Minimum-time quantum control protocols can be obtained from the quantum brachistochrone formalism [Carlini, Hosoya, Koike, and Okudaira, Phys. Rev. Lett. 96, 06053, (2006)]. We point out that the original treatment implicitly applied the variational calculus with fixed boundary conditions. We argue that the genuine quantum brachistochrone problem involves a variational problem with a movable endpoint, contrary to the classical brachistochrone problem. This formulation not only simplifies the derivation of the quantum brachistochrone equation but introduces an additional constraint at the endpoint due to the boundary effect. We present the general solution to the full quantum brachistochrone equation and discuss its main features. Using it, we prove that the speed of evolution under constraints is reduced with respect to the unrestricted case. In addition, we find that solving the quantum brachistochrone equation is closely connected to solving the dynamics of the Lagrange multipliers, which is in general governed by nonlinear differential equations. Their numerical integration allows generating time-extremal trajectories. Furthermore, when the restricted operators form a closed subalgebra, the Lagrange multipliers become constant and the optimal Hamiltonian takes a concise form. The new class of analytically solvable models for the quantum brachistochrone problem opens up the possibility of applying it to many-body quantum systems, exploring notions related to geometry such as quantum speed limits, and advancing significantly the quantum state and gate preparation for quantum information processing.

I. INTRODUCTION

The ability to control quantum systems lies at the heart of various quantum technologies, such as quantum computation [1–3], quantum state preparation [4–8], quantum metrology [9–13], shortcut to adiabaticity [14–17], measurement-based state stabilization [18], and dynamical decoupling [13, 19], among others.

One protocol that stands out among the different approaches to quantum control is based on the quantum brachistochrone (QB) and was initiated by Carlini, Hosoya, Koike, and Okudaira (CHKO) [4, 5] more than a decade ago. Motivated by the classical brachistochrone problem, its quantum counterpart aims at finding the evolution which takes the minimum time between two given quantum states or quantum gates under given resources, such as a fixed norm of the Hamiltonian and a limited set of available Hamiltonian controls. The QB program by CHKO results in a differential equation with boundary conditions, which we shall refer to as the CHKO equation in what follows. It has inspired a number of theoretical works [20–26] and experiments [27]. The QB problem has close connections to other fundamental notions in nonequilibrium quantum physics, such as the quantum speed limit for driven systems [28, 29] and counterdiabatic driving [14, 15, 17].

At present, many aspects of the understanding and formulation of the QB remain to be elucidated. The QB problem was proposed by CHKO exploiting the analogy with its classical counterpart. The classical brachistochrone problem is solved by the variation calculus with fixed boundary conditions [30]. In this work, we reexamine the QB problem formulated by CHKO and find the fixed boundary condition is also implicitly assumed when performing the variational calculus. We point out that, unlike its classical counterpart, the genuine QB problem should be formulated as a variational problem with a movable endpoint, stemming from the U(1) transformation illustrated in Fig. 1. As a result, the genuine QB problem should be solved via variational calculus with movable boundaries. After accounting for the boundary effect, the variational calculus with a movable boundary condition still yields the CHKO equation as its governing equation, but with an additional constraint at the final time, unrecognized in preceding studies. This constraint is necessary for clarifying the notion of locally time-extremal trajectories. Indeed, trajectories that violate this constraint have been mistakenly classified as locally time-extremal in previous literature. Moreover, as a by-product of our formalism, the derivation of the CHKO equation for a given system is simplified dramatically with respect to previous treatments.
Developing efficient numerical algorithms for the QB problem is notoriously difficult \[22, 31\]. Numerical calculations of the QB problem reported to date remain limited to systems with a few qubits. Solving the QB for a many-body system, even numerically, is a formidable task. The underlying reason for this difficulty is the lack of an analytic understanding of the structure of the solutions to the QB problem. Here, we analyze the general features of the full QB equation, and find general analytical expressions for the optimal Hamiltonian and unitary evolution operator, deriving the governing equations of the full QB problem in terms of the dynamics of the Lagrangian multipliers. We exactly pin down the challenge of solving the full QB problem in terms of the dynamics of the Lagrangian multipliers. We prove that the speed of evolution is in general reduced when constraints are introduced in Sec. VII and discuss a class of analytically solvable examples in Sec. VIII, before closing the manuscript with a summary of the main conclusions.

II. THE CHKO EQUATION

Throughout this work, we consider systems with a finite Hilbert space dimension \(N\). The QB problem involves finding the optimal Hamiltonian that generates a time evolution from the initial state \(|\psi_i\rangle\) to the final state \(|\psi_f\rangle\) in the shortest possible time under given constraints. Before formulating the problem, we first note the redundancy of the gauge degree of freedom. If \(H(t)\) is the optimal Hamiltonian, then shifting \(H(t)\) by any time-dependent scalar also yields the optimal Hamiltonian. Fixing such a gauge degree of freedom yields the constraint

\[\text{Tr}[H(t)] = 0.\]  

Furthermore, if the norm of \(H(t)\) is unbounded, one can always scale \(H(t)\) so that the minimum time is zero \[4\]. This observation motivates the norm constraint \(\text{Tr}[\dot{H}^2(t)] \leq 2\omega^2\). As argued in \[22\], when this inequality is not saturated, one can always rescale the Hamiltonian such that the trajectory \(|\psi(t)\rangle\) is unchanged and traversed in a shorter time. Therefore, one should consider the following equality constraint,

\[f_0(H(t)) = \frac{1}{2} \text{Tr}[H^2(t)] - \omega^2 = 0.\]  

In addition, the controls available in a given system may be limited. This is typically the case in many-body quantum systems \[12, 34, 35\], where the Hamiltonian \(H(t)\) may lack certain operators, such as those involving long-range or multiple-body interactions. This motivates the following constraint

\[f_j(H(t)) = \text{Tr}[H(t)X_j] = 0, \quad j \in [1, M],\]  

where \(X_j\)'s are the traceless orthonormal and Hermitian generators of the \(su(N)\) Lie algebra, satisfying \(\text{Tr}(X_iX_j) = N\delta_{ij}\). Finally, the underlying equation of motion should be satisfied by the controlled dynamics. Under unitary evolution, the trajectory \(|\psi(t)\rangle\) is generated by the Hamiltonian \(H(t)\) according to the Schrödinger equation

\[i |\dot{\psi}(t)\rangle = H(t) |\psi(t)\rangle.\]  

Given the above constraints, CHKO \[4\] constructed the following action

\[S_{\text{CHKO}}(\psi, H, |\chi\rangle, \lambda_j) = \sum_{\alpha=T, C, S} \int_0^T L_\alpha \, dt,\]  

involving the time, constraint, and Schrödinger Lagrangians defined as

\[L_T = \frac{\sqrt{\Delta E}}{\Delta E}, \quad L_C = \sum_j \lambda_j f_j(H(t)),\]  

\[L_S = \langle \chi(t)|H(t)|\psi(t)\rangle - i \langle \chi(t)|\dot{\psi}(t)\rangle + \text{h.c.},\]  

where \(\lambda_j\) is an integrator parameter to be determined. The \(L_T\) term ensures that the integral is bounded as \(T \rightarrow \infty\). The \(L_C\) term introduces constraints on the Hamiltonian, and finally, the \(L_S\) term yields the Schrödinger equation. The minimization of \(S_{\text{CHKO}}\) with respect to \(H(t)\) leads to the so-called CHKO equation.

We next review the basic results in Refs. \[4, 5\] by CHKO in Sec. II. In Sec. III, we carefully examine that boundary condition in the variational calculus that CHKO employed and found that as an analogy to the classical QB problem, CHKO assumed the fixed boundary condition in the QB problem while the genuine QB should be formulated as a variational problem with the endpoint movable. We further show that one can derive the CHKO equation without the assumption that the boundary conditions are fixed, significantly simplifying the calculation in the original CHKO formalism. In Sec. IV, we account for the effect of the movable endpoint in the CHKO action and show that the moving boundary will introduce an additional constraint at the final time. In Sec. V, we derive the optimal Hamiltonian and optimal unitary evolution for the QB problem as well as the governing differential equations for the Lagrangian multipliers. We prove that the
respective. Here, \( g_{ii} \equiv \langle \dot{\psi}(t) | \dot{\psi}(t) \rangle - | \langle \dot{\psi}(t) | \psi(t) \rangle |^2 \) is the Fubini-Study metric [36] and \( \Delta E(t) = \sqrt{\text{Var}[H^2(t)]} |_{\dot{\psi}(t)} \) characterizes the speed of quantum evolution [28]. Minimization of the action \( \delta S_{\text{CHKO}} = 0 \) yields the Euler-Lagrangian equation

\[
\sum_{n} \frac{\partial L_{\alpha}}{\partial (\dot{\psi}(t))} - \frac{d}{dt} \frac{\partial L_{\alpha}}{\partial (\dot{\psi}(t))} = 0, \quad \sum_{n} \frac{\partial L_{\alpha}}{\partial (\dot{H}(t))} = 0, \quad (8)
\]

where \( \alpha = T, C, S \). After performing algebraic simplifications, CHKO arrived at the following equation

\[
[F(t) + i[H(t), F(t)]] | \psi(t) \rangle = 0, \quad (9)
\]

\[
\{F(t), P(t)\} = F(t), \quad (10)
\]

where \( P(t) = | \psi(t) \rangle \langle \psi(t) | \) and \( F(t) = \sum_{j} \lambda_j(t) \partial f_j / \partial H(t) \). Multiplying both sides of Eq. (10) by \( O(t) \) from the left and taking the trace on both sides, we see that

\[
\langle O(t) F(t) \rangle + \langle F(t) O(t) \rangle = \text{Tr}[O(t) F(t)], \quad (11)
\]

where \( \langle \cdot \rangle \) denotes the average over the state \( | \psi(t) \rangle \) throughout this work. In particular,

\[
\langle F(t) \rangle = \text{Tr}[F(t)] = \lambda_0(t) \text{Tr}[H(t)] + \sum_{j \geq 1} \lambda_j(t) \text{Tr} (X_j) = 0. \quad (12)
\]

CHKO showed that it is sufficient to satisfy Eq. (9) at all times if

\[
F(t) + i[H(t), F(t)] = 0, \quad (13)
\]

\[
\{F(0), P(0)\} = F(0), \quad (14)
\]

which can be explicitly verified by noting that \( F(t) = U(t) F(0) U(t)^\dagger \), where \( U(t) \) is the time-evolution operator generated by the Hamiltonian \( H(t) \). We refer to Eqs. (13)-(14) as the CHKO equation in the following. In fact, as we show in Appendix A, Eq. (9) also implies Eq. (13) and therefore they are equivalent.

