$\phi_a'' = \sum_{i=1}^{Q}\varphi''(a_i)\mathcal{P}^{(i)}, \tag{43}$$

where $\mathcal{P}^{(i)} \in \mathrm{End}(\mathfrak{g})$ is the orthogonal projector onto the subspace $\mathfrak{l}_a^{(i)}$. A straightforward calculation shows that for φ given in Eq. (41) one has $\varphi''(a_i) = 0$ for $i = 1, \dots, q$ and $\varphi''(a_i) = 1$ for $q < i \leqslant Q$. Therefore, with $\varphi(z)$ given by Eq. (41) we have

$$\hat{\omega} = \mathcal{P}^{\perp} + \mathcal{P}^{(B)} = \mathcal{P}_B, \tag{44}$$

where $\mathcal{P}^{(B)} = \mathcal{P}^{(q+1)} + \dots + \mathcal{P}^{(Q)}$.

Finally, substituting the Lax matrices into the Lax equation and (36) and gathering coefficients at different powers of λ, we obtain the following set of equations:

$$[\hat{a}, \hat{b}] = 0, \quad [\hat{a}, \hat{\omega}(\hat{l})] = [\hat{b}, \hat{l}],$$
$$\dot{\hat{l}} = [\hat{l}, \hat{\omega}(\hat{l})] + [\hat{s}, \hat{b}], \quad \dot{\hat{s}} = [\hat{s}, \hat{\omega}(\hat{l})]. \tag{45}$$

The first pair of equations is satisfied automatically thanks to the definitions (31) and (34). In the second pair of equations we use the the definition of $\hat{t} = \hat{l} + \hat{s}$, the fact that $\hat{b} = \hat{a} = \epsilon \hat{p}$, and the specific form of $\hat{\omega}$, Eq. (44) to obtain

$$\frac{d}{dt}\hat{t} = [\hat{t}, \mathcal{P}_B\hat{t}] + \epsilon[\hat{s}, \hat{p}]. \tag{46}$$

Taking the $\varepsilon \to 0$ limit we finally obtain the brachistochrone equation in the form (26), with the *AB* decomposition given by Eq. (38). ■

C. Cases admitting for reduction to a linear system

There are two special types of the decomposition (38), which admit for a straightforward reduction to a linear system.

Type I. In *AB* decompositions of this type, the $\mathfrak{b}$ subspace is a subalgebra of $\mathfrak{g}$. This is achieved by choosing $\mathfrak{l}_a^{(A)} = 0$ and $\mathfrak{l}_a^{(B)} = \mathfrak{l}_a$ in Eq. (38). This case was analyzed in the literature [19] and we discuss it here in the section on time-independent Lagrange multipliers.

Type II. By choosing $\mathfrak{l}_a^{(A)} = \mathfrak{l}_a$ and $\mathfrak{l}_a^{(B)} = 0$ one gets $\mathfrak{b} = \mathfrak{l}^{\perp}$. Clearly, in this case the $\mathfrak{b}$ subspace is not a subalgebra of $\mathfrak{g}$. However, the system (10) can still be reduced to a linear one.

Proposition 2. Consider the AB decomposition such that $\mathfrak{b} = \mathfrak{l}^{\perp}$. Then the dynamical variables, which are the projections of $\hat{t}$ onto the $\mathfrak{l}_a$ subspace are integrals of motion. Furthermore, the system of ODEs (10) reduces to a linear system with time-dependent coefficients.

Proof. If $\mathfrak{l}_a^{(B)} = 0$, then $\mathcal{P}_B\hat{t} = \hat{l}^{\perp}$ is the orthogonal projection of $\hat{t}$ onto $\mathfrak{l}^{\perp}$. In this case, the orthogonal projection $\hat{l}_a$ of $\hat{t} = \hat{s} + \hat{l}$ onto the subspace $\mathfrak{l}_a$ is a constant of motion. To see that, consider the commutator $[\hat{s} + \hat{l}, \hat{l}^{\perp}]$ on the right-hand side of Eq. (26). The only potentially nontrivial projection of this commutator on the $\mathfrak{l}_a$ subspace is due to the element $\hat{x} = [\hat{l}_a, \hat{l}^{\perp}]$. However, this element lies in $\mathfrak{l}^{\perp}$ because for any $\hat{l}_a' \in \mathfrak{l}_a$ one has $\mathrm{Tr}(\hat{l}_a'\hat{x}) = \mathrm{Tr}(\hat{l}^{\perp}[\hat{l}_a', \hat{l}_a]) = 0$, where we use the cyclicity of trace and the fact that $\mathfrak{l}_a$ is closed under the Lie bracket.

We further note that the system of equations for the dynamical variable $\hat{l}^{\perp}$ takes the form

$$\frac{d}{dt}\hat{l}^{\perp} = [\hat{l}_a, \hat{l}^{\perp}]. \tag{47}$$

Since $\hat{l}_a$ are integrals of motion, this is a linear system, which has an explicit solution in the form

$$\hat{l}^{\perp}(t) = e^{\hat{l}_a t}\hat{l}^{\perp}(0)e^{-\hat{l}_a t}. \tag{48}$$

The remaining equation for the $\hat{s}$ component of $\hat{t}$ takes the form

$$\frac{d}{dt}\hat{s} = [\hat{s}, \hat{l}^{\perp}(t)], \tag{49}$$

where $\hat{l}^{\perp}(t)$ is given by Eq. (48). This is a linear equation with variable coefficients, which is formally solved in the form of a time-ordered exponential. ■

Protocols derived based on Proposition 2 fall under the type-II protocols. An example of such a construction is presented in the Appendix for the su(3) algebra.

