Quantum brachistochrone for multiple qubits

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Abstract

Efficient control of qubits plays a key role in quantum information processing. In the current work, an alternative set of differential equations are derived for an optimal quantum control of single or multiple qubits with or without interaction. The new formulation enables a great reduction of the computation load by eliminating possible redundant complexity involved in previous algorithms. A relaxation technique is designed for numerically detecting optimal paths involving entanglement. Interesting continuous symmetries are identified in the Lagrangian, which indicates the existence of physically equivalent classes of paths and may be utilized to remove neutral directions in the Jacobian of the evolution. In the 'ground state' solution among the set of optimal paths, the time-reversal symmetry of the system shows up, which is expected to be universal for the symmetry-related initial and final state.

1. Introduction

Ever since people realized that quantum computers are much more powerful than their classical counterparts [1, 2], researchers have been working hard to bring it to life for years, which is making considerable progress and leads to a dramatic increase in the complexity of controllable quantum systems, from prototyped small quantum devices to machines possibly with thousands of qubits [3]. Undoubtedly, in order to reduce the impact of dissipation or decoherence that is always present in such complex systems, people continue to work on time-optimal control strategy, which minimizes the necessary traversing time required to reach a quantum target (namely, a quantum state or a unitary operation) and proves to be important for building efficient gates in quantum computer architectures. Therefore, a lot of research about the quantum speed limit (QSL) has been reported, which gives a lower bound of the time needed for a quantum system to travel from the initial to the final state and is estimated with the average energy or its variance [4–7]. In addition, time optimal control provides a physical framework [8] for defining complexity of quantum algorithms, probably superior to traditional ones [9]. For example Nielsen et al. proposed a new quantum computing criterion by using the Riemannian geometry and transforming the problem of finding an optimal quantum trajectory into a geometric one in the space of Hamiltonians [10], and revealed that the complexity of a quantum gate is related to the problem of optimal control [11].

In a series of works on the QSL [4–7], the estimation of minimum evolution time is quite general and applicable to many different situations, in which, however, the optimal evolution path is not given explicitly. In the literature, the Grape algorithm and the Krotov algorithm are very popular for locating optimal evolution path. In the Grape algorithm [12, 13], the initial and the target state evolve forward and backward respectively for the same amount of time to obtain two state sequences and the control variables are updated by iteratively minimizing the difference between the two sequences. The Grape algorithm relieves the limitation in the number of control variables and thus enjoys high flexibility. However, the convergence is slowing down when the deviation tend to a local. Also, an improper selection of step size often leads to a
tortuous search route. In order to overcome this difficulty, the Krotov method \cite{13–16} introduces a second term to penalize the undesired effects. A key feature of the algorithm is that all information is utilized at each time step which often consistently reduces the objective functional and accelerates the iteration. However, when parameters are too small, its convergence rate deteriorates, and sometimes even worsely the algorithm turns unstable. One interesting way of optimal solution searching with constraints on Hamiltonian invokes interesting theories such as Pontryagin maximum principle \cite{17} or the geometry of unitary group \cite{18–20}. A significant piece of work was reported by Carlini \cite{21}, who derived a quantum brachistochrone equation (QBE) with variational method which is widely used and plays a crucial role \cite{22–27} in classical systems. The scheme produces a Schrödinger equation together with the optimal control strategy under an energy constraint. Except for some special cases \cite{28–30}, analytic solutions are hard to obtain and hence numerical solution is the only resort. A scheme based on a geometric point of view is designed recently \cite{31}, which depicts the quantum brachistochrone paths as geodesics on the constraining manifold and tackles the problem by solving a family of geodesic equations. However, there is an infinite number of geodesic families present even for locally time-optimal solutions, which makes the scheme less convenient to use. Another drawback is the complexity of the commutators introduced by different terms in the Hamiltonian in the Euler–Lagrange equation (see equation (2) in reference [31]). As a result, the computation load for multiple qubits could get very high and hardly be applied in practice. The problem of how to implement an effective dimension reduction to efficiently steer quantum bits is worth further exploration.

In this paper, we uncover the source of computational complexity from the perspective of a variational principle, and in the process propose an alternative set of equations with much improved efficiency, especially for multiple qubits with limited control parameters. We first slightly extend the formulation in reference \cite{21} and derive all the necessary equations for later convenience. By introducing a set of new variables, the redundancy originated from the commutation relation between operators gets eliminated, which enables a very efficient computation of optimal paths in the presence of multiple qubits. A relaxation scheme is designed and implemented to solve the problem involving quantum entanglement when interaction between different bits comes into play. With several continuous symmetries identified in the Lagrangian formulation, it is possible to remove the annoying neutral directions in the numerical computation. In all the examples we tried, the simplest optimal paths seem to always bear the time-reversal symmetry if the initial and target state are related by a symmetry of the Hamiltonian.