### III. FIXED BOUNDARY VERSUS MOVABLE BOUNDARY

In the CHKO formalism [4], the evolution time, i.e., \( \int_0^T L_T dt \) is optimized over all the possible trajectories which traverse from an initial state \( | \psi_i \rangle \) to a target state \( | \psi_f \rangle \) under the constraints (2)-(4). Note that in the constrained variational problem, before introducing the Lagrange multipliers, the only independent function is \( | \psi(t) \rangle \).

Here, we point out that in the genuine QB problem, when \( | \psi(t) \rangle \rightarrow | \dot{\psi}(t) \rangle = | \dot{\psi}(t) \rangle + i | \dot{\psi}(t) \rangle \), there is also an infinitesimal change in the evolution time, which must be accounted for in the integral upper limit of the CHKO action (5). Taking into account the boundary effects requires the variational calculus with movable boundaries, distinct from the one with fixed boundaries. However, the Euler-Lagrangian equation (6)-(7) from which the CHKO equation is obtained does not contain information on whether the boundary is moving or not. The fixed boundary condition is implicitly assumed in the CHKO formalism.

To see this, let us unveil the original optimization problem corresponding to the CHKO action (5) before introducing the Lagrange multipliers. It consists of finding the extremum of \( \int_0^T L_T dt \), under the constraints that \( | \psi(t) \rangle \) and \( H(t) \) satisfy Eqs. (2)-(4), where \( T \) is kept as some constant. Note that under the constraint of the Schrödinger equation (4), Amadan and Aharonov [28] obtained that \( \sqrt{\int_0^T L_T dt} = T \). It is worth noting that although the original CHKO formalism requires the calculation of \( \partial L_T / \partial (\dot{\psi}(t)) \), \( \partial L_T / \partial (\dot{\psi}(t)) \) and \( (| \psi(t) \rangle \langle \psi(t) |) \) [see e.g. Eq. (2) of Ref.[4]], when the endpoint \( T \) is kept fixed, \( \delta S_T \) actually vanishes regardless of the variations of \( | \dot{\psi}(t) \rangle \) and \( | \dot{H}(t) \rangle \),

\[
\delta S_T = \delta \int_0^T L_T dt = \delta T = 0. \quad (15)
\]

Equation (15) not only allows us to reproduce the CHKO equation, which validates our observation that the endpoint is implicitly assumed in the CHKO formalism, but also simplifies the derivation dramatically without performing the tedious variational calculus of \( \partial L_T / \partial (\dot{\psi}(t)) \), \( \partial L_T / \partial (\dot{\psi}(t)) \) and \( \partial L_T / \partial (\dot{H}(t)) \). In Eq. (8), one only needs to consider the contribution from \( \alpha = S \) and \( \alpha = C \), ignoring the contribution from \( \alpha = T \). This results in the following Euler-Lagrange equation

\[
H(t) | \chi(t) \rangle = i | \chi(t) \rangle, \quad (16)
\]

\[
F(t) + (| \psi(t) \rangle \langle \chi(t) | + | \chi(t) \rangle \langle \psi(t) |) = 0. \quad (17)
\]

Taking trace on both sides of Eq. (17) yields

\[
\langle \psi(t) | \chi(t) \rangle + \langle \chi(t) | \psi(t) \rangle = 0. \quad (18)
\]

Applying \( | \psi(t) \rangle \) to Eq. (17), one obtains

\[
| \chi(t) \rangle = - \langle \chi(t) | \psi(t) \rangle | \psi(t) \rangle - F(t) | \psi(t) \rangle. \quad (19)
\]

Substituting Eq. (19) back to Eq. (17), we then find

\[
F(t) - P(t) | \psi(t) \rangle - P(t) | \psi(t) \rangle | \chi(t) \rangle - P(t) F(t) - F(t) P(t) = 0. \quad (20)
\]

According to Eq. (18), we obtain Eq. (10). Next, we take derivative on both sides of Eq. (17) and using Eq. (16), we find

\[
F(t) + (| \psi(t) \rangle \langle \chi(t) | + | \psi(t) \rangle \langle \psi(t) |) = 0. \quad (21)
\]

Using the Schrödinger equation for \( | \psi(t) \rangle \) and Eq. (16), yields the relation

\[
| \dot{\psi}(t) \rangle \langle \chi(t) | + | \psi(t) \rangle \langle \chi(t) | = - i [H(t), | \psi(t) \rangle \langle \chi(t) |], \quad (22)
\]

whence it follows that

\[
| \dot{\psi}(t) \rangle \langle \chi(t) | + | \psi(t) \rangle \langle \chi(t) | + \text{h.c.} = - i [H(t), | \psi(t) \rangle \langle \chi(t) |]. \quad (23)
\]
where in the last step we have used Eq. (17). Thus, combining the above equation with Eq. (21), we obtain Eq. (13). The derivation of the CHKO presented here offers a dramatic simplification of the original one, once the proper interpretation of the endpoints in the variational calculus is recognized.

In Ref. [5], CHKO also derived an equation for quantum gates. The result is agrees with Eq. (13), but without the initial condition (14) and with a different boundary condition $U(T) = T \exp \left[-i \int_0^T H(t)dt\right] \sim U_f$, up to some $U(1)$ phase. Following a similar procedure to the one presented here, one can also rederive the CHKO result for quantum gates with minimum efforts, as we show in Appendix B.

IV. THE FULL QUANTUM BRACHISTOCHRONIQUE EQUATION

In this section, we show that in addition to the CHKO equation, the full QB equation involves an additional constraint at the final time $T$ stemming from the effect of the movable boundaries. Our goal is to

$$\text{optimize } \int_0^T dt,$$  

provided that $|\psi(t)\rangle$ and $H(t)$ satisfy the Schrödinger equation (4), and that $H(t)$ fulfills the constraints (2)-(3) and the boundary condition

$$|\psi(0)\rangle = |\psi_i\rangle,$$

$$|\psi(T)\rangle \sim |\psi_f\rangle.$$  

However, at variance with the situation in ordinary variational calculus, the boundary condition at $T$ is not fixed.

For a general movable boundary condition, $|\psi(t)\rangle \rightarrow |\tilde{\psi}(t)\rangle = |\psi(t)\rangle + i\delta\psi(t)$ at $T \rightarrow T + \delta T$, as shown in Fig. 1, one readily finds that

$$\tilde{\psi}(\tilde{T}) = e^{i\delta\theta(T)}|\psi(T)\rangle,$$

where $\delta\theta(T)$ should be an arbitrary variation. We emphasize that the value of the variational trajectory $|\tilde{\psi}(t)\rangle$ at the new final time is proportional to the old trajectory $|\psi(T)\rangle$ at the old final time with the proportionality constant being a phase close to the identity. Therefore, we conclude that

$$|\psi(T)\rangle = -i \langle\tilde{\psi}(T)|\delta T + i\delta\theta(T)|\psi(T)\rangle.$$  

Finally, we remark that that $|\tilde{\psi}(T)\rangle$ introduces a change of the total time $\delta T$ at the end point. Without introducing the Lagrange multipliers, $|\tilde{\psi}(T)\rangle$ depends on $|\psi(t)\rangle$. In this case, a change in the Hamiltonian leads to a change of the evolution time $T$. However, after introducing the Lagrange multipliers, $H(t)$ and $|\psi(t)\rangle$ are independent functions. Only the variation of $|\psi(t)\rangle$ leads to a change of the total evolution time.

Given these considerations, the variation of the CHKO action reads

$$\delta S_{\text{CHKO}} = \delta T + \int_0^{T+\delta T} L_S(|\psi(t)\rangle + i|\delta\psi(t)\rangle)dt - \int_0^T L_S(|\psi(t)\rangle)dt$$

$$+ \int_0^T L_S(|\psi(t)\rangle)dt - \int_0^T L_S(|\psi(T)\rangle)dt$$

$$= \delta T + L_S(|\psi(T)\rangle)\delta T + \int_0^T \delta\psi(t)\left(\frac{\partial L_S}{\partial |\psi(t)\rangle} - \frac{d}{dt}\frac{\partial L_S}{\partial \langle\psi(t)\rangle}\right)dt + \langle\delta\psi(t)|\dot{\psi}(t)\rangle_{t=0}.$$  

Substituting Eq. (28) and noting that

$$|\delta\psi(0)\rangle = 0,$$

$$L_S\left(|\psi(T)\rangle, |\psi(T)\rangle\right) = 0,$$

$$\frac{\partial L_S}{\partial |\psi(t)\rangle} - \frac{d}{dt}\frac{\partial L_S}{\partial \langle\psi(t)\rangle} = H(t)|\dot{\psi}(t)\rangle - i|\dot{\psi}(t)\rangle,$$

we arrive at

$$\delta S_{\text{CHKO}} = \int_0^T \langle\delta\psi(t)|\dot{\psi}(t)\rangle \left(\frac{\partial L_S}{\partial |\psi(t)\rangle} - \frac{d}{dt}\frac{\partial L_S}{\partial \langle\psi(t)\rangle}\right)dt$$

$$+ \left(1 - i\langle\psi(T)|\dot{\psi}(T)\rangle\right)\delta T + i\delta\theta(T)\langle\psi(T)|\dot{\psi}(T)\rangle.$$  

Thus $\delta S_{\text{CHKO}} = 0$ yields not only Eq. (16), but also two addi-
tional equations,
\[ i \langle \psi(T)|\dot{\chi}(T) \rangle = 1, \quad \text{(34)} \]
\[ \langle \psi(T)|\chi(T) \rangle = 0. \quad \text{(35)} \]

Using the Schrödinger equation into Eq. (34) yields
\[ \langle \psi(T)|H(T)|\chi(T) \rangle + 1 = 0, \quad \text{(36)} \]
which together with Eq. (19) and Eq. (35) leads to
\[ \langle \psi_f|H(T)F(T)|\psi_f \rangle = 1. \quad \text{(37)} \]

Equation (37) is one of our central results and constitutes an additional non-trivial constraint due to the moving boundary, unrecognized in the previous literature. An analogous constraint also exists in the context of generating a target quantum gate, see Appendix C.

The reader may wonder what happens when both the initial and the final boundary conditions are movable, i.e., \( \langle \psi_f(0) = e^{i\theta_f}|\psi_f \rangle \) and \( \langle \psi_f(T) = e^{i\theta_f}|\psi_f \rangle \). Obviously, trajectories satisfying these boundary conditions can be identified with trajectories satisfying \( \langle \psi_f(0) = |\psi_f \rangle \) and \( \langle \psi_f(T) = e^{i\theta_f}|\psi_f \rangle \), with the Hamiltonian and time-evolution operator remaining unchanged. This is tantamount to imposing the boundary conditions in Eqs. (25)-(26). Therefore, it is sufficient to consider the case where the initial state is fixed while the final boundary condition is movable, according to the \( U(1) \) gauge transformation.