The *AB* decompositions we presented rely on the Cartan decomposition of su(n) algebras. In the next section we

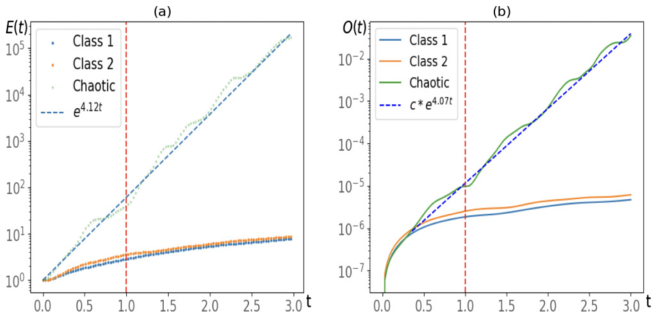

FIG. 1. Stability of brachistochrone equations for su(4). (a) Given a particular $\hat{U}_d$ the respective $\mathbf{x}(0)$ are found for the three protocols. The stability of those initial points are shown after averaging $E(t)$ for 2000 random small $\mathbf{d}$. (b) The time dependence of $O^i(t)$ for the same $\hat{U}_d$. The dashed lines fit the chaotic $E(t)$, providing estimations for the effective Lyapunov exponent.

present examples for $n = 3, 4$, but it can be extended for arbitrary n. A question of practical importance, which is worth mentioning here, is how the integrable protocols could be realized with local operators in multiqubit systems. This brings up the issue of the construction of pseudo-Cartan decompositions of su(2^n) with maximally local gates: a mathematical problem, where few results are known today [39].

IV. NUMERICAL STABILITY

Stability of equations of motion

We embarked on the search for integrable brachistochrone equations due to their inherent stability. A well-known issue in general nonlinear problems is the instability of trajectories under slightly varied initial conditions. Specifically, if we solve equations with initial conditions $\mathbf{x}'(0) = \mathbf{x}(0) + \mathbf{d}$ with $|\mathbf{d}| \ll |\mathbf{x}(0)|$ the respective variation for the solutions versus time $DH(t) = ||\mathbf{x}'(t) - \mathbf{x}(t)||$. Stability can be quantified using the following measure:

$$E(t) \equiv \frac{|DH(t)|}{|DH(0)|}. \tag{50}$$

In Fig. 1(a) we show how $E(t)$ of the brachistochrone equations (12) behave for the three different cases. The initial conditions have been chosen so that they realize a particular $\hat{U}_d$ for the integrable decompositions of types I and II, and a general chaotic case, respectively. We observe that for a generic AB decomposition, even for SU(4) case, we observe Lyapunov exponents $\lambda_e \geqslant 1$, i.e., $E^{\rm ch}(t) \propto \exp(\lambda_e t)$. where the "ch" superscript refers to the particular general chaotic decomposition. This indicates that the chaotic behavior becomes relevant for the brachistochrone problem since it kicks in for time $t < 1$.

To exclude the role of exceptional perturbations, we sampled many different perturbations and we sampled $DH(t)$ over them. Moreover, we tried numerous other AB decompositions. We confirm, therefore, the expected exponential divergence for a general AB decomposition.

It is instructive to see how the instability of the brachistochrone equations (12) propagates to the generated unitary operator through Eq. (1). To this end we look into the following measure of the divergence of to nearby trajectories

$$O^i(t) = \left\langle \left|\left| \log\left(\left(\hat{U}_b^i\right)^\dagger(\mathbf{x}_0, t)\hat{U}_b^i[\mathbf{x}_0 + \mathbf{d}, t]\right)\right|\right|_F \right\rangle_{\mathbf{d}}. \tag{51}$$

Here $U_b^i(\mathbf{x}_0, t)$ is the generated unitary operator at time t for the initial conditions $\mathbf{x}_0$ to the boundary value problem of Eq. (12) for the ith case (integrable or chaotic). By doing so [see Fig. 1(b)], we can see when the nonlinear behavior appears for the chaotic case. For short-enough times, the divergence of $\hat{U}_b(\mathbf{x}_0 + \mathbf{d})$ from $\hat{U}_b(\mathbf{x}_0)$ is linear for all three cases. For the chaotic one, we confirm this stops at time $t \approx \lambda_e^{-1}$. We confirm, therefore, that indeed the instability of the brachistochrone equation propagates to the generated unitary operator.

This comes as no surprise. If we assume

$$\hat{U}_b^i(\mathbf{x}_0 + \mathbf{d}, t) = \hat{U}_b^i(\mathbf{x}_0, t)\hat{u}(t), \tag{52}$$

where the unitary operator $\hat{u}$ is the (conjugate transpose) of the argument in the log of O^i. It obeys the Schrödinger equation

$$i\partial\hat{u} = \left(\hat{U}_b^i(\mathbf{x}_0, t)\right)^\dagger \hat{\Delta}\hat{U}_b^i(\mathbf{x}_0, t)\hat{u}, \quad \hat{u}(0) = \mathbb{I}, \tag{53}$$

where $\hat{\Delta} = \hat{H}(t)' - \hat{H}(t)$ is the difference of the two Hamiltonians for different initial conditions. This means that $\hat{u}$ is driven by the Hamiltonian (in the rotated frame) $\hat{U}_b^\dagger(\mathbf{x}_0, t)\hat{\Delta}\hat{U}_b(\mathbf{x}_0, t)$. Therefore, one can explain why there is similar (albeit latent) Lyapunov exponent for the same equation.