The paper is organized as follows. In section 2.1 Lagrangian formation of the QBE is reproduced with an introduction of uncontrollable terms (the coefficients of which are fixed values). All the necessary variational equations are derived and written in convenient vector forms. The solution of these equations is derived analytically and verified numerically in section 3, in the absence of interaction. To deal with multiple qubits with interaction, a new set of equations are written down in section 4 with a change of variables, which achieves a great reduction of complexity. The evolution of the entanglement along an optimal path is always unimodal, which is demonstrated in all the examples in section 5. Our findings are summarized in the final section.

2. The variational principle

Without loss of generality, the Hamiltonian of a quantum system that is of interest could be written as:

\[
H = \sum_{j=1}^{m} \xi_j(t)A_j,
\]

where \(\xi_j(t)\)'s are real numbers and \(A_j\)'s are Hermitian operators that satisfy \(\text{Tr}A_j = 0\) and \(\text{Tr}(A_jA_k) = \delta_{jk}(j,k \leq m)\). The traceless Hamiltonian could be divided into two parts: the controllable part \(\mathcal{A} = \sum_{j=1}^{n} \xi_j(t)A_j\) with each \(\xi_j(j = 1, \ldots, n)\) subject to external control and the uncontrollable part \(\mathcal{B} = \sum_{j=n+1}^{m} \xi_j(t)A_j\) with \(\xi_j\)'s being constant or changing in a pre-determined way, often used to model interaction between qubits. For later convenience we use \(u\) and \(v\) to label coefficients of the controllable part \(u = (\xi_1, \xi_2, \ldots, \xi_n, 0, \ldots, 0)^t\) and the uncontrollable part \(v = (0, 0, \ldots, \xi_{t+1}, \xi_{t+2}, \ldots, \xi_m)^t\), and hence \(\xi = u + v\). In this work, we build a formulation applicable to the general case which includes both components.
2.1. A variational scheme for the QBE

The action integral is written as [21]:

\[ S(\psi) = \int \frac{\sqrt{\langle \psi | (1 - P) | \psi \rangle}}{\Delta E} + i(\phi | \psi \rangle + \langle \phi | H | \psi \rangle + c.c) + \lambda \left( \sum_{j=1}^{m} \xi_j^2 - \omega^2 \right) + \sum_{j=m+1}^{\lambda_j (\xi_j - Q_j)} \]  

(2)

where \( P(t) = |\psi(t)\rangle \langle \psi(t) | \) is the projection to the state \( |\psi(t)\rangle \) which is a normalized wavefunction defined in the configuration space, \( \phi \) is an auxiliary wavefunction and c.c denotes complex conjugates.

(\( \Delta E \))\(^2 \equiv \langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2 \) is the energy variance. Parameters \( \lambda \) and \( \lambda_j \) are Lagrange multipliers and all \( \{ \lambda_j \}_{j=1,2,\ldots,n} \) are set to zero, \( \omega \) is a given constant, the \( Q_j \)'s denote the coupling constants in the Hamiltonian and the Planck's constant \( h \) is chosen to be 1 for simplicity.

Now we take the variation of the action equation (2) to obtain the equation of motion and all the constraints imposed to the variables.

(a). The variation with respect to \( \phi \) gives

\[ i\psi = H|\psi\rangle, \]

(3)

which is the usual Schrödinger equation. In the projective space \( CP^{m-1} \), the Fubini–Study line element is written as \( ds^2 = |\langle 1 - P | d|\psi\rangle|^2 \), which measures the displacement in the angular direction. Here, it is easy to check that \( ds^2 = (\Delta E)^2 dt^2 \). Hence, the first part of equation (2) refers to the total time of the process and the other parts embody differential or other constraints.

(b). Here, we take the variation with respect to \( \lambda \) and \( \lambda_j \) separately, resulting in \( \frac{1}{2} \sum_{j=1}^{m} \xi_j^2 = \omega^2 \), which defines the size of the Hamiltonian as a finite energy constraint, and \( \xi_j = Q_j \) (\( n < j \leq m \)), which depicts the influence of generic interactions.