\section{V. THE GOVERNING EQUATIONS FOR THE FULL QUANTUM BRACHISTOCHRONE EQUATION}

Having found the additional constraint due to the effect of a moving boundary, we now discuss how to solve the complete set of QB equations, including the CHKO equation (13)-(14), the constraints (1)-(3), the boundary conditions in Eq. (26), and Eq. (37). We shall divide the solution process into two stages:

(i) In the first stage, we consider \( \lambda_j(t)(j \geq 0) \) and \( H(t) \) as unknown functions, treating \( \lambda_0(t) \) and \( H(0) \) as fixed and solve the constraints (1)-(3) together with Eq. (13). We derive the expression of \( H(t) \) and \( U(t) \) in terms of the Lagrange multipliers \( \lambda_j(t)(j \geq 0) \), whose dynamics is given by a nonlinear differential equation.

(ii) In the next stage, we consider \( \lambda_j(0)(j \geq 0) \), \( H(0) \) and \( T \) as unknowns and solve Eq. (14) subject to the boundary conditions in Eq. (26) and Eq. (37).

To gain some qualitative understanding of the solution, let us count the number of constraints and the number of unknowns in the CHKO equation at both stages. In the first stage, the number of independent equations is \( N^2 + M + 1 \), which is the same as the number of unknowns. Since the norm constraint (2) is nonlinear, the number of solutions, provided that they exist, should be multiple in general. In fact, as one can see from Eqs. (42)-(44), the differential equations involving \( \lambda_j(t) \) are highly nonlinear. In the second stage, the number of independent equations is \( N^2 + M + 4 \), while the number of unknowns is \( N^2 + M + 2 \). Therefore, we see that the presence of Eq. (37) imposes a compatibility condition among the coefficients \( \lambda_j(0) \) and \( H(0) \). Violation of the compatibility condition could mean that the extremal-time trajectory does not exist, which can be expected when the Hamiltonian is highly restricted. For example, if the Hamiltonian is local, it may not be able to generate a trajectory between an initially separable state and a final entangled state.

Takahashi [37] found the solution to Eq. (13), using Lewis-Riesenfeld invariants [38, 39]. Using the fact that the solution in the first stage admits a compact form, it is shown in Appendix D that the Hamiltonian and the evolution operator are respectively given by

\[ H(t) = \frac{1}{\lambda_0(t)} \left[ \lambda_0(0)\tilde{H}(t) + \sum_{j \geq 1} \lambda_j(0)\tilde{X}_j(t) \right] - G(t), \quad \text{(38)} \]

\[ U(t) = V(t) \exp \left\{ -i \int_0^t \left[ \lambda_0(0)H(0) + \sum_{j \geq 1} \lambda_j(0)X_j \right] \frac{d\tau}{\lambda_0(t)} \right\}. \quad \text{(39)} \]

Here, \( \tilde{O}(t) = V(t)O(t)V^+(t) \) is the operator in the frame generated by the restricted operators, \( V(t) \) satisfies the Schrödinger-like equation

\[ \dot{V}(t) = iG(t)V(t), \quad \text{(40)} \]

with the initial condition \( V(0) = I \) and the generator

\[ G(t) \equiv \sum_{j \geq 1} \lambda_j(t) \frac{1}{\lambda_0(t)}X_j. \quad \text{(41)} \]

Further, \( \lambda_j(t) \) satisfy

\[ \dot{\lambda}_j(t) = \frac{1}{N} \sum_{l \geq 1} \lambda_l(t)\eta_{jl}(t), \quad \text{(43)} \]

where \( \mathcal{F}_{jl} \equiv i[X_j, X_l] \)

\[ \eta_{jl}(t) = \text{Tr}[H(t)\mathcal{F}_{jl}]. \quad \text{(44)} \]

Equations (38)-(43) constitute another central results of this work. We note an important symmetry of Eqs. (38)-(43).

\[ \lambda_0(t) \rightarrow \tilde{\lambda}_j(t) = \frac{1}{c} \lambda_j(t), \quad \eta_{jl}(t) \rightarrow \tilde{\eta}_{jl}(t) = \eta_{jl}(t), \quad \text{(45)} \]

\[ H(t) \rightarrow \tilde{H}(t) = H(t), \quad U(t) \rightarrow \tilde{U}(t) = U(t), \quad \text{(46)} \]

as long as \( c \neq 0 \).

In the second stage, one may assume that \( \lambda_0(0) = 0 \). Therefore

\[ F(0) = \sum_{j \in Y} \mu_j\mathcal{F}_j + \sum_{j \in X} \lambda_j(0)\mathcal{X}_j, \quad \text{(47)} \]

\[ H(0) = \sum_{j \in Y} \mu_j\mathcal{F}_j, \]
where $\mathcal{Y}_j$ are the allowed orthonormal generators, and $X$ and $Y$ denote the sets of indices for the disallowed operators and the allowed operators, respectively. Furthermore, the norm constraint implies that

$$N \sum_{j \in Y} \mu_j^2 = 2 \omega^2. \tag{48}$$

We define

$$|\tilde{\psi}_j \rangle \equiv |\psi_j \rangle - \langle \psi_i | \psi_j \rangle |\psi_i \rangle \tag{49}$$

and

$$|\psi_j \rangle \equiv \frac{|\tilde{\psi}_j \rangle}{\| |\tilde{\psi}_j \rangle \|} = \frac{|\tilde{\psi}_j \rangle}{\sin \Omega_B}, \tag{50}$$

where

$$\cos \Omega_B \equiv |\langle \psi_i | \psi_j \rangle| \in [0, 1], \tag{51}$$

$$\phi \equiv \text{arg} \langle \psi_i | \psi_j \rangle, \tag{52}$$

and $\Omega_B \in [0, \pi/2]$ is the Bures angle [1]. The remaining orthonormal basis is denoted by $|e_k \rangle_{k=1}^N$ with $|e_1 \rangle = |\psi_i \rangle$ and $|e_2 \rangle = |\psi_j \rangle$. Equation (14) indicates that $F(0)$ should have the following representation in the orthonormal basis $|e_k \rangle_{k=1}^N$

$$F(0) = \begin{bmatrix}
0 & \times & \times & \cdots & \times \\
\times & \times & \cdots & \times \\
\vdots & \vdots & \ddots & \vdots \\
\times & \times & \cdots & 0
\end{bmatrix}, \tag{53}$$

where $\times$ denotes matrix elements that are in general not zero. Thus, the values of $\mu_i(0)$ and $\lambda_i(0)$ are chosen such that Eqs. (53) and (26) are satisfied. Equation (37) can be split into two parts

$$\text{Re} \langle \psi_j | H(T) F(T) \psi_j \rangle = 1, \tag{54}$$

$$\text{Im} \langle \psi_j | H(T) F(T) \psi_j \rangle = 0. \tag{55}$$

The first part (54) can be always satisfied by setting $c = \text{Re} \langle \psi_j | H(T) F(T) \psi_j \rangle$ in the symmetry transformation (45)-(46) and renormalizing $\lambda_i(0)$’s. However, the second part, Eq. (55) cannot be gauged away by renormalizing $\lambda_i(0)$’s and therefore imposes a nontrivial constraint on the Lagrange multipliers. In fact, whether Eq. (55) holds or not does not depend on the choice of $\lambda_i(0)$ or $\lambda_j(0)$. This constraint has been ignored previously in the literature.

With Eq. (13), Eq. (55) can be rewritten as

$$\langle \psi_j | [H(T), G(T)] \psi_j \rangle = 0, \tag{56}$$

where we have used $[H(t), F(t)] = \lambda(0)[H(t), G(t)]$. In terms of the initial state

$$\langle \psi_j | [iU'(T) U(T), U'(T) G(T) U(T)] \psi_j \rangle = 0. \tag{57}$$

Previous works have shown that solving the CHKO equation numerically is notoriously difficult [22, 31]. The problem is particularly complex at the many-body level. Yet, we note that the solution process in the second stage is almost trivial since all the equations are algebraic equations about $\lambda_j(0)$ and $H(0)$. The challenges in numerically solvingQB problem arise from determining self-consistently the dynamics of the Lagrange multipliers, which are governed by the nonlinear differential equations Eqs. (42)-(43). This is the reason why analytic examples of the QB problem are very rare and remain limited to very simple cases. Nevertheless, using the results above we report a class of new analytic examples of the QB in Sec. VIII.

Next, instead of solving the QB problem completely, we propose a method to generate time-extremal trajectories numerically. To reach this goal, we first leave the final state undetermined; it will be eventually specified by imposing Eq. (26). In leaving the final state unfixed, one can focus on the highly nontrivial part of solving the QB problem, i.e., determining the dynamics of the Lagrange multipliers:

1. For an initial state $|\psi_i \rangle$, we choose an initial Hamiltonian $H(0)$ that bears the form of Eqs. (47)-(48) so that it satisfies Eqs. (1)-(3) at $t = 0$. Eq. (14) implies that $F(0)$ must have the structure of Eq. (53), which introduces additional constraints between $\mu_j$’s and $\lambda_i(0)$’s, as discussed in Appendix E. Section VIII B provides an example of how this step is performed in an analytic example where the dynamics of the Lagrange multipliers are constants.

2. Choosing the initial values of $\mu_j$’s and $\lambda_i(0)$ that satisfy the constraints in Step 1, one can generate
the time-optimal trajectories by numerically integrating Eqs. (40-43). The numerical integration will stop until it reaches some time $T$ such that Eq. (55) is satisfied with $\text{Re} \langle \psi(T)|H(T)F(T)|\psi(T)\rangle \neq 0$. We note that Eq. (54) can be satisfied by choosing $c = \text{Re} \langle \psi(T)|H(T)F(T)|\psi(T)\rangle$ and then renormalizing $\lambda_f(t)$ to $\lambda_f(t)$. Upon setting $|\psi_f\rangle$ equal to $|\psi(T)\rangle$, we find a time-extremal trajectory between $|\psi_i\rangle$ and $|\psi_f\rangle$.

Although our numerical recipe here does not give the optimality of the trajectories globally, it makes the generation of time-extremal trajectories possible. The full QB problem may be solved numerically by combining our algorithms here with some other searching algorithms that can select the global minimum-time trajectories among all the local extremal ones.