Lyapunov instability is a fundamental manifestation of chaos in brachistochrone problems with nonintegrable AB decompositions. However, a given AB decomposition is not generally characterized by a given largest Lyapunov exponent. Rather, the Lyapunov exponent is a function of the initial condition of the trajectory. To illustrate this point we investigate the statistics of the largest Lyapunov exponents in a chaotic system with a given AB decomposition. First, we notice that the brachistochrone equations (12) are invariant under the transformation $\mathbf{a}' \to \kappa\mathbf{a}$, $\boldsymbol{\lambda}' \to \kappa\boldsymbol{\lambda}$, $t' \to t/\kappa$ where $\kappa \in \mathbb{R}^+$. This means that, under this transformation, the left-hand side of

$$\frac{||\mathbf{x}_1(t) - \mathbf{x}_0(t)||}{||\mathbf{x}_1(0) - \mathbf{x}_0(0)||} \approx \exp(\gamma_0 t) \tag{54}$$

remains invariant, while the right-hand side becomes $\exp(\kappa\gamma_0 t)$. Therefore, the transformed solution has a Lyapunov exponent $\lambda_e' = \kappa\gamma_0$. For this reason it is only meaningful to talk about the distribution of Lyapunov exponents on the basin of initial conditions defined by the constraint $||\mathbf{x}_0|| = 1$.

In Fig. 2 we show the distribution of Lyapunov exponents for random sampling of $\mathbf{x}_0'$s with $||\mathbf{x}_0|| = 1$. For random sampling we assume the probability distribution invariant under the adjoint action of SU(n).

We observed that, for a chaotic protocol, close initial conditions diverge exponentially, while integrable protocols diverge polynomially. We expect, thus, between these two a qualitative difference regarding the closeness of two different unitary operators $\hat{U}_0, \hat{U}_1$ derived from close initial configurations $[\mathbf{a}_0(0), \boldsymbol{\lambda}_0(0)]$, $[\mathbf{a}_1(0), \boldsymbol{\lambda}_1(0)]$, respectively. Thus we introduce the measure

$$\mathcal{F}^i(\hat{U}_0, \mathbf{d}) = \left|\left| \log\left\{\left[(\hat{U}_0)^\dagger\hat{U}_b^i(\mathbf{x}_0 + \mathbf{d}, 1)\right]\right\}\right|\right|_F, \tag{55}$$

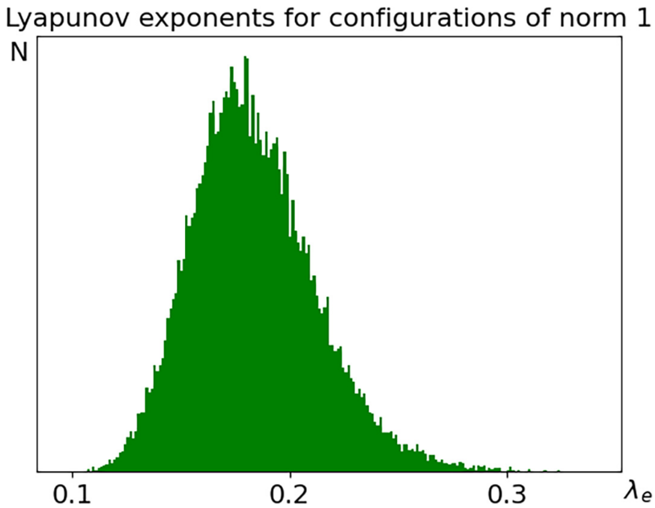

FIG. 2. Histogram of Lyapunov exponents for an SU(4) chaotic *AB* decomposition. The histogram of distribution of Lyapunov exponents for configurations $\mathbf{x}_0$ with $||\mathbf{x}_0|| = 1$. Twenty-five thousand random configurations are sampled.

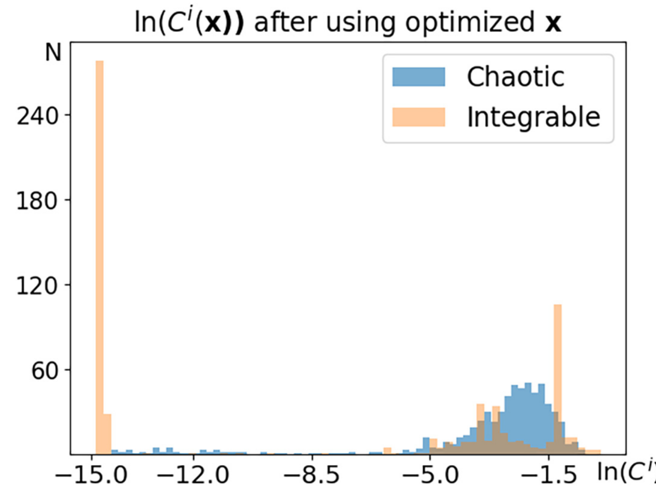

FIG. 4. Histogram of the eventual values of $\ln C^i(\mathbf{x})$ for an SU(4) chaotic and integrable *AB* decomposition. Some random initial values $\mathbf{x}_0$ are used along with standard optimizing routines, giving the final $\mathbf{x}$.