(c). The variation with respect to \( \psi \) gives

\[ \frac{d}{dt} \left[ \frac{H - \langle H \rangle}{2(\Delta E)^2} \right] |\psi\rangle - i|\dot{\psi}\rangle + H|\psi\rangle = 0, \]

(4)

where \( \langle \cdot \rangle \) refers to the average with respect to |\psi\rangle. Equations (3) and (4) are seen in the literature [21] but the equations below appear new.

(d). The variation with respect to \( H \) could now be taken as multivariate change with respect to \( \{ \xi_j \}_{j=1,2,\ldots,m} \), resulting in

\[ D_j = \frac{1}{2\Delta E^2} \sum_k F_{jk} \xi_k - \lambda_j \xi_j - \lambda_j' \quad \text{(with } \lambda_j' = 0 \text{ for } j \leq n), \]

(5)

where \( F_{jk} = \langle A_j A_k + A_k A_j \rangle - 2 \langle A_j \rangle \langle A_k \rangle \), \( D_j = \langle \phi | A_j | \psi \rangle \) and c.c and \( \sum \) stands for \( \sum_{k=1}^{m} \) which is also the case in all the following equations. The detailed derivation of equation (5) has been relegated to appendix A. Next, we derive the equations of motion for \( \lambda \) and \( \{ \xi_j \}_{j=1,2,\ldots,m} \).

A multiplication of both sides of equation (5) with \( \{ \xi_j \}_{j=1,2,\ldots,m} \), the controllable components, and then a summation over \( j \) results in

\[ \lambda = \frac{1 - \mathbf{D} \cdot \xi - \sum_{j=n+1}^{m} \left( \sum_k \frac{F_{jk} \xi_k}{\Delta E^2} - D_j \xi_j \right)}{\omega^2}, \]

(6)

where \( \mathbf{D} \cdot \xi = \sum_{j=1}^{m} D_j \xi_j \) and \( \omega^2 = \sum_{j=1}^{m} \xi_j^2 \) is constant (the constraint on the controllable part of the Hamiltonian). Noticing that \( \{ \xi_j \}_{j=n+1,\ldots,m} \equiv 0 \), we obtain:

\[ \lambda = \frac{\sum_{j=n+1}^{m} \left\{ \frac{\xi_j}{\Delta E^2} \left[ \sum_k (F_{jk} \xi_k + \tilde{F}_{jk} \xi_k) - \frac{\tilde{F}_{jk}}{\Delta E^2} \tilde{F}_{jk} \right] + D_j \xi_j \right\}}{\omega^2}, \]

(7)

where \( \tilde{F} = \xi \cdot F \) and \( \tilde{F}_{jk} = \sum_k F_{jk} \xi_k \). Here we used the fact that \( \frac{d}{dt} \mathbf{D} \cdot \xi = 0 \) (details in appendix B), \( \xi \cdot \mathbf{C} = \mathbf{C} \cdot \xi = 0 \) (details in appendix C) and

\[ \frac{d}{dt} D_j = \frac{1}{2\Delta E^2} \left( \sum_k F_{jk} \xi_k - \tilde{F}_{jk} \tilde{F}_{jk} \right) + \sum_k C_{jk} \xi_k, \]

(8)
where $C_k$ satisfies $[H, A_j] = -i \sum_k C_k A_k$, with $C_k$ being a real number. For a detailed derivation of equation (8), please check appendix D. Feeding equation (8) into equation (7) results in

$$
\dot{\lambda} = \frac{\sum_{j=0}^m \sum_{k=1}^{m+1} \xi_j C_k \left( D_k - \frac{E_j}{2 \Delta E} \right)}{\omega^2},
$$

with $\dot{F} = C \cdot F + F \cdot C^T$ (appendix E). Taking the time derivative of both sides of equation (5), and together with equation (8), we get

$$
\dot{u} = -\frac{C \cdot D}{\lambda} + \frac{C \cdot F \cdot \xi}{2 \lambda \Delta E^2} + \frac{(v \cdot C \cdot X')}{\lambda \omega^2} u.
$$

(10)

With equations (8), (9), (10) and the Schrödinger equation (3), the optimal path can be calculated now.