VI. FREE EVOLUTION

To illustrate how the QB solution can be found by making use of the two stages presented in Sec. V, we consider the simplest case with $M = 0$. We refer to this case as the free evolution, since it is free from the operator constraint (2), and refer to the case $M \geq 1$ as the operator-restricted evolution, given that it is subject to the operator constraint (3). The free evolution was previously discussed by CHKO [4]. However, several subtleties in the problem are not discussed by CHKO, including the constraint of the moving boundary effect (37).

Since in this case $\lambda_f(t) = 0$, $j \geq 1$, the dynamics of the Lagrangian multiplier in the first stage becomes trivial, $\lambda_0(t) = \lambda_0(0) \equiv \lambda_0$. Furthermore, $V(t) = 1$ and therefore Eqs. (38)-(39) become

$$H_F(t) = H_F, \quad U_F(t) = e^{-iH_FT},$$

where $H_F$ is some time-independent Hamiltonian. The solution in the first stage readily follows. Let us now discuss the solution in the second stage. Equation (14) becomes

$$H_F|\psi_i\rangle \langle \psi_i| + |\psi_f\rangle \langle \psi_f| H_F = H_F.$$  \hspace{1cm} (60)

For $N = 2$, according to Eq. (53), in the orthonormal basis $\{|\psi_i\rangle, |\psi_f\rangle\}$, $H_F$ becomes

$$H_F = \begin{bmatrix} 0 & h_{if} \\ h_{fi}^* & 0 \end{bmatrix}. \quad (61)$$

Eq. (2) implies that $|h_{if}|^2 = \omega^2$, so we can denote $h_{if} = \omega e^{-i\varphi}$. Therefore

$$H_F = \omega(\cos \varphi \sigma_x^{\text{eff}} + \sin \varphi \sigma_y^{\text{eff}}), \quad (62)$$

where

$$\sigma_x^{\text{eff}} = |\psi_i\rangle \langle \psi_f^+| + |\psi_f^+\rangle \langle \psi_i|, \quad \sigma_y^{\text{eff}} = -i \left(|\psi_i\rangle \langle \psi_f^+| - |\psi_f^+\rangle \langle \psi_i|\right).$$  \hspace{1cm} (63)

In the basis $\{|\psi_i\rangle, |\psi_f^\perp\rangle\}$,

$$|\psi_i\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\psi_f^\perp\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |\psi_f\rangle = \frac{\cos \Omega_B e^{i\varphi}}{\sin \Omega_B},$$

and Eq. (62) becomes $H_F = \omega(\cos \varphi \sigma_x^{\text{eff}} + \sin \varphi \sigma_y^{\text{eff}})$. It is then straightforward to compute

$$e^{-iH_FT} \left|\psi_i\right\rangle = \left(-i \sin(\omega T)e^{i\varphi}\right).$$

Thus, the boundary condition (26) can be satisfied if and only if

$$T = \frac{\Omega_B}{|\omega|} + \frac{2\pi k}{|\omega|}, \quad k \in \mathbb{N},$$

$$\varphi = 2\pi l - \left(\phi - \frac{\pi}{2}\right), \quad l \in \mathbb{Z}. \quad (68)$$

The optimal Hamiltonian is thus given by

$$H_F = \omega(\sin \varphi \sigma_x^{\text{eff}} - \cos \varphi \sigma_y^{\text{eff}}),$$

with the global minimum time being $\Omega_B/\omega$. Upon defining $|\psi_f^\perp\rangle = ie^{-i\varphi} |\psi_f^\perp\rangle$, Eq. (69) reduces to Eq. (13) in Ref. [4].

In this work, we shall stick to Eq. (69) because it explicitly displays the role of the phase angle $\varphi$, which plays a role in the restricted evolution, as we shall see in Sec. VIII. It is also worth noting that when $\langle \psi_i | \psi_f \rangle = 0$, $\phi$ can be chosen arbitrarily and there is an infinite family of optimal Hamiltonians in this case.

Furthermore, we note that

$$\text{Re} \langle \psi_f | H_F | \psi_f \rangle = \frac{1}{\lambda_0} \langle \psi_f | H_F^2 | \psi_f \rangle = 2\lambda_0 \omega^2 = 1. \quad (70)$$

Equation (54) indicates that $\lambda_0 = 1/(2\omega^2)$. In addition, for this particular example, Eq. (55) is satisfied automatically. The fact that Eq. (54) imposes the exact value of $\lambda_0$ was noted in [4].

Finally, we argue that Eq. (69) is also the optimal Hamiltonian for general $N$-level systems. The argument builds on the fact that

$$T = \int ds \frac{\Delta E(t)}{\omega}, \quad (71)$$

and thus the minimum-time trajectory is also the minimum-length trajectory. On the other hand, any trajectory that is outside of the subspace $\text{span}(|\psi_i\rangle, |\psi_f^\perp\rangle)$ will take longer than its projected trajectory onto this subspace. There may not be a unique way of constructing the target Hamiltonian that generates the projected trajectory. For example, with the method of counter-diabatic driving [14-17], one can construct the generating Hamiltonian for any given trajectory $|\psi(t)\rangle$ as follows: First, one constructs a set of orthonormal trajectories $\{|\psi_{\sigma}(t)\rangle\}$, $\langle \psi_{\sigma}(t)|\psi_{\sigma}(t)\rangle = \delta_{\sigma m}$ with $|\psi_{\sigma}(t)\rangle = |\psi(t)\rangle$. Then, the target Hamiltonian is derived as $H(t) = iU(t)U^\dagger(t)$ with

$$U(t) = \sum |\psi_{\sigma}(t)\rangle \langle \psi_{\sigma}(t)|.$$  \hspace{1cm} (72)

Thus, for general $N$-level systems, it suffices to consider the subspace $\text{span}(|\psi_i\rangle, |\psi_f^\perp\rangle)$, with the optimal Hamiltonian in this subspace being also given by Eq. (69).
VII. THE SPEED OF EVOLUTION UNDER CONSTRAINTS

Having discussed the general solutions to the QB problem, let us calculate the speed of evolution according to Eqs. (38, 39). The importance of the speed of evolution cannot be overemphasized in quantum information processing. For example, it is generally conjectured that with more constraints, the speed of evolution will be reduced in general when compared to the free evolution [4, 32]. Nevertheless, a rigorous and systematic study on how the speed of evolution for time-optimal trajectories is affected under constraints has not been reported in the literature, to the best of our knowledge. Next, we rigorously prove this assertion.

Theorem 1. The speed of evolution under constraints, in general, can not exceed \( \omega \).

Proof. The speed of evolution can be rewritten as
\[
\Delta E^2(t) = \text{Var}[F(t)/\lambda_0(t) - G(t)]_{\|\phi(0)\|}.
\]
Using Eq. (11), one finds that
\[
\langle F^2(t) \rangle - \lambda_0(t) \langle F(t)G(t) \rangle + G^2(t)
\]
\[
= \frac{1}{2} \text{Tr}[F^2(t)] - \lambda_0(t) \text{Tr}[F(t)G(t)]
\]
\[
= \frac{1}{2} \text{Tr}[F^2(t)] - \lambda_0^2(t) \text{Tr}[G^2(t)]
\]
\[
= \omega^2 \lambda_0^2(t) - \frac{1}{2} \lambda_0^2(t) \text{Tr}[G^2(t)].
\]
Therefore,
\[
\Delta E^2(t) = \omega^2 - \left( \text{Tr}[G^2(t)]/2 - \text{Var}[G(t)]_{\|\phi(0)\|} \right).
\]
We recall the following inequality, often used in quantum metrology [12, 40–43],
\[
\text{Var}[G(t)]_{\|\phi(0)\|} \leq \left[ \frac{g_{\text{max}}(t) - g_{\text{min}}(t)}{2} \right]^2
\]
where \( g_k(t) \) is the eigenvalue of \( G(t) \). Thanks to it,
\[
\text{Tr}[G^2(t)]/2 - \text{Var}[G(t)]_{\|\phi(0)\|} \geq \left[ \frac{g_{\text{max}}(t) - g_{\text{min}}(t)}{2} \right]^2 + \sum_{k \neq \text{max}, \text{min}} \frac{g_k^2(t)}{2} \geq 0,
\]
which concludes the proof. \( \square \)

According to Eq. (71), the distance of the minimum-time trajectory for the free evolution is also the minimum-distance trajectory. In addition, Theorem 1 indicates that the speed in the free evolution is maximum. Therefore we have the following corollary:

Corollary 2. Free evolution generates the global minimum-time trajectory among all the time-extremal trajectories.

Given a set of restricted operators \( \{X_j\} \), depending on the initial and final states, it may occur that the optimal Hamiltonian for free-evolution given by (69) is still a legitimate optimal Hamiltonian that does not contain the disallowed operators \( \{X_j\} \), which corresponds to the solution of Lagrangian multipliers \( \lambda_j(t) = 0 \) for all \( j \). On the other hand, according to Corollary 2, the free evolution is the global minimum-time trajectory. In this case, the restricted operators are not really in effect and the dynamics of the evolution is then trivially restricted. For the dynamics to be non-trivially restricted, we have the following theorem:

Theorem 3. The extremal evolution is non-trivially restricted by the set \( \{X_j\} \) if and only if there exists at least one operator \( X_j \) in the restricted set such that
\[
\text{Im} \left[ \langle \psi_j^\perp | X_j | \psi_i \rangle e^{-i\theta} \right] \neq 0,
\]
Proof. To exclude the case of \( \lambda_j(t) = 0 \) for all \( j \), there must be some operator \( X_j \) such that \( \text{Tr}[H_t X_j] \neq 0 \). Otherwise, the optimal Hamiltonian is the one for the free evolution, i.e., Eq. (69). To see this, we note that
\[
\text{Tr}[H_t X_j] = i(\langle \psi_j^\perp | X_j | \psi_i \rangle e^{-i\theta} - \text{h.c.}).
\]
Thus, to exclude the case of free evolution, Eq. (77) must be satisfied. \( \square \)

VIII. A CLASS OF ANALYTICALLY SOLVABLE EXAMPLES FOR RESTRICTED EVOLUTION

In this section, we consider an important class of solvable examples of the QB problem where the \( \{X_j\} \) forms a closed subalgebra. The results are summarized in the following theorem:

Theorem 4. If the restricted operators form a closed Lie subalgebra of \( su(N) \), i.e.,
\[
\mathcal{X}_k \in \text{span}\{X_j\}, \forall k, l,
\]
for all the time-extremal trajectories the Lagrange multipliers are time-independent. The optimal Hamiltonian and the unitary evolution operators can then be expressed as
\[
H(t) = e^{Gt}H(0)e^{-Gt},
\]
\[
U(t) = e^{Gt}e^{-i[H(0) + Gt]},
\]
where \( |\psi_j^\perp\rangle \) and \( \phi \) are defined in Eqs. (50) and (52), respectively, and where \( G \) is defined in Eq. (41) but is independent of time.