where $\mathbf{x}_0$ is the configuration that generates $\hat{U}_0$ through the brachistochrone equations for some particular protocol, and $\mathbf{d}$ is a small perturbation. The index i refers to which protocol is used (an integrable or a chaotic one). For a fixed $\mathbf{x}_0$, we are going to constrain ourselves to $\mathbf{d}$ of fixed (small) norm. Essentially $\mathbf{x}_0$ determines the nature of the measure (55). Thus, as we explained above, the norm of $\mathbf{x}_0$ is the parameter that determines the closeness of the measure $\mathcal{F}^i$. When the norm of configuration $\mathbf{x}_0$ is sufficiently small the statistical behavior of $\ln(\mathcal{F})$ between integrable and chaotic protocols for different $\mathbf{d}$ [see Fig. 3(a)] will not be significant. However, when the norm of $\mathbf{x}_0$ becomes bigger, there is an exponential separation and small deformations of configurations lead to bigger $\mathcal{F}$ [Fig. 3(b)]. The difference in the behavior between the two cases is because for small Lyapunov exponents (small norm of $\mathbf{x}_0$) the chaos does not play an important role by the end of the protocol (for times $t \approx 1$).

This observation hints at the impact of the increase in the rank of the unitary group and the number of constraints on the numerical hardness of computing the brachistochrone reaching an arbitrary unitary $\hat{U}_d$. Generally, the higher the dimensionality of the Hilbert space, the greater the norm of the typical driving Hamiltonian. Furthermore, by introducing extra constraints one replaces "physical" degrees of freedom with Lagrange multipliers, which typically take bigger values. Both factors essentially increase the norm of the configurations $\mathbf{x}_0$, which makes the brachistochrone path to a given $\hat{U}_d$ more unstable, as we established previously. We would like to stress, however, that no quantitative claim is made at this point and is an open question to be investigated.

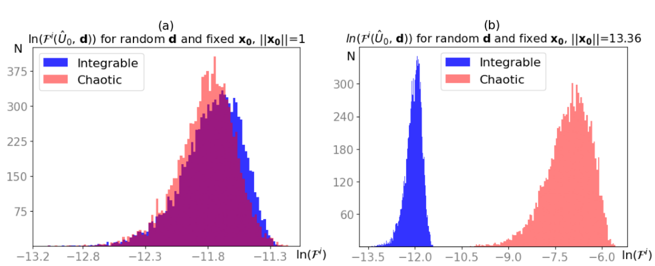

FIG. 3. Histogram of $\ln[\mathcal{F}^i(\hat{U}_0, \mathbf{d})]$ for an integrable and a chaotic SU(4) *AB* decomposition and a given $\hat{U}_0$ (generated by $\mathbf{x}_0$) over random deformations $\mathbf{d}$. Panel (a): A configuration $\mathbf{x}_0$ is used norm 1 is used. The behavior of $\mathcal{F}$ between chaotic and integrable is qualitatively the same. (b) A $\mathbf{x}_0$ is used that solves the boundary value problem for some some random operator (i.e., not close enough to the identity operator). We observe some exponential separation between the integrable and the chaotic one.

Instability with respect to small variations in the initial conditions makes the boundary value problem a numerically hard task. Essentially it turns out to be an optimization problem, where a high precision of the parameter landscape is required to converge to the desired unitary operator. To quantify this we introduce the cost function

$$C^i_{\hat{U}_0}(\mathbf{x}) := ||\log[\hat{U}_0^\dagger \hat{U}_{b,i}(\mathbf{x}, 1)]||_F. \tag{56}$$

After fixing $\hat{U}_0$ and the *AB* decomposition, the minimization of C requires some minimization routine. We employed certain preconstructed ones for the the chaotic and the integrable cases, respectively. Since certain initial guesses may get stuck at some local minima, and not at the global one, we sampled over many initial points $\mathbf{x}_0$ and study their statistics. From Fig. 4 one can see that for the integrable case, there are many initial guesses that converge to the desired solution, with certain accuracy (of order of 10^{-6}). However, in the chaotic case the optimization gets stuck to suboptimal solutions and need extra resources to reach to the desired solution. So we deduce how immensely more difficult is to solve the boundary value problem for a generic decomposition, even for the SU(4) group, let alone higher ones.

V. CONCLUSION

We investigated quantum brachistochrone equations describing the optimal realization of an SU(n) gate with the help of a protocol utilising a constrained set of driving Hamiltonians. We found that, for a certain class of driving Hamiltonians, the quantum brachistochrone equation can be viewed as a limiting case of a completely integrable system known as the generalized Euler-Arnold top. We give an explicit prescription for the associated AB decomposition of the algebra of physical observables into the space of driving Hamiltonians and its orthogonal complement.

To demonstrate the utility of the completely integrable AB decompositions, we compare the numerical stability of generic brachistochrone equations with the completely integrable ones. In contrast to the integrable case, generic brachistochrone equations are found to exhibit exponential divergence of nearby trajectories characteristic of chaotic behaviour. We quantify such divergence by the Lyapunov exponents and investigate the statistical distribution and scaling properties of such exponents for small groups. We propose arguments as to why such exponential divergence poses an increasing numerical challenge for the solution of the boundary value problem as one increases the size of the unitary group or the number of constraints. This should motivate further investigation of completely integrable protocols and their small nonintegrable deformations.