Here let’s discuss a special case with $H \in \mathcal{A}$, namely $\xi = u$, which means that all parts are controllable and thus $v = 0$. It is obvious that this case is simple since

$$
D_k = \frac{1}{2 \Delta E^2} \sum_k F_k u_k - \lambda u_k,
$$

(11)

$$
\frac{d}{dt} D_k = \frac{1}{2 \Delta E^2} \left( \sum_k F_k u_k - \dot{F}_k \frac{\dot{u}}{\Delta E^2} \right) + \sum_k C_k D_k.
$$

(12)

Hence equation (9) implies that $\dot{\lambda} = 0$. equation (10) could be reduced to

$$
\dot{u} = -\frac{C \cdot D}{\lambda} + \frac{C \cdot F \cdot u}{2 \lambda \Delta E^2}
$$

(13)

Considering $u \cdot C = 0$ (appendix C) and feeding equation (11) into equation (13) leads to a trivial solution $\dot{u} = 0$, which indicates that $u$ is a constant vector and the evolution corresponds to a simple rotation with a fixed axis on the Bloch sphere.

2.2. Gauge symmetries in the Lagrangian

In this section, we discuss the gauge symmetries in the Lagrangian equation (2), which create neutral directions in the evolution and may bring complication in numerical calculation. First, consider a transform $\hat{U}_1: \phi \to \phi + i a \psi$, $a \in \mathcal{R}$, with which the Lagrangian becomes

$$
S' = S + \int dt (a(\psi') \psi - ia(\psi'H\psi) + c.c.).
$$

(14)

The expression $(\psi|\psi) + c.c.$ is a total differentiation, which could be integrated out. With the Hermiticity of $H$, the extra integral in equation (14) vanishes and hence $\hat{U}_1$ is a symmetry transform. Next, we consider another transform $\hat{U}_2: \phi \to \frac{\lambda + b}{\lambda} \phi$, $\lambda \to \lambda + b$, $\mathbf{X} \to \frac{\lambda + b}{\lambda} \mathbf{X}'$, $b \in \mathcal{R}$ which turns equation (2) into

$$
S(\psi, H, \phi, \lambda, \mathbf{X}) = \int dt \frac{\sqrt{(\psi' | (I - P) \psi)}}{\Delta E} + \frac{\lambda + b}{\lambda} \left[ (\phi|\phi) + (\phi'H\psi) + c.c.) + \lambda \left( \sum_{j=1}^m \frac{E_j^2}{2} - \omega^2 \right) + \sum_{j=m+1}^n \lambda_j (\xi_j - Q_j) \right],
$$

(15)

which only changes the values of the invisible Lagrange multipliers $\phi, \lambda, \mathbf{X}$ while the equation for the observables $\psi, u$ remain intact. Actually, it is most obvious in the simplified formulation equation (18) below, where $\Omega, \ u, \ \Omega, \ \dot{u}$ keep invariant under the transform $\hat{U}_2$. Hence $\hat{U}_2$ is a symmetry transform.

3. The evolution of Hamiltonian as a rotation

The equation $\xi \cdot C = 0$ tell us that $v \cdot C = -u \cdot C$. Substituting the equation (5) into equation (10) results in

$$
\dot{u} = (I - P_u) \frac{C \cdot \mathbf{X}'}{\lambda}.
$$

(16)

where $I$ is the identity matrix and $P_u$ is the projection operator $\frac{u | u}{| u |^2}$ ($\omega^2 = \sum_{j=1}^m E_j^2 = \sum_{j=1}^m u_j^2 = |u|^2$). Here we use the Dirac notation to emphasize the projection, whereas $u$ is actually real. With the fact that
$v = 0$, it is easy to check that $\xi \cdot \dot{\xi} = u \cdot \dot{u} = 0$. And the uncontrollable part of the time derivative of equation (5) similarly gives the evolution of $X'$

$$\dot{X'} = C \cdot X' + \frac{v \cdot C \cdot X'}{\omega^2} v = (I + \frac{|v|^2}{|u|^2} P_v) \cdot C \cdot X', \quad (17)$$

where $P_v = \frac{v}{|v|^2}$ and $|v|^2$ is a real constant. After, defining $\Omega = -\frac{2}{\sqrt{|X'|}} X'$, the angular velocity of the rotation of $u$ can be described with $\Omega$. Furthermore, the QBE problem can be characterized with a simpler set of equations

$$\dot{u} = \frac{\sqrt{1_r I}}{2} (I - P_v) \cdot C \cdot \Omega$$

$$\dot{\Omega} = (I + \frac{|v|^2}{|u|^2} P_v) \cdot C \cdot \Omega - \frac{\sqrt{1_r I}}{2\omega^2} (v \cdot C \cdot \Omega) \Omega \quad (18)$$

along with the Schrödinger equation $\dot{\psi} = -iH\psi$.