Proof. Since the optimal \( H(t) \) is the linear combination of the basis \( \mathcal{Y}_j \), Eq. (79) implies that
\[
\text{Tr}[H(t) \mathcal{X}_k] = 0,
\]
whence it follows that \( \eta_j(t) = 0 \). According to Eqs. (42)-(43), the dynamics of the Lagrangian multipliers becomes trivial.
as they are constant in time $A_j(t) = A_j(0)$ and $G(t)$ is time-independent. Therefore
\[ \frac{1}{A_0} \sum_{j=1} A_j \dot{X}_j(t) = V(t) \left( \frac{1}{A_0} \sum_{j=1} A_j X_j \right) V(t) = V(t) G V(t) = G. \]  
(83)

In this case Eqs. (38)-(39) simplify and one finds
\[ \text{Tr}[H(t) [\mathcal{X}_1]] = \text{i} \text{Tr}(H(t)[\mathcal{X}_1, G]) = 0, \]  
(84)

where we have used $\dot{O}(t) = [G, \dot{O}(t)]$ and $[\mathcal{X}_1, G] \in \text{span}\{X_j\}$ due to the closure of $\text{span}\{X_j\}$. By mathematical induction, it follows that
\[ \text{Tr} \left[ \frac{d\text{Tr} H(t)}{dt} \mathcal{X}_1 \right] = \text{i} \text{Tr}(H(t)[\mathcal{X}_1, G], G], \cdots G]) = 0, \forall n. \]  
(85)

Eq. (85) provides a further consistent check of Eq. (82): as long as one chooses $\text{Tr}[H(0)\mathcal{X}_1] = 0$, thanks to Eq. (85) and the continuity of $H(t)$, Eq. (82) always holds at later times. □

A few comments are in order. First, when $\text{span}\{X_j\}$ does not form a closed subalgebra, the solution can be complicated as $G(t)$ will become time-dependent, which presents some analytical difficulty in solving the Schrödinger-like equation (40). Second, as mentioned in Sec. V, solving the dynamics of the Lagrangian multiplier in stage (i) is then difficult. Theorem 4 specifies the new class of examples in which the Lagrangian multiplier in stage (i) is then difficulty in solving the Schrödinger-like equation (40). Practically, when the number of restricted operators is large, which may make the calculation tedious. Theorem 5 below indicates that under the condition that the boundary constraints (26), (86) are independent (dependent) of $\mu$, $\lambda$ is equivalent to removing the corresponding constraints. This can be easily shown by noting that $L_j^{\mu,\lambda} = 0$ implies that $\lambda^{\mu,\lambda} = 0$.

**Theorem 5.** Setting the free Lagrange multipliers to zero is essentially equivalent to removing the corresponding constraints. This can be easily shown by noting that $L_j^{\mu,\lambda} = 0$ implies that $\lambda^{\mu,\lambda} = 0$.

**Proof.** The proof of the theorem is rather straightforward: Setting the free Lagrange multipliers to zero is essentially equivalent to removing the corresponding constraints. This can be easily shown by noting that $L_j^{\mu,\lambda} = 0$ implies that $\lambda^{\mu,\lambda} = 0$.

The term $\int_0^T \lambda^{\mu,\lambda}(H(t)) dt$ vanishes in the constraint action, which is effectively equivalent to the case in which the constraint $f_j(H(t)) = 0$ is absent.

Furthermore, we observe that the global minimum-time trajectory for the case containing more constraints is also the locally time-extremal trajectory in the case in which some of the constraints are removed. Therefore, setting the free Lagrange multipliers to be zero cannot increase the global minimum of the evolution time.

With the same arguments, one can easily deduce an analogous corollary for the constrained Lagrange multipliers:

**Corollary 6.** Setting the constrained Lagrange multipliers in Eqs. (80)-(81) be zero, but still preserves the norm constraint (2) (at $t = 0$) and the boundary constraints (26), (86), will not increase the globally minimum-time.

We next illustrate the application of these theorems in representative examples.

**A. $M = 1$**

In the case of $M = 1$, we find $\mathcal{X}_1 = 0$, which of course forms a trivial subalgebra. So the dynamics of the Lagrangian multiplier can be trivially solved, i.e., $\lambda(t) = \lambda(0) \equiv \lambda_0$ and $\lambda_1(t) = \lambda(0) \equiv \lambda_0$. Eqs. (80)-(81) become
\[ H(t) = \exp [\text{i} \lambda_1 X_1(t)], \]  
(87)
\[ U(t) = \exp [\text{i} \lambda_1 X_1(t)] \exp [-\text{i} (H(0) + \lambda_1 X_1(t)], \]  
(88)

Without loss of generality one can choose $\lambda_0 = 0$. As we have mentioned, thanks to Eqs. (45)-(46), $\lambda_0$ and $\lambda_0$ can be renormalized to $\lambda_1$ and $\lambda_0$, respectively, in order to satisfy Eq. (54) without changing $H(t)$ and $U(t)$. $\tilde{F}(t)$ is computed from the normalized Lagrange multipliers $\lambda_1(t)$ while $F(t)$ is computed from the unnormalized Lagrange multipliers $\lambda_1(t)$.

Eqs. (87)-(88) generalize the restricted in example for two-level system by CHKO [4] to $N$-level systems. One can take $X_1 = \sigma_z$, which is the example presented in [4]. Following the Step 1 in the recipe in Sec. V, we consider
\[ H(0) = \mu_x \sigma_x + \mu_y \sigma_y, \]  
(89)
\[ F(0) = \mu_x \sigma_x + \mu_y \sigma_y + \lambda_1 \sigma_z. \]  
(90)

For the initial state $|\psi_i\rangle = |e_1\rangle = |+x\rangle$ and $|e_2\rangle = |\psi_i\rangle = |-x\rangle$, Eq. (14) implies that
\[ \langle e_1 | F(0) | e_1 \rangle = - \langle e_2 | F(0) | e_2 \rangle = \mu_x = 0. \]  
(91)

Eq. (48) implies that $\mu_x = \omega$. Thus Eqs. (87)-(88) become
\[ H(t) = \omega \exp [\text{i} \lambda_1 \sigma_z(t)] \sigma_z \exp [-\text{i} \lambda_1 \sigma_z(t)], \]  
(92)
\[ U(t) = \exp [\text{i} \lambda_1 \sigma_z(t)] \exp [-\text{i} (\omega \sigma_z + \lambda_1 \sigma_z(t)]]]. \]  
(93)

Reference [4] assumes that after the renormalization of $\lambda_1$ and $\lambda_0$, all the pairs of $(\lambda_1, T)$ would give rise to a locally time-extremal trajectory between the initial state $|\psi_i\rangle$ and $U(T) |\psi_i\rangle$.
as Eq. (55) is not taken into account. As one can see from Fig. 2(b), there are pairs of \((\lambda_1, T)\) that violate Eq. (55). These trajectories, that satisfy the CHKO equation (13)-(14), the constraints (1)-(3) and the boundary condition (26), are not, even locally, extremal trajectories. This aspect was ignored in Ref. [4] for this simple case with \(N = 2\).

One can readily calculate that in the basis of \(|0\rangle, |1\rangle\),

\[
|\psi(T)\rangle = \frac{1}{\sqrt{2}} \left( e^{i\lambda_1 T} \cos(\lambda_1 T) - e^{i\lambda_1 T} e^{\theta_0} \sin(\lambda_1 T) \right),
\]

where

\[
\Lambda_1 \equiv \sqrt{\lambda_1^2 + \omega^2}, \quad \cos \theta_1 \equiv \omega/\Lambda_1, \quad \sin \theta_1 = \lambda_1/\Lambda_1.
\]

A straightforward calculation of the l.h.s. of Eq. (86) implies that

\[
\lambda_1 \cos(2\lambda_1 T) = 0. \tag{96}
\]

According to Theorem 3, in this case \(|\psi_f\rangle = \langle X_1 | \phi_i\rangle = (-\lambda |\sigma_x\rangle + x) = 1\). Thus, if \(\phi = 2\pi m, \pi + 2\pi m\) with \(m \in \mathbb{Z}\), the constraint has no effect. This is consistent with the fact that setting \(\lambda_1 = 0\) and equating \(|\psi(T)\rangle \sim |\psi_f\rangle\) will lead to \(\phi = 2\pi m, \pi + 2\pi m\). In this case, Eq. (96) is trivially satisfied as one can see from Fig. 2 (b). The genuine restricted evolution with \(\lambda_1 \neq 0\) has not been discussed before. Yet, this is the simplest case where there is only one restricted operator. When we have freedom to choose the final state \(|\psi_f\rangle\), any choice of \(\lambda_1 \neq 0\) such that \(\cos(2\lambda_1 T) = 0\) will generate a local-time extremal trajectory between \(|\psi_i\rangle\) and \(|\psi_f\rangle = |\psi(T)\rangle\).

What if the final state is a priori known? With Eq. (65), in the basis of \(|0\rangle, |1\rangle\), the final state can be parameterized as follows:

\[
|\psi_f\rangle = \frac{1}{\sqrt{2}} \left( e^{i\theta} \cos \Omega_B + 1 \sin \Omega_B \right), \tag{97}
\]

Now we would like to satisfy both Eq. (86) and Eq. (26). Equation (96) implies that

\[
\Lambda_1 T = \frac{\pi}{4} + \frac{k\pi}{2}, \quad k \in \mathbb{N}. \tag{98}
\]

To satisfy Eq. (26), we would like to have \(\rho(T) = \rho_f\), where \(\rho(T) = |\psi(T)\rangle \langle \psi(T)|\) and \(\rho_f = |\psi_f\rangle \langle \psi_f|\). Using Eq. (98), this leads to

\[
(-1)^k \cos \theta_1 = -\cos \phi \sin(2\Omega_B), \tag{99}
\]

\[
(-1)^k \sin \theta_1 \sin(2\lambda_1 T) = \cos(2\Omega_B), \tag{100}
\]

\[
(-1)^k \sin \theta_1 \cos(2\lambda_1 T) = \sin \phi \sin(2\Omega_B). \tag{101}
\]

Our goal now is to find a solution for \(\lambda_1\) and \(T\) so that Eqs. (98-101) are satisfied consistently. Taking the ratio between Eq. (100) and Eq. (101), we find

\[
\lambda_1 T = \frac{1}{2} \left[ \arccot \left( \sin \phi \tan(2\Omega_B) \right) + i\pi \right], \quad l \in \mathbb{Z}. \tag{102}
\]