Notwithstanding the intriguing link between integrable brachistochrone equations and the classical integrable models, many questions remain unanswered. For instance, it is unclear how far one can advance with the program of developing an explicit solution of the completely integrable brachistochrone equations, in particular, with finding an explicit relationship between the initial conditions and the generated unitary operator at the end of the protocol. One systematic approach to this problem employs the Baker-Akhiezer functions and a factorisation method based on the matrix Riemann-Hilbert problem [32,33]. Furthermore, even if a formal algebraic solution to the boundary value problem is found, the actual computation of the initial conditions may still present a certain challenge as is evidenced by Eq. (19). It is also important to note that the completely integrable cases of AB decompositions identified here may not cover all integrable brachistochrone problems, making further investigation into this area an interesting and relevant problem in its own right.

ACKNOWLEDGMENTS

We would like to thank M. Semenyakin for helpful discussions. This publication is part of the project Adiabatic Protocols in Extended Quantum Systems, Project No. 680-91-130, which is funded by the Dutch Research Council (NWO).

APPENDIX A: ACQUIRING THE BRACHISTOCHRONE EQUATIONS

Let's consider the action with the Lagrange multipliers $\{\lambda_i\}$:

$$S_0 = \int_0^T dt\left(\frac{1}{2}Tr(\partial_t\hat{U}\,\partial_t\hat{U}^\dagger) + i\sum_\kappa \lambda_\kappa Tr(B_k\partial_t\hat{U}\hat{U}^\dagger)\right). \tag{A1}$$

To facilitate our computations we adopt the index notation. This way the matrix multiplication and Tr operation get simpler. The integrand, then, is written

$$s = \frac{1}{2}(\partial\hat{U})_{ab}(\partial\hat{U}^\dagger)_{ba} + i\sum_\kappa \lambda_\kappa (B_\kappa)_{ab}(\partial\hat{U})_{bc}(U^\dagger)_{ca}. \tag{A2}$$

We are going to vary the "field" U to minimize the action s. To keep it short we separate the action in two parts, $s_{1,2}$, respectively,

$$\delta s_1 = \tfrac{1}{2}(\partial\delta\hat{U})_{ab}(\partial\hat{U}^\dagger)_{ba} + \tfrac{1}{2}(\partial\hat{U})_{ab}(\partial\delta\hat{U}^\dagger)_{ba}. \tag{A3}$$

Up to boundary terms, δs_1 can be written as

$$\delta s_1 = -\tfrac{1}{2}((\partial^2\hat{U}^\dagger)_{ba}(\delta\hat{U})_{ab} + (\partial^2\hat{U})_{ab}(\delta\hat{U}^\dagger)_{ba}). \tag{A4}$$

Meanwhile the variation of s_2:

$$\delta s_2 = i\sum_\kappa(\lambda_\kappa(B_\kappa)_{ab}(\partial\delta\hat{U})_{bc}(\hat{U}^\dagger)_{ca} + \lambda_\kappa(\hat{B}_\kappa)_{ab}(\partial\hat{U})_{bc}(\delta\hat{U}^\dagger)_{ca}). \tag{A5}$$

Again up to boundary terms

$$\delta s_2 = i\sum_\kappa(-\dot{\lambda}_\kappa(\hat{B}_\kappa)_{ab}(\delta\hat{U})_{bc}(\hat{U}^\dagger)_{ca} - \lambda_\kappa(\hat{B}_\kappa)_{ab}(\delta\hat{U})_{bc} \times (\partial\hat{U}^\dagger)_{ca} + \lambda_\kappa(\hat{B}_\kappa)_{ab}(\partial\hat{U})_{bc}(\delta\hat{U}^\dagger)_{ca}). \tag{A6}$$

We want to collect all the variation wrt δU. So we need to take into consideration $\hat{U}\hat{U}^\dagger = \mathbb{I} \Rightarrow \delta\hat{U}\hat{U}^\dagger + \hat{U}\delta\hat{U}^\dagger = 0 \Rightarrow \delta\hat{U}^\dagger = -\hat{U}^\dagger\delta\hat{U}\hat{U}^\dagger$. Moreover using the Tr properties, we can rewrite $\delta s_1 = \delta\hat{U}_{ab}T^1_{ba}$, $\delta s_2 = \delta\hat{U}_{ab}T^2_{ba}$:

$$T^1 = -\frac{1}{2}(\partial^2\hat{U}^\dagger - \hat{U}^\dagger\partial^2\hat{U}\hat{U}^\dagger), \tag{A7}$$

$$T^2 = -i\sum_\kappa\lambda_\kappa\partial\hat{U}^\dagger\hat{B}_\kappa - i\sum_\kappa\dot{\lambda}_\kappa\hat{U}^\dagger\hat{B}_\kappa - i\sum_\kappa\lambda_\kappa\hat{U}^\dagger\hat{B}_\kappa\partial\hat{U}\hat{U}^\dagger. \tag{A8}$$

So essentially the "equation of motion" is $T^1 + T^2 = 0$. To simplify it further, we use $\partial\hat{U}^\dagger = -\hat{U}^\dagger\partial\hat{U}\hat{U}^\dagger$. So we will have

$$T^1 = \hat{U}^\dagger\partial^2\hat{U}\hat{U}^\dagger + \tfrac{1}{2}(\partial\hat{U}^\dagger\partial\hat{U}\hat{U}^\dagger + \hat{U}^\dagger\partial\hat{U}\partial U^\dagger). \tag{A9}$$

Multiplied with $\hat{U}\ T^1$ becomes

$$UT^1 = \partial^2\hat{U}\hat{U}^\dagger + \tfrac{1}{2}(\hat{U}\partial U^\dagger\partial\hat{U}\hat{U}^\dagger + \partial\hat{U}\partial U^\dagger). \tag{A10}$$