According to appendix C, $C$ can be conveniently determined, which in specific circumstances may provide possible routes to analytic solutions. As a specific case, in the case without entanglement, the phase space can be divided into separate Bloch spheres of qubits. Then, according to equation (18), the equation of a single qubit in three-dimensional space is appreciably simplified to

$$\dot{u} = \Omega \times \xi - u \cdot (\Omega \times \xi) \quad \textbf{u} = \Omega \times \textbf{u}.$$ Meanwhile, the uncontrollable part is generally limited to no more than one dimension per qubit, or there will be no solution for most boundary conditions. As a result, $\Omega$ is in the direction of $X'$ which is along $v$ in the case of three dimensions. Here the cross product holds for each $SO(3)$ Bloch sphere, which indicates that $u$ is rotating with the angular velocity $\Omega$.

As $\Omega$, $v$ is in the same direction for a single qubit. After multiplying $\Omega$ with equation (18) we see that $\Omega$, the rotation speed of $u$, is a constant vector. In fact, in this case $X' = 0$ and thus $\Omega = 0$, $\dot{u} = 0$ as given in the previous section. It is easy to see that the spin vector $\langle \sigma \rangle$ ($\sigma_{j=\{x,y,z\}}$ are the Pauli matrices) is rotating around $\textbf{u}$, and the evolution of wave function is analytically computed with rotation matrices.

### 4. A reduced scheme to the QBE

In practice, there are usually a large number of uncontrollable terms in the Hamiltonian. However, for the convenience of computation and design, most interaction terms are fixed. In this case the number of control parameters is appreciably low, while, the computation complexity of the conventional numerical methods remains as high. To address and eliminate the redundant complexity, here we propose an alternative approach, reintroducing the Lagrange multiplier $\phi$ previously replaced by $D$.

In general situations we see that the tremendous complexity is mainly brought in by the factor $C \cdot D$, since the commutation relation (D6) will incur a large number of or sometimes even infinitely many $A_i$'s and thus $D_i$'s in the QBE equations when there are multiple interacting qubits. It is seen that most of the previous searching schemes [21, 31] are confronted with this problem but no special attention has been paid. Here, we introduce an efficient new scheme based on the fact that $C \cdot D$ is immediately derivable from $\phi$. Technically, consider

$$\phi' = \phi - \frac{1}{2\Delta E^2} (H - \langle H \rangle) \psi, \quad (19)$$

then equation (5) turns to

$$D'_j = \langle \phi' | A_j | \psi \rangle + \text{c.c.} = -\lambda_j \xi_j - \lambda'_j, \quad \text{with } \lambda'_j = 0 \text{ for } j \leq n. \quad (20)$$

Thus $C \cdot D'_j = C \cdot \langle \phi' | A_j | \psi \rangle + \text{c.c.}$. Furthermore, it is much easier to evolve $\phi'$ than $\phi$ since equation (4) yields

$$i\phi' - H\phi' = \frac{i}{2\Delta E^2} [(H - \langle H \rangle) \psi - \frac{\dot{F} \cdot \xi}{\Delta E^2} (H - \langle H \rangle) \psi], \quad (21)$$

which gives

$$i\phi' = H\phi'. \quad (22)$$
In analogy to previous derivations in section 3, it is easy to check that equation (18) now holds in an alternative form
\[
\dot{\psi} = -iH\psi, \\
\dot{\phi} = H\phi', \\
\dot{\lambda} = -\frac{\mathbf{v} \cdot \mathbf{C} \cdot \mathbf{X}'}{2\alpha^2}, \\
\dot{u} = (I - P_u) \cdot \mathbf{C} \cdot \mathbf{X}', \\
i\phi' = H\phi', \\
\mathbf{H} = \sum_{j} C_{ij} D_j = \langle \phi' | [H, A_i] | \psi \rangle + \text{c.c.},
\]
where from equation (20), \( \mathbf{C} \cdot \mathbf{X}' = -\mathbf{C} \cdot \mathbf{D}' \) with \( \sum_{j} C_{ij} D_j = \langle \phi' | [H, A_i] | \psi \rangle + \text{c.c.} \), which could be evaluated directly with the computed states \( \phi' \) and \( \psi \) and the known \( H \) and \( A_i \)'s. In conclusion, the whole QBE problem is fully described by equation (23). Terms like \( \mathbf{C} \cdot \mathbf{F} \cdot \mathbf{\xi}/2\Delta E^2 \) in \( \mathbf{C} \cdot \mathbf{D} \) are eliminated now because of the introduction of the state variable \( \phi' \), and hence the previous large number of equations needed to evaluate \( \mathbf{C} \cdot \mathbf{D} \) are simply replaced by the evolution of \( \phi' \). Since the number of degrees of freedom of vector \( \phi' \) is much smaller than that of matrix \( \mathbf{C} \).