Substituting Eq. (102) into Eqs. (95), (98), we find

\[
T(k, l) = \frac{1}{|\omega|} \sqrt{\frac{\pi}{4} + \frac{k^2\pi^2}{2}} - \frac{1}{4} \left( \arccot \left( \sin \phi \tan(2\Omega_B) \right) + i\pi \right)^2,
\]

\[
\sin \theta_1 = \frac{\arccot \left( \sin \phi \tan(2\Omega_B) \right)}{2 + ln/2} \frac{\pi/4 + k\pi/2}{\pi/4 + k\pi/2}. \tag{104}
\]

Clearly, \(k \in \mathbb{N}\) and \(l \in \mathbb{Z}\) must satisfy the constraint that the expression under the square root on the r.h.s. of Eq. (103) is positive. Finally, we note that with Eq. (98), Eq. (100) implies Eq. (101) and Eq. (99) or vice versa. Therefore, the pair \((k, l)\) also needs to satisfy Eq. (100), which leads to the following compatibility condition:

\[
\frac{2 (\arccot \left( \sin \phi \tan(2\Omega_B) \right) / |\pi + l|)}{(1 + 2k) \sqrt{1 + [\cot(2\Omega_B)]^2 (\csc \phi)^2}} = \sin(2\Omega_B) \sin \phi, \tag{105}
\]

where \(\phi \neq 2\pi m, \pi + 2\pi m\) with \(m \in \mathbb{Z}\) since the free evolution is excluded. The global minimum time can be obtained by finding \(\min_{k, l} T(k, l)\) such that the pair \((k, l)\) satisfies Eq. (105) with \(k \in \mathbb{N}, l \in \mathbb{Z}\).

### B. A two-qubit example with multiple constraints

In this section, we consider an example in which the set of restricted operators contain more than one operators and form a Lie sub algebra. For the sake of simplicity, we shall index the Pauli operators by number 1, 2, 3 rather than \(x, y, z\). Let us consider a two-qubit example, where

\[
\{X_j\} \in \{\sigma_1^x, \sigma_2^x, \sigma_1^y, \sigma_2^y, \sigma_1^z, \sigma_2^z\}, \quad \alpha = 1, 2, 3, \quad i = 1, 2. \tag{106}
\]

In this case, both single-qubit operations and any two-qubit operations involving \(\sigma_1^i(\sigma_2^i)\) operation on any of the qubits
are forbidden. Explicit computation yields
\begin{align}
[\sigma_1^\alpha, \sigma_2^\beta, \sigma_1^\beta, \sigma_2^\alpha] &= 0, \quad \alpha, \beta = 2, 3, \\
i[\sigma_1^\alpha, \sigma_2^\beta, \sigma_1^\beta, \sigma_2^\alpha] &= -2\sigma_1^\alpha, \\
i[\sigma_1^\alpha, \sigma_2^\beta, \sigma_1^\beta, \sigma_2^\alpha] &= 2\sigma_1^\beta, \\
i[\sigma_1^\alpha, \sigma_2^\beta, \sigma_1^\beta, \sigma_2^\alpha] &= 2\epsilon_{\alpha\beta\gamma\delta}\sigma_1^\gamma\sigma_2^\delta, \quad \alpha, \beta = 2, 3.
\end{align}
(107) (108) (109) (110) (111)

Thus, \(\text{span}(X_i)\) forms a closed subalgebra of \(su(4)\) and the Lagrange multipliers are constants. We simply denote \(\lambda_j \equiv \lambda_j(0)\). Once again, we can choose \(\lambda_0 = 1\) for the ease of calculation. As we have mentioned previously, one can always renormalize \(\lambda_j\)’s according to Eqs. (45)-(46) such that (54) is satisfied while keeping \(H(t)\) and \(U(t)\) unchanged. Theorem 4 gives then the optimal Hamiltonian
\begin{align}
H(t) &= \sum_{(\alpha,\beta) \in X} \mu_{\alpha\beta} e^{i\sum_{\gamma\delta} \lambda_\gamma \sigma_\gamma^\alpha \sigma_\delta^\beta} e^{i\sum_{\gamma\delta} \lambda_\delta \sigma_\gamma^\beta \sigma_\delta^\alpha} \\
U(t) &= e^{i\sum_{\gamma\delta} \lambda_\gamma \sigma_\gamma^\alpha \sigma_\delta^\beta} e^{-i\sum_{\gamma\delta} \lambda_\delta \sigma_\gamma^\beta \sigma_\delta^\alpha} e^{i\sum_{\gamma\delta} \lambda_\delta \sigma_\gamma^\beta \sigma_\delta^\alpha}.
\end{align}
(112) (113)

where
\begin{align}
X &= \{10, 20, 30, 01, 01, 02, 03, 11, 12, 21, 13, 31\}, \\
Y &= \{22, 33, 23, 32\}.
\end{align}
(114) (115)

As we have mentioned, due to Eq. (14), \(\lambda_{\alpha\beta}\) and \(\mu_{\alpha\beta}\) are not independent. For example, if we start with the ground state \(|\psi_1\rangle = |\psi_1\rangle = |11\rangle\) and \(|\psi_2\rangle = |\psi_2\rangle = |00\rangle\) so that the final state is
\begin{align}
|\psi_f\rangle &= \cos \Omega_B e^{i\phi} |00\rangle + \sin \Omega_B |11\rangle.
\end{align}
(116)

Among all the restricted operators, we already find
\begin{align}
\langle 11|\sigma_1^\gamma|22\rangle = 0, \quad \langle 11|\sigma_1^\gamma\sigma_2^\delta|22\rangle = \langle 11|\sigma_1^\gamma|22\rangle = 0 = \langle 11|\sigma_1^\gamma\sigma_2^\delta|22\rangle = i.
\end{align}
(117)

According to Theorem 3, regardless the values of \(\phi\), the optimal time-evolution is restricted. We choose the remaining basis as \(|e_3\rangle = |10\rangle\) and \(|e_4\rangle = |01\rangle\).

Furthermore, we show in Appendix E that Eq. (14) leads to the following constraints among the coefficients.
\begin{align}
\mu_{13} &= 0, \quad \lambda_{30} = \lambda_{03} = 0, \\
\mu_{23} + \lambda_{30} &= 0, \quad \lambda_{13} + \lambda_{10} = 0, \\
\mu_{32} + \lambda_{02} &= 0, \quad \lambda_{31} + \lambda_{01} = 0, \\
\mu_{22} + \lambda_{11} &= 0, \quad \lambda_{12} - \lambda_{21} = 0.
\end{align}
(118) (119) (120) (121)

Eq. (48) indicates that
\begin{align}
\mu_{23} + \mu_{32} + \mu_{22} &= \frac{\omega^2}{2}.
\end{align}
(122)

Thus, the free parameters are \(\lambda_{13}, \lambda_{31}, \lambda_{12}\) and \(\lambda_{21}\). According to Theorem 5, they can be set to be zero, provided the boundary constraints (26), (86) are satisfied, which will be manifestly true later but is assumed for now. The calculation can be further reduced. Among the three Lagrange multipliers left, we choose \(\lambda_{11} \neq 0\) with \(\lambda_{20} = \lambda_{02} = 0\). If such a choice can satisfy boundary constraints (26), (86), according to Corollary 6, it provides the globally minimum-time trajectory. The reason we do not set \(\lambda_{11} = 0\) is that it will result in a local Hamiltonian in the qubits that cannot general nonlocal evolution. Therefore, an entangled state cannot be generated and Eq. (26) is violated. With this choice, Eqs. (112)-(113) become
\begin{align}
H &= \frac{\omega}{\sqrt{2}} \sigma_1^2, \\
U(t) &= \exp \left[ -\frac{\omega t}{\sqrt{2}} \sigma_1^2 \right],
\end{align}
(123) (124)
with
\begin{align}
G &= -\frac{\omega}{\sqrt{2}} \sigma_1^2.
\end{align}
(125)

A straightforward application of the Baker-Campell-Hausdorff formula shows that Eqs. (126)-(127) is satisfied. The time evolution reads
\begin{align}
U(T)|\psi_i\rangle = \cos(\omega T/\sqrt{2})|11\rangle + i \sin(\omega T/\sqrt{2})|00\rangle.
\end{align}
(128)

In this case, Eq. (86) is trivially satisfied. Upon setting \(|\psi_f\rangle \sim U(T)|\psi_i\rangle\), which leads to
\begin{align}
\phi = -\frac{\pi}{2} + 2k\pi, \quad k \in \mathbb{Z},
\end{align}
(129)
the boundary condition (26) is also satisfied. Therefore, we find the globally minimum-time evolution is
\begin{align}
T &= \frac{\sqrt{2}\Omega_B}{\omega}.
\end{align}
(129)

In comparison to the free evolution, the constraints make the time-optimal evolution longer by a factor \(\sqrt{2}\).

Similar calculations can be done for other initial and final states, e.g., \(|\psi_i\rangle = |01\rangle\) and \(|\psi_f\rangle = |10\rangle\), \(|\psi_i\rangle = |+x, +x\rangle\) and \(|\psi_f\rangle = |-x, -x\rangle\), \(|\psi_i\rangle = |+x, -x\rangle\) and \(|\psi_f\rangle = |-x, +x\rangle\), etc. We would like to remark that although we only give two analytic examples, the class where restricted operators form a closed Lie algebra is rich. In particular, we expect this class to contain analytically solvable instances of the QB problem in many-body restricted Hamiltonians, of relevance to the study of quantum speed limits in many-body quantum systems [32, 33].

IX. CONCLUSION

In summary, we argued that unlike the classical brachistochrone problem, the final boundary condition in the QB
problem should be considered as movable according to the $U(1)$ gauge transformation and the QB should be solved by variational calculus with movable boundary conditions. The effect of the movable endpoint introduces an additional constraint, unrecognized in the original formulation of QB by CHKO \cite{4} and ensuing literature. Furthermore, we have also provided an alternative derivation of the QB equations based on the proper observation of the boundary condition. An advantage of the current approach is that it requires much less effort than the original derivation by CHKO.

Using it, we have reported a general expression for the optimal Hamiltonian and optimal unitary evolution operator and derived the governing equation for the dynamics of the Lagrange multipliers in the QB problem. We have also proposed a numerical algorithm that generates time-extremal trajectories, taking into account the additional constraint at the final time. Furthermore, we have identified an important class of analytically solvable examples of the QB problem where the restricted operators form a closed Lie algebra. In this case, the Lagrange multipliers become constants and the optimal Hamiltonian and optimal unitary operators take a simple form. This opens up the possibility to study QB in many-body systems. We have illustrated with specific examples that the effect of the moving endpoint cannot be ignored in general. Indeed, doing so can lead to an erroneous identification of the time-extremal trajectories.