The terms in the parentheses are equal (use two times the property $\partial\hat{U}\hat{U}^\dagger = -\hat{U}\partial\hat{U}^\dagger$). Actually, the entire term $i\hat{U}T^1 = \partial_t\hat{H}$. Similar manipulation of $\hat{U}T^2$ gives

$$\hat{U}T^2 = \sum_\kappa(\lambda_\kappa\hat{H}\hat{B}_\kappa - i\dot{\lambda}_\kappa\hat{B}_\kappa - \lambda_\kappa\hat{B}_\kappa\hat{H}) = \sum_\kappa(\lambda_\kappa[\hat{H},\hat{B}_\kappa] - i\dot{\lambda}_\kappa\hat{B}_\kappa). \tag{A11}$$

As a whole $i\hat{U}(T^1 + T^2) = 0$ gives

$$\partial_t\hat{H} + \sum_\kappa(i\lambda_\kappa[\hat{H},\hat{B}_\kappa] + \dot{\lambda}_\kappa\hat{B}_\kappa) = 0. \tag{A12}$$

This is the known quantum brachistochrone equation. Also the second term we introduced implies:

$$Tr(\hat{H}\hat{B}_k) = 0, \quad \forall k. \tag{A13}$$

Note. The variation of action S_0 is equivalent to the variation of the action S_1:

$$S_1 = \int dt \left(\sqrt{\mathrm{Tr}(\partial U \partial U^\dagger)} + \sum_i \lambda_i \mathrm{Tr}(\partial \hat{U} \hat{U}^\dagger) \right). \tag{A14}$$

The only thing that changes is that $S_0(\lambda_i) \to S_1(\lambda_i/\|H\|_F^2)$; but as we show in a next section the Frobenius norm of H remains constant along a trajectory. This means that we should need to rescale the Lagrange multipliers.

APPENDIX B: EXAMPLE OF A LINEARIZABLE *AB* DECOMPOSITION

We consider the su(3) algebra and its pseudo-Cartan decomposition $\mathfrak{g} = \mathfrak{l} + \mathfrak{p}$ such that $\hat{s} \in \mathfrak{p}$ and $\hat{l} \in \mathfrak{l}$ are parametrized as follows:

$$\hat{s} = \begin{pmatrix} 0 & 0 & z_1 \\ 0 & 0 & z_2 \\ z_1^* & z_2^* & 0 \end{pmatrix}, \quad \hat{l} = \begin{pmatrix} r_1 & \psi_1 & 0 \\ \psi_1^* & r_2 & 0 \\ 0 & 0 & -(r_1 + r_2) \end{pmatrix}. \tag{B1}$$

Note that the subgroup $\mathfrak{l} \cong \mathrm{su}(2) \times \mathfrak{u}(1)$. Now let's fix the element $\hat{a}$. Let that be (arbitrarily)

$$\hat{a} = \begin{pmatrix} 0 & 0 & a_1 \\ 0 & 0 & 0 \\ a_1 & 0 & 0 \end{pmatrix}, \tag{B2}$$

where $a_1 \in \mathbb{R}$. From that we infer that the subset $\mathfrak{l}_a$ consists of the single (linearly independent) element

$$\hat{X} = \frac{1}{\sqrt{3}} \mathrm{diag}(1, -2, 1). \tag{B3}$$

Therefore $L_p = \sum_i m_i Y_i$, where $L_p \in \mathfrak{l}_a^\perp$ and $\mathfrak{l}_a^\perp$:

$$\mathfrak{l}_a^\perp := \mathrm{span}\left\{ \hat{Y}_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{Y}_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{Y}_3 = \mathrm{diag}(1, 0, -1) \right\}. \tag{B4}$$

Moreover, the generic invariant polynomial can be generated by

$$\phi = \sum_i c_i Tr((\hat{s} + \hat{l})^i), \tag{B5}$$

for arbitrary $\{c_i\}$. From that on can define $b = d\phi(a)$ (i.e., the gradient of ϕ at a). If one includes at least powers 2,3 basically what they get is

$$b = \kappa_1 a + \kappa_2 X, \tag{B6}$$

κ_i's are arbitrary (and dependent on all c_i). From this, we can get ω. In particular,

$$\omega(l) = \begin{cases} \mu X, & \text{if } l \in \mathfrak{l}_a, \\ ad_b(ad_a)^{-1} l, & \text{if } l \in \mathfrak{l}_a^\perp, \end{cases} \tag{B7}$$

again μ is related to c (but independent from κ_i's). Let's see that what happens first with $(ad_a)^{-1}$. We want some operator Z that $i[a, Z] = l$ (physics convention with multiplication with i). So Z for each of the three cases is

$$Z = \begin{cases} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{i}{a_1} \\ 0 & -\frac{i}{a_1} & 0 \end{pmatrix}, & \text{if } l = Y_1, \\ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{a_1} \\ 0 & -\frac{1}{a_1} & 0 \end{pmatrix}, & \text{if } l = Y_2, \\ \begin{pmatrix} 0 & 0 & \frac{i}{2a_1} \\ 0 & 0 & 0 \\ \frac{-i}{2a_1} & 0 & 0 \end{pmatrix}, & \text{if } l = Y_3. \end{cases} \tag{B8}$$