Now a two-point boundary value problem with equation (23) is left for us to solve. To begin with, we count the number of independent variables. The number of different variables in equation (23) is \( N = N_u + N_{\phi'} + N_{\lambda} + N_\psi + N_{\psi'}, \) while the number of the constraints is \( N' = N_u + N_{\psi'} + 2N_\psi + 1 \) given by equation (20) (\( N_u + N_{\psi'} \) constraints), the energy constraint \( \sum_{j=1}^{n} \xi_j^2 = \omega^2 \), the prescribed initial and final states \( \psi(0) = \psi_u \) and \( \psi(T) = \psi_{\text{target}} \) (2\( N_\psi \) constraints). Thus we have \( N = N' \) (where \( N_\lambda = 1 \) and \( N_{\phi'} = N_\psi \)). Here we evaluate the number of differential equations that we have to solve. In the work of reference [31], the number of equations is \( N_u \) (accessible space) + \( N_{\psi'} \) (forbidden space) + \( N_\psi \). In our method, this number is \( N_u + N_\psi + N_{\phi'} + N_{\lambda} \). Very often, especially for multiple qubits \( N_{\phi'} + N_{\lambda} \leq N_{\psi'} \).

The difference increases with the number of qubits, as we will see in the following examples. Obviously, our method needs to solve fewer equations in complex situations, which is due to the introduction of the variable \( \phi' \).

In order to steer the final state \( \psi(T) \) to the target state \( \psi_{\text{target}} \) by adjusting the initial conditions and the flight time \( T \), the famous shooting method (explained in appendix F) and the idea of ‘relaxation’ will be carefully used in finding the optimal path when Hamiltonian \( H \) contains interaction terms. We give more details about relaxation below.

When it comes to large-scale qubit systems, the shooting method per se can be too costly and need a good trial solution that is sufficiently close to the exact solution. In order to overcome those shortcomings we suggest a ‘relaxation’ method to meet the boundary conditions step by step. First, one starts from the case without interaction, solving the problem with separate qubits. With interaction present, secondly, we invite part of the interactions back and use the no-interaction solution as the initial condition (i.e. taking the first-step coupling constant \( J = 0.01 \) in our examples), so a new solution in case of the weak interaction is obtained, which can be used as the initial condition for the case with a little bit stronger interaction. Repeat this process until the full interaction is restored and an optimal path is then obtained. This is a relaxation process since the effective Hamiltonian in the computation is gradually relaxed to the desired one.

5. Examples

5.1. One-qubit Bloch sphere

Here we first try to search for local optimal paths of single-qubit evolution on the Bloch sphere. The goal is to flip the spin state of a single Fermion from \(| + \rangle \langle x |) to | - \rangle \langle x |.

Assuming \( \hbar = 1 \), the Hamiltonian with the full control is
\[
H = -\mu_{\Omega} \cdot \mathbf{B} \equiv \frac{\gamma}{2} \mathbf{\sigma} \cdot \mathbf{B} = -\frac{\gamma}{2}(B_x\sigma_x + B_y\sigma_y + B_z\sigma_z),
\]
where \( \gamma = g\frac{\alpha}{ \mu_{\text{B}} } \) is the gyromagnetic ratio and \( q \) is the charge carried by the particle. Since \( \gamma \simeq -2 \), then
\[
H \simeq \mathbf{B} \cdot \mathbf{\sigma}.
\]

Based on previous discussions section 3, the evolution path of \( \psi \) can be analytically addressed, as a rotation with the angular velocity \( \omega_{\text{eff}} \) around an axis \( \mathbf{u} \) rotating itself at \( \Omega \). The effective angular velocity \( \omega_{\text{eff}} \) of spin vector is determined as
\[
\omega_{\text{eff}} = 2\mathbf{B} = \frac{2}{\sqrt{1H}} \mathbf{u} = \sqrt{2u},
\]
where $B$ is an effective magnetic field and the Hamiltonian $H = \sigma \cdot B = \sum_{j} A_j n_j$. This is derived from the fact that the SU(2) element of a rotation with $\Delta \phi$ is $e^{i \Delta \phi \omega \sigma_z}$. In the frame of reference rotating with $\Omega$, the motion of $\psi$ is viewed as a fixed-axis rotation with the angular velocity $\Omega' = \omega_{\text{eff}} - \Omega$.