Our results here open the door to investigate the geometry of the evolution of many-body quantum systems. Many questions are open based on our results here, such as the combination of the recipe for generating time-extremal trajectories proposed here with other algorithms to develop a full numerical framework to solve the CHKO equation, the study of the QB in many-body quantum systems combined with many-body techniques, and the application of the analytical findings reported here to the optimal generation of a target quantum gate.

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\section*{Appendix A: The equivalence between Eq. (9) and Eq. (13)}

The solution to Eq. (13) is

$$F(t) = U(t)F(0)U^\dagger(t),$$

where $U(t)$ is the unitary evolution generated by $H(t)$. One can easily check that $F(t)$ satisfies Eq. (9). Let us proof the converse. Obviously, the second equation of Eq. (9) implies the initial condition in Eq. (13). Our goal now is to prove the differential equation Eq. (13). Equation (9) is equivalent to

$$\{\dot{F}(t) + i[H(t), F(t)]\}\mathcal{P}(t) = 0,$$  \hspace{1cm} (A2)

$$U^\dagger(t)F(t), \mathcal{P}(t)U(t) = \bar{F}(t),$$  \hspace{1cm} (A3)

where

$$\bar{F}(t) \equiv U^\dagger(t)F(t)U(t),$$  \hspace{1cm} (A4)

and $\mathcal{P}(t) = U(t)\mathcal{P}(0)U(t)$ with $\mathcal{P}(0) = |\psi_i\rangle\langle \psi_i|$.\footnote{Eq. (A2) can be further rewritten as}

$$U^\dagger(t)\{\dot{F}(t) + i[H(t), F(t)]\}U(t)\mathcal{P}(0) = 0.$$  \hspace{1cm} (A5)

According to Eq. (A4), it can be readily obtained

$$\dot{\bar{F}}(t) = iU^\dagger(t)[H(t), F(t)]U(t) + U^\dagger(t)\bar{F}(t)U(t).$$  \hspace{1cm} (A6)

Substituting Eq. (A6) into Eq. (A5) yields

$$\dot{\bar{F}}(t)\mathcal{P}(0) = 0,$$  \hspace{1cm} (A7)

from which we conclude that $\bar{F}(t)\mathcal{P}(0)$ is a constant of motion, that is

$$\bar{F}(t)\mathcal{P}(0) = \bar{F}(0)\mathcal{P}(0).$$  \hspace{1cm} (A8)
Furthermore, we note the relations
\[
U^\dagger(t)F(t)\mathcal{P}(t)U(t) = F(t)\mathcal{P}(0), \quad (A9)
\]
\[
U^\dagger(t)\mathcal{P}(t)F(t)U(t) = \mathcal{P}(0)F(t). \quad (A10)
\]
Using them Eq. (A3) can be rewritten as
\[
\{\tilde{F}(t), \mathcal{P}(0)\} = \tilde{F}(t). \quad (A11)
\]
Combining Eq. (A8) with Eq. (A11), it follows that
\[
\tilde{F}(t) = F(0)\mathcal{P}(0) + \mathcal{P}(0)\tilde{F}(0), \quad (A12)
\]
which is a constant of motion. As a result, \(\dot{\tilde{F}}(t) = 0\) leads to Eq. (13) in the main text.

### Appendix B: Rederiving the CHKO equation for quantum gate implementation with minimum efforts

In Ref. [5], to study the QB equation for quantum gates, CHKO constructed the following action:
\[
S_{\text{CHKO}}(\phi, H, \mathcal{P}, \lambda_i) = \sum_{\alpha = T, S, C} \int_0^T L_\alpha \, dt, \quad (B1)
\]
where the time, Schrödinger, and the constraint Lagrangians are defined as
\[
L_T = \frac{\sqrt{g_{tt}}}{v(t)}, \quad (B2)
\]
\[
L_S = \text{Tr}\left\{ \Lambda(t)\left[ i\tilde{U}(t)U^\dagger(t) - H(t) \right] \right\}, \quad (B3)
\]
\[
L_C = \sum_j \lambda_j(t)f_j(H(t)), \quad (B4)
\]
with the boundary conditions
\[
U(0) = 1, \quad (B5)
\]
\[
U(t_f) \sim U_f, \quad (B6)
\]
Again, one can always make the Hamiltonian traceless, i.e., \(\text{Tr}[H(t)] = 0\). Further,
\[
g_{tt}(t) \equiv \text{Tr}[\tilde{U}(t)\tilde{U}(t)] + \frac{1}{N} \left( \text{Tr}[\tilde{U}^\dagger(t)U(t)] \right)^2 \quad (B7)
\]
is the metric on the manifold of quantum unitary matrices induced by the Hilbert space norm which is invariant under \(U(1)\)-gauge transformation. CHKO computed the speed of \(v(t)\) by substituting the Schrödinger equation into Eq. (B7) and obtained
\[
v(t) = \frac{1}{\sqrt{g_{tt}}} = \frac{1}{\sqrt{\text{Tr}[H^2(t)]}}. \quad (B8)
\]
As we have discussed in the main text, to derive the CHKO equation, there is no need to perform the variational calculus with respect to \(L_T\). One can directly set \(\delta S_{TT} = 0\). On the other hand, since \(S_C\) is independent of \(U\), it can be readily found that \(\delta S_C = 0\) under the the variation of \(U\). Next, we would like to compute \(\delta S_S\).

For the Lagrangian \(L = L(U, \dot{U}, U^\dagger, \dot{U}^\dagger)\), minimization of the action yields
\[
\delta \int_0^T L \, dt = \int_0^T dt \text{Tr}\left\{ \frac{\partial L}{\partial U} \delta U + \frac{\partial L}{\partial U^\dagger} \delta U^\dagger + \frac{\partial L}{\partial U} \frac{dt}{dt} \delta U + \frac{\partial L}{\partial U^\dagger} \frac{dt}{dt} \delta U^\dagger \right\}
\]
\[
= \int_0^T dt \left[ \text{Tr}\left( \left. \frac{\partial L}{\partial U} \delta U \right|_{t=0} + \left. \frac{\partial L}{\partial U^\dagger} \delta U^\dagger \right|_{t=0} \right) + \text{Tr}\left( \frac{\partial L}{\partial U} \delta U \right) \right]_{t=0}^{t=T} \quad (B9)
\]
Note that due to $UU^\dagger = \mathbb{1}$, $\delta U^\dagger$ and $\delta U$ are related to each other as follows:

$$\delta U^\dagger = -U^\dagger \delta U U^\dagger. \quad (B10)$$

Using Eq. (B10), we thus obtain

$$\delta \int_0^T L dt = \int_0^T dt \text{Tr} \left[ \left( \frac{\partial L}{\partial U} - \frac{d}{dt} \frac{\partial L}{\partial \dot{U}} - U^\dagger \frac{\partial L}{\partial U^\dagger} \dot{U} + U^\dagger \frac{d}{dt} \frac{\partial L}{\partial \dot{U}^\dagger} \right) \delta U \right]$$

$$+ \text{Tr} \left[ \left( \frac{\partial L}{\partial U} - U^\dagger \frac{\partial L}{\partial U^\dagger} \right) \delta U \right] \bigg|_{t=0}^{T}. \quad (B11)$$

Taking $L = L_S$ and applying the fixed boundary condition, we arrive at

$$\delta S_S = -i \int_0^T dt \text{Tr} \left[ U^\dagger (t) \left\{ \dot{\Lambda}(t) + \Lambda(t) \dot{U}(t) + U(t) \dot{U}^\dagger (t) \Lambda(t) \right\} \delta U(t) \right]$$

$$= -i \int_0^T dt \text{Tr} \left[ U^\dagger (t) \left\{ \dot{\Lambda}(t) + i[H(t), \Lambda(t)] \right\} \delta U(t) \right], \quad (B12)$$

where we have used $H(t) = i U(t) U^\dagger (t)$. Therefore, the Euler-Lagrange equation for $U(t)$ is

$$\dot{\Lambda}(t) + i[H(t), \Lambda(t)] = 0. \quad (B13)$$

Keeping $U$ fixed, one can easily find the identities

$$\delta S_S = - \int_0^T \text{Tr} \left( \Lambda(t) \delta H(t) \right) dt, \quad (B14)$$

$$\delta S_C = \int_0^T \text{Tr} (F(t) \delta H(t)) dt. \quad (B15)$$

The Euler-Lagrange equation for $H(t)$ is

$$\Lambda(t) = F(t). \quad (B16)$$

Obviously, Eqs. (B13), (B16) imply Eq. (13) in the main text.

**Appendix C: Derivation of the full quantum brachistochrone equation for quantum gate implementation**

As with Eq. (27), one can show that

$$\dot{U}(T) - U(T) = \dot{U}(T) \delta T + \delta U(T). \quad (C1)$$

The boundary condition (B6) again dictates that

$$\dot{U}(T) = e^{i\delta \theta(T)} U(T),$$

and we find

$$\delta U(T) = -\dot{U}(T) \delta T + i \delta \theta(T) U(T). \quad (C2)$$

This equation is also discussed in Ref. [25], though the issue of the moving boundary is not explicitly mentioned there. When varying $U(t)$ while keeping $H(t)$ fixed, we find

$$\delta S_S = \int_0^{T+\delta T} L_S(U + \delta U) dt - \int_0^T L_S(U) dt$$

$$= L_S(U) \delta T + \delta \int_0^T L_S(U + \delta U) dt - \int_0^T L_S(U) dt$$

$$= L_S(U) \delta T + i \text{Tr} \left[ U^\dagger (t) \Lambda(t) \delta U(t) \right] \bigg|_{t=0}^{T} - i \int_0^T dt \text{Tr} \left[ U^\dagger (t) \left\{ \dot{\Lambda}(t) + i[H(t), \Lambda(t)] \right\} \delta U(t) \right]. \quad (C3)$$
Therefore, the relation
\[ \delta S_{CHKO} = \delta T + \delta S_S = 0 \quad \text{(C4)} \]
yields not only the CHKO equation (13), but also
\[ i \text{Tr} \left[ U^\dagger(T) \Lambda(T) U(T) \right] = 1, \quad \text{(C5)} \]
and
\[ \text{Tr} \left[ U^\dagger(T) \Lambda(T) U(T) \right] = 0. \quad \text{(C6)} \]
With the Schrödinger equation and Eq. (B16), Eq. (C5) becomes
\[ \text{Tr} \left[ H(T) F(T) \right] = 1. \quad \text{(C7)} \]
Eq. (C6) is satisfied automatically since \( \text{Tr}[F(t)] = 0 \) at all times.