Consequently the last step is to get simply $i[b, Z]$ for the three different cases

$$\omega(l) = \begin{cases} \mu X & \text{if } l \in \mathfrak{l}_a, \\ \frac{\kappa_1}{a_1} Y_1 & \text{if } l = Y_1, \\ \frac{\kappa_1}{a_1} Y_2 & \text{if } l = Y_2, \\ \frac{\kappa_1}{a_1} Y_3 & \text{if } l = Y_3. \end{cases} \tag{B9}$$

Note that to reach to this result we had to set $\kappa_2 = 0$ since with nonzero κ_2 it would generate components of ω that do not belong in $\mathfrak{l}$. With this is mind, we are able to write down the final differential equations. By using the linearity of $\omega(l)$:

$$\dot{l} = [l, \omega(l)] + [s, b], \quad \dot{s} = [s, \omega]. \tag{B10}$$

If we take the $a_1 \to 0$ limit (that is the matrix $a \to 0$). The system of equations becomes the brachistochrone equation

$$\dot{l} + \dot{s} = [l + s, \omega]. \tag{B11}$$

Note that the limit is legitimate since ω remains finite in that limit. With this, we can set $\mu = 0, \kappa_1 = \alpha_1$ o make ω a projector onto the $\mathfrak{l}^\perp$. This way we create a new integrable protocol. The system of equations one has to solve is

$$\begin{pmatrix} \dot{a}_1 \\ \dot{a}_2 \\ \dot{a}_3 \\ \dot{a}_4 \\ \dot{l} \\ \dot{m}_1 \\ \dot{m}_2 \\ \dot{m}_3 \end{pmatrix} = \begin{pmatrix} -a_2 m_2 - a_3(m_1 + 2m_3) \\ a_1 m_2 - a_3(m_1 + m_3) \\ a_2 m_1 - a_3 m_2 + 2a_1 m_3 \\ a_1 m_1 + a_3 m_2 + a_2 m_3 \\ 0 \\ \sqrt{3} l m_2 \\ -\sqrt{3} l m_1 \\ 0 \end{pmatrix},$$

$$\hat{H}(t) = \begin{pmatrix} \frac{l}{\sqrt{3}} & 0 & a_1 - ia_3 \\ 0 & -\frac{2l}{\sqrt{3}} & a_2 - ia_4 \\ a_1 + ia_3 & a_2 + ia_4 & \frac{l}{\sqrt{3}} \end{pmatrix}. \tag{B12}$$

Note that the system is linear. In particular, m_1, m_2 can be solved exactly and are some linear combinations of $\sin(\sqrt{3}lt), \cos(\sqrt{3}lt)$. Also since m_3 is time-independent, the system of a_i becomes a driven linear system. The explicit solution is given by

$$\begin{pmatrix} a_1(t) \\ a_2(t) \\ a_3(t) \\ a_4(t) \end{pmatrix} = \mathcal{T} \exp\left(\int_0^t \hat{M}(t')dt' \right) \begin{pmatrix} a_1(0) \\ a_2(0) \\ a_3(0) \\ a_4(0) \end{pmatrix}, \quad \hat{M}(t) = \begin{pmatrix} 0 & -m_2(t) & -2m_3(t) & -m_1(t) \\ m_2(t) & 0 & -m_1(t) & -m_3(t) \\ 2m_3(t) & m_1(t) & 0 & -m_2(t) \\ m_1(t) & m_3(t) & m_2(t) & 0 \end{pmatrix}. \tag{B13}$$

Since the matrix $\hat{M}$ is antisymmetric, we know that the matrix remains finite and there are not exponential divergences.

[1] T. Caneva, M. Murphy, T. Calarco, R. Fazio, S. Montangero, V. Giovannetti, and G. E. Santoro, Optimal control at the quantum speed limit, Phys. Rev. Lett. **103**, 240501 (2009).

[2] F.-Q. Dou, M.-P. Han, and C.-C. Shu, Quantum speed limit under brachistochrone evolution, Phys. Rev. Appl. **20**, 014031 (2023).

[3] N. Khaneja, R. Brockett, and S. J. Glaser, Time optimal control in spin systems, Phys. Rev. A **63**, 032308 (2001).

[4] D. Dong and I. R. Petersen, Quantum control theory and applications: A survey, IET Control Theory & Applications **4**, 2651 (2010).

[5] C. P. Koch, U. Boscain, T. Calarco, G. Dirr, S. Filipp, S. J. Glaser, R. Kosloff, S. Montangero, T. Schulte-Herbrüggen, D. Sugny, and F. K. Wilhelm, Quantum optimal control in quantum technologies. Strategic report on current status, visions and goals for research in Europe, EPJ Quantum Technol. **9**, 19 (2022).

[6] M. A. Nielsen, M. R. Dowling, M. Gu, and A. C. Doherty, Quantum computation as geometry, Science **311**, 1133 (2006).

[7] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information: 10th Anniversary Edition* (Cambridge University Press, Cambridge, England, 2010).

[8] D. Guéry-Odelin, A. Ruschhaupt, A. Kiely, E. Torrontegui, S. Martínez-Garaot, and J. G. Muga, Shortcuts to adiabaticity: Concepts, methods, and applications, Rev. Mod. Phys. **91**, 045001 (2019).

[9] D. Girolami, How difficult is it to prepare a quantum state? Phys. Rev. Lett. **122**, 010505 (2019).

[10] P. Yuan and S. Zhang, Optimal (controlled) quantum state preparation and improved unitary synthesis by quantum circuits with any number of ancillary qubits, Quantum **7**, 956 (2023).