For instance, consider the numerically simulated case [21] where $\psi(0) = |+x\rangle$, $\psi_{\text{target}} = |-x\rangle$, $B(0)$ is the constraints $T_r(\omega \sigma_z)$ in the $\Omega B R \Omega$ around $\psi = H + \text{displaced as well in figure 1.}$ From previous discussions, we know that in this case optimal path is naturally a geodesic curve (see figure 1 (left), which shows one of the many geodesic state and the geodesic solution is simple according to the discussion in section 5.1 above. Here, we focus on the oscillating solutions under the anisotropic constraint featuring

$\langle \sigma \rangle(t) = R(\phi, \theta, \Psi) \cdot \langle \sigma \rangle(0) = \begin{pmatrix}
\cos \Omega t & \cos \Omega' t & \sin \Omega t & \sin \Omega' t \\
-\sin \Omega t & -\sin \Omega' t & \cos \Omega t & \cos \Omega' t \\
\omega_{\text{eff}} & -\omega_{\text{eff}} & \omega_{\text{eff}} & \omega_{\text{eff}} \\
\sin \Omega t & \sin \Omega' t & \cos \Omega t & \cos \Omega' t
\end{pmatrix}, \quad (26)
$

where the values of $\Omega$ and $\Omega'$ are twice as much as those in reference [21]. Equation (26) gives a family of analytic solutions if we choose $(\Omega T, \Omega' T, \frac{\omega_{\text{eff}}}{\Omega}) = (k\pi, l\pi, \frac{k}{\sqrt{l^2-k^2}})$, where $l, k$ are non-negative integers and $l + k$ is odd. The case $k = 0$ corresponds to the geodesic solution with no anisotropic constraints and cases of $k \neq 0$ correspond to the oscillating solutions with $l - 1$ nodes. We will denote $L = l - 1$ for later convenience. The oscillating curve in figure 1 plots the solution with $k = 1, L = 0$ and 1.

The simulated paths obtained by our numerical method are consistent with the analytical solution and displaced as well in figure 1. From previous discussions, we know that in this case $\mathbf{u} = 0$, i.e. $\mathbf{B} = 0$. So the optimal path is naturally a geodesic curve (see figure 1 (left), which shows one of the many geodesic solutions). The red line on the equatorial plane (marked by the green grid inside the sphere) indicates the evolution of the external magnetic field $\mathbf{B}$, which does not change throughout the evolution. In principle, the constraints $T_r(H\sigma_j) = 0$ allow oscillating solutions with $\mathbf{B} \neq 0$. Let’s take the case of $H = B_x \sigma_x + B_y \sigma_y + B_z \equiv 0$ as an example. In numerical computation, we use the shooting method to identify the initial value $\phi_0$ of the prescribed boundary conditions $\psi(0) = |+x\rangle, \psi(T) = |-x\rangle$. Figure 1 (right) shows the resulting optimal path which oscillates with one node on the equator, where $\Omega = (0, 0, \frac{2k}{l})$. The evolution of $\mathbf{B}$ (the area swept by the red line in figure 1 (right)) corroborates the theory of rotation in section 3. Of course, it is not hard to get a locally optimal path with more than one node, which we will not show here.

### 5.2. Two-qubit Bloch sphere

In the case of two qubits without interaction, two Bloch spheres may be used to represent a non-entangled state and the geodesic solution is simple according to the discussion in section 5.1 above. Here, we focus on the oscillating solutions under the anisotropic constraint featuring $B_z = 0$. We give an example with

$$H = B_x^{(1)} \sigma_x^{(1)} + B_y^{(1)} \sigma_y^{(1)} + B_x^{(2)} \sigma_x^{(2)} + B_y^{(2)} \sigma_y^{(2)}.$$

(27)
Similarly, our purpose is to flip both qubits (where $\psi(0)^{(1)} = | + x \rangle$ and $\psi^{(1)}_{\text{target}} = | - x \rangle$ for qubit one, $\psi(0)^{(2)} = | + y \rangle$ and $\psi^{(2)}_{\text{target}} = | - y \rangle$ for qubit two). Obviously, these two qubits are both reversing their states, and because $x$- and $y$- directions are totally equivalent these qubits should share the same energy at the ground state (namely $\omega^{(1)}_{\text{eff}} = \omega^{(2)}_{\text{eff}}$). Figure 2 shows a local optimal solution of the constrained two-qubit system with $L = 1$. $\Omega^{(1)} = (0, 0, -\sqrt{3} \omega)$, $\Omega^{(2)} = (0, -\sqrt{3} \omega, 0)$. It is apparent that the evolution of $B$ turns out to be a rotation as expected. (Since the numerical solution is consistent with the analytical one, it will not be distinguished in the following. Also, we can obtain longer paths with larger $L$, not shown here.)