**Appendix D: Derivation of the governing equations for the QB equation**

In the most general case, the constraints are \( \text{Tr}[H(t)] = 0 \) and Eqs. (2)-(3) in the main text. Therefore
\[ F(t) = \lambda_0(t)[H(t) + G(t)], \quad \text{(D1)} \]
where
\[ G(t) = \frac{1}{\lambda_0(t)} \sum_{j \geq 1} \lambda_j(t) X_j. \quad \text{(D2)} \]
Now let us solve the CHKO equation Eq. (13). The solution is
\[ F(t) = U(t) F(0) U^\dagger(t), \quad \text{(D3)} \]
where
\[ i \dot{U}(t) = H(t) U(t). \quad \text{(D4)} \]
Substituting Eq. (D1) into Eq. (D3), we obtain
\[ \lambda_0(t) [H(t) + G(t)] = U(t) F(0) U^\dagger(t). \quad \text{(D5)} \]
Multiplying both sides by \( U(t) \), we find
\[ i \dot{U}(t) + G(t) U(t) = \frac{1}{\lambda_0(t)} U(t) F(0). \quad \text{(D6)} \]
Therefore, we consider the Hamiltonian.
\[ H(t) = i \dot{U}(t) U^\dagger(t) = -G(t) + \frac{1}{\lambda_0(t)} U(t) F(0) U^\dagger(t). \quad \text{(D7)} \]
Eq. (D6) is a first-order differential equation with initial condition \( U(0) = I \) and thus have unique solution. When \( M = 1 \), where \( G(t) \) commutes at all times, the solution to Eq. (D6) is
\[ U(t) = \exp \left[ i \int_0^t G(\tau) d\tau \right] \exp \left[ -i F(0) \int_0^t \frac{d\tau}{\lambda_0(\tau)} \right]. \quad \text{(D8)} \]
For the case \( M \geq 2 \), while \( G(t) \) does not commute at all times, the formal solution admits the form
\[ U(t) = \mathcal{T} \exp \left[ i \int_0^t G(\tau) d\tau \right] \exp \left[ -i F(0) \int_0^t \frac{d\tau}{\lambda_0(\tau)} \right], \quad \text{(D9)} \]
where \( \mathcal{T} \) denotes the time-ordering operator. For the sake of simplicity, we denote
\[ V(t) = \mathcal{T} \exp \left[ i \int_0^t G(\tau) d\tau \right]. \quad \text{(D10)} \]
and note that it satisfies Eq. (40) in the main text. Therefore, upon substituting the expression for \( F(0) \), we establish Eq. (39) in the main text.

One can check that Eq. (D9) is indeed a solution to Eq. (D6), given that
\[
\dot{U}(t) = iG(t)U(t) - i\frac{1}{\lambda_0(t)} U(t)F(0).
\]

Thus, Eq. (D7) becomes
\[
H(t) = \frac{1}{\lambda_0(t)} V(t)F(0)V^\dagger(t) - G(t).
\]

Upon substituting the expression for \( F(0) \) and \( G(t) \), we find Eq. (38) in the main text.

Eq. (D12) satisfies the constraints \( \text{Tr}[H(t)] = 0 \) and by default given Eq. (D1). To satisfy the norm constraint (2) in the main text, we compute
\[
\text{Tr}[H^2(t)] = \text{Tr}[G^2(t)] + \frac{\text{Tr}[F^2(0)]}{\lambda_0^2(t)} - \frac{2}{\lambda_0(t)} \text{Tr}[G(t)F(t)] = 2\omega^2,
\]
where we have used the fact that
\[
F(t) = U(t)F(0)U^\dagger(t) = V(t)F(0)V^\dagger(t).
\]

We note that
\[
\text{Tr}[G^2(t)] = N\frac{\sum_{j=1}^N \lambda_j^2(t)}{\lambda_0^2(t)},
\]
\[
\text{Tr}[F^2(t)] = 2\omega^2 \lambda_0^2(t) + N \sum_{j=1}^N \lambda_j^2(t),
\]
and that \( \text{Tr}[F^2(t)] \) is a conserved quantity, so we have
\[
2\omega^2 \lambda_0^2(t) + N \sum_{j=1}^N \lambda_j^2(t) = 2\omega^2 \lambda_0^2(0) + N \sum_{j=1}^N \lambda_j^2(0).
\]

Thus, Eq. (D13) becomes
\[
\text{Tr}[G(t)F(t)] = \frac{N \sum_{j=1}^N \lambda_j^2(t)}{\lambda_0(t)}.
\]

To satisfy the constraint (3), we have
\[
\text{Tr}[H(t)X_j] = \frac{1}{\lambda_0(t)} \left[ \text{Tr}[X_jF(t)] - \lambda_j(t)N \right] = 0,
\]
which leads to
\[
\text{Tr}[X_jF(t)] = N \lambda_j(t), \quad \forall \ j \geq 1.
\]

Since Eq. (D20) implies Eq. (D18), we note that only Eq. (D17) and Eq. (D20) are independent. Since Eq. (42) holds at the initial time, it will be satisfied if its first derivatives on both sides are equal at all times. This leads to the following differential equation
\[
2\omega^2 \lambda_0(t) \dot{\lambda}_0(t) + N \sum_{j=1}^N \lambda_j(t) \dot{\lambda}_j(t) = 0.
\]

Similarly, Eq. (D20) is satisfied initially. So taking time derivatives on both sides of Eq. (D20) and using the fact that
\[
\dot{F}(t) = -i[H(t), F(t)] = -i \lambda_0(t)[H(t), G(t)],
\]
together with the identity \( \text{Tr}(ABC) = \text{Tr}(CAB) \), yields the differential equation
\[
\dot{\lambda}_j(t) = \frac{1}{N} \sum_{l=1}^N \lambda_l(t) \eta_j(t),
\]
where
\[
\eta_j(t) = \text{Tr}[H(t)X_j^\dagger].
\]

Substituting Eq. (D22) into Eq. (D21), we obtain Eq. (42) in the main text.
Appendix E: Determine the form of $F(0)$ and $H(0)$ using Eq. (14) for the two-qubit example

According to Eq. (47), one should choose the initial Hamiltonian as,

\[
H(0) = \mu_{22}\sigma_1^0\sigma_2^0 + \mu_{33}\sigma_1^3\sigma_2^3 \\
+ \mu_{23}\sigma_1^2\sigma_2^2 + \mu_{32}\sigma_1^1\sigma_2^1,
\]

and

\[
F(0) = H(0) + \lambda_{10}\sigma_1^0 + \lambda_{20}\sigma_1^2 + \lambda_{30}\sigma_1^3 \\
+ \lambda_{01}\sigma_2^1 + \lambda_{02}\sigma_2^2 + \lambda_{03}\sigma_2^3 + \lambda_{11}\sigma_1^1\sigma_2^1 \\
+ \lambda_{12}\sigma_1^1\sigma_2^2 + \lambda_{13}\sigma_1^1\sigma_2^3 + \lambda_{23}\sigma_1^2\sigma_2^1 + \lambda_{33}\sigma_1^3\sigma_2^3,
\]

where we have set $\lambda_0 = 1$. We consider $|e_1\rangle = |\psi_i\rangle = |11\rangle$ and $|e_2\rangle = |\psi_f\rangle = |00\rangle$. Note that $\langle e_k|\sigma^\varphi_i\sigma^\varphi_j|e_k\rangle = 0$ as long as $\alpha$, $\beta$ are both not equal to 3. Therefore, we find that $\langle e_k|X_i|e_k\rangle = 0$ except for $X_i = \sigma_1^2$ or $\sigma_2^3$. Using $\langle e_1|F(0)|e_1\rangle = 0$ leads to

\[
\mu_{33} - \lambda_{30} - \lambda_{03} = 0.
\]

Similarly, for $k \geq 2$, $\langle e_k|F(0)|e_k\rangle = 0$ lead to

\[
\mu_{33} + \lambda_{30} + \lambda_{03} = 0, \quad \mu_{33} - \lambda_{30} + \lambda_{03} = 0, \quad \mu_{33} + \lambda_{30} - \lambda_{03} = 0,
\]

from which we find Eq. (118) in the main text.

One can also readily find that

\[
\langle 00|\sigma^\varphi_i\sigma^\varphi_j|10\rangle = 0, \quad \beta \neq 3, \quad \langle 00|\sigma^\varphi_i\sigma^\varphi_j|10\rangle = 1, \quad \langle 00|\sigma^\varphi_i\sigma^\varphi_j|10\rangle = -i,
\]

which leads to $\langle e_2|F(0)|e_1\rangle = -i(\mu_{23} + \lambda_{20}) + \lambda_{13} + \lambda_{10} = 0$. On the other hand, we note $\mu_{\alpha\beta}$ and $\lambda_{\alpha\beta}$ must be real, so we obtain Eq. (119) in the main text.

Similarly, we observe

\[
\langle 00|\sigma^\varphi_i\sigma^\varphi_j|01\rangle = 0, \quad \beta \neq 3, \quad \langle 00|\sigma^\varphi_i\sigma^\varphi_j|01\rangle = 1, \quad \langle 00|\sigma^\varphi_i\sigma^\varphi_j|01\rangle = i,
\]

which leads to Eq. (120) in the main text. At this point, we find

\[
H(0) = \mu_{22}\sigma_1^0\sigma_2^0 + \mu_{23}\sigma_1^2\sigma_2^2 + \mu_{32}\sigma_1^1\sigma_2^1
\]

and

\[
F(0) = \mu_{22}\sigma_1^0\sigma_2^0 + \mu_{23}\sigma_1^2\sigma_2^2 + \mu_{32}\sigma_1^1\sigma_2^1 \\
+ \lambda_{10}\sigma_1^0 + \lambda_{20}\sigma_1^2 + \lambda_{01}\sigma_2^1 + \lambda_{02}\sigma_2^2 \\
+ \lambda_{10}\sigma_1^0 - \lambda_{01}\sigma_2^1 + \lambda_{02}\sigma_2^2 \\
+ \lambda_{11}\sigma_1^1\sigma_2^1 + \lambda_{12}\sigma_1^1\sigma_2^2 + \lambda_{21}\sigma_1^2\sigma_2^1.
\]

Finally, we note that

\[
\langle 10|\sigma^\varphi_i\sigma^\varphi_j|01\rangle = 1, \quad \langle 10|\sigma^\varphi_i\sigma^\varphi_j|01\rangle = 1, \quad \langle 10|\sigma^\varphi_i\sigma^\varphi_j|01\rangle = -i, \quad \langle 10|\sigma^\varphi_i\sigma^\varphi_j|01\rangle = i,
\]

which leads to Eq. (121) in the main text.

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