[11] A. Carlini, A. Hosoya, T. Koike, and Y. Okudaira, Time-optimal quantum evolution, Phys. Rev. Lett. **96**, 060503 (2006).

[12] B. Russell and S. Stepney, Zermelo navigation in the quantum brachistochrone, J. Phys. A: Math. Theor. **48**, 115303 (2015).

[13] J. Geng, Y. Wu, X. Wang, K. Xu, F. Shi, Y. Xie, X. Rong, and J. Du, Experimental time-optimal universal control of spin qubits in solids, Phys. Rev. Lett. **117**, 170501 (2016).

[14] Z. Han, Y. Dong, B. Liu, X. Yang, S. Song, L. Qiu, D. Li, J. Chu, W. Zheng, J. Xu, T. Huang, Z. Wang, X. Yu, X. Tan, D. Lan, M.-H. Yung, and Y. Yu, Experimental realization of universal time-optimal non-abelian geometric gates, arXiv:2004.10364.

[15] Y. Dong, C. Feng, Y. Zheng, X.-D. Chen, G.-C. Guo, and F.-W. Sun, Fast high-fidelity geometric quantum control with quantum brachistochrones, Phys. Rev. Res. **3**, 043177 (2021).

[16] A. Carlini, A. Hosoya, T. Koike, and Y. Okudaira, Time-optimal cnot between indirectly coupled qubits in a linear Ising chain*, J. Phys. A: Math. Theor. **44**, 145302 (2011).

[17] A. Carlini and T. Koike, Time-optimal transfer of coherence, Phys. Rev. A **86**, 054302 (2012).

[18] A. Carlini and T. Koike, Time-optimal unitary operations in ising chains: Unequal couplings and fixed fidelity, J. Phys. A: Math. Theor. **46**, 045307 (2013).

[19] J. Yang and A. del Campo, Minimum-time quantum control and the quantum brachistochrone equation, arXiv:2204.12792.

[20] R. Burden and J. Faires, *Numerical Analysis* (Brooks/Cole Cengage Learning, San Francisco, CA, 2011).

[21] J. Stoer and R. Bulirsch, *Introduction to Numerical Analysis*, Texts in Applied Mathematics (Springer, New York, 2002).

[22] J. Nocedal and S. J. Wright, *Numerical Optimization*, 2nd ed., (Springer, New York, 2006).

[23] X. Wang, M. Allegra, K. Jacobs, S. Lloyd, C. Lupo, and M. Mohseni, Quantum brachistochrone curves as geodesics: Obtaining accurate minimum-time protocols for the control of quantum systems, Phys. Rev. Lett. **114**, 170501 (2015).

[24] D. Wang, H. Shi, and Y. Lan, Quantum brachistochrone for multiple qubits, New J. Phys. **23**, 083043 (2021).

[25] E. Ott, *Chaos in Dynamical Systems* (Cambridge University Press, Cambridge, England, 2002).

[26] E. N. Lorenz, Deterministic nonperiodic flow, J. Atmos. Sci. **20**, 130 (1963).

[27] A. A. Kolmogorov, Preservation of conditionally periodic movements with small change in the Hamilton function, *Stochastic Behavior in Classical and Quantum Hamiltonian Systems: Volta Memorial Conference, Como, 1977* (Springer, New York, 1979), pp. 51–56.

[28] J. Möser, On invariant curves of area-preserving mappings of an annulus, Nachr. Akad. Wiss. Göttingen **II**, 1 (1962).

[29] V. I. Arnol'd, Proof of a theorem of an kolmogorov on the invariance of quasi-periodic motions under small perturbations of the Hamiltonian, Russian Mathematical Surveys **18**, 9 (1963).

[30] V. I. Arnol'd, Small denominators and problems of stability of motion in classical and celestial mechanics, Russian Mathematical Surveys **18**, 85 (1963).

[31] J. Moser, On the construction of almost periodic solutions for ordinary differential equations, in *Proceedings of the International Conference on Functional Analysis and Related Topics, Tokyo* (Springer, New York, 1969), pp. 60–67.

[32] M. R. A. Semenov-Tian-Shansky, Reduction of Hamiltonian systems, affine Lie algebras and Lax equations II., Invent Math. **63**, 423 (1981).

[33] A. G. Reyman and M. A. Semenov-Tian-Shansky, *Group-Theoretical Methods in the Theory of Finite-Dimensional Integrable Systems in Dynamical Systems VII* (Springer, New York, 1994).

[34] R. A. Bertlmann and P. Krammer, Bloch vectors for qudits, J. Phys. A: Math. Theor. **41**, 235303 (2008).

[35] F. Albertini and D. D'Alessandro, Notions of controllability for bilinear multilevel quantum systems, IEEE Transactions on Automatic Control **48**, 1399 (2003).

[36] A. Carlini, A. Hosoya, T. Koike, and Y. Okudaira, Time-optimal unitary operations, Phys. Rev. A **75**, 042308 (2007).

[37] M. Gu, A. Doherty, and M. A. Nielsen, Quantum control via geometry: An explicit example, Phys. Rev. A **78**, 032327 (2008).

[38] S. Helgason, *Differential Geometry, Lie Groups, and Symmetric Spaces* (Academic, New York, 1979).

[39] N. Khaneja and S. J. Glaser, Cartan decomposition of $SU(2^n)$ and control of spin systems, Chem. Phys. **267**, 11 (2001).