Actually, the local solutions can be derived analytically as long as the interaction terms are missing in the Hamiltonian. According to the rotation picture, the analytical approach can be applied to no-interacting many-qubit systems with an arbitrarily large number of qubits. Here in figure 2 the solution corresponds to $(k^{(1)}, L^{(1)}) = (k^{(2)}, L^{(2)}) = (1, 1)$ as the oscillating solution in figure 1 (right), so they naturally share the same geometric property. Later on, these solutions would be good initial guesses in the presence of interaction in the searching algorithm based on the idea of relaxation (see 4).

### 5.3. Two or three qubits with interaction

In the case of a single qubit or double qubits without interaction, it is easy to obtain the solutions analytically, which are very regular. With interaction, however, it is very difficult to obtain such an analytical solution, and thus we resort to the numerical method discussed in appendix F. In this section, three different cases are investigated together with a general description of the consequences brought by possible entanglement in the wave functions.

Case 1, the initial and final spin states are the same as in section 5.2, but there is an extra interaction term in the Hamiltonian

$$H = B_x^{(1)} \sigma_x^{(1)} + B_y^{(1)} \sigma_y^{(1)} + B_y^{(2)} \sigma_y^{(2)} + B_y^{(2)} \sigma_y^{(2)} + J_y \sigma_y^{(1)} \sigma_y^{(2)},$$

where $J_y = 1$ is a fixed interaction constant. In the numerical computation, in order to utilize a reasonable initial condition, we gradually increase the value of $J_y$ from 0.01 to 1 with a step-size 0.01. After the interaction term $J_y$ is introduced, the wave function $\psi(t)$ is no longer separable, but becomes entangled. Following the work in the literature [32, 33], we may define an entanglement index $E_p$ for the two subsystems $A$ and $B$,

$$E_p(|\psi\rangle_{AB}) = -\text{Tr}_A(\rho_A \log_2 \rho_A) - \text{Tr}_B(\rho_B \log_2 \rho_B),$$

where $\rho_A = \text{Tr}_B(|\psi\rangle_{AB} \langle \psi|)$ is the reduced density matrix of the pure state $|\psi\rangle_{AB}$ over subsystem $A$, and $\rho_B$ has a similar definition. Figures 3(a)–(d) depict the entanglement of $\psi(t)$ with $L = 1, 3, 2, 4$, which have a common feature: the entanglement of the wave function connecting the two separable states (the initial and the target state) increases first, reaches a maximum and then decreases back to zero. The entanglement evolution profile for $L = 1, 3$ (figures 3(a) and (b)) is symmetric and the maximum is exactly at the symmetry point, while for $L = 2, 4$ (figures 3(c) and (d)), the profile is skewed. Given a suitable initial value of $\phi_0$, the computation converges exponentially when approaching an optimal path (See figure 5(c)). Next, we keep the initial state unchanged and set the target state as an entangled one with $E_p = 0.6061$. The wavefunction $\psi(t)$ connecting the two states is computed with $J = 1, 0.9, 0.65$, the entanglement evolution
Figure 3. The time evolution of the entanglement $E_p$ of $\psi(t)$ for different $J_{yy}$ and $L = 1$ (a), 3 (b), 2 (c), 4 (d) with the Hamiltonian given by equation (28). $t/T$ represents the normalized time where $T$ is the total time. The initial state is $|+\rangle_x (1)$ $|+\rangle_y (2)$ and the final state is $|-\rangle_x (1)$ $|-\rangle_y (2)$ for qubits 1 and 2.

Figure 4. The evolution of the entanglement $E_p(t)$ of wavefunction $\psi(t)$ from the initial state $\psi(0) = (0.5, 0.5i, 0.5, 0.5i)^T$ to the final state $(-0.216558 - 0.450669i, 0.528077 + 0.256587i, 0.070204 + 0.391403i, -0.294949 + 0.400223i)$ with $L = 1$, $J = 0.65, 0.9, 1$, $T = 0.6837, 1.1517, 1.5816$ and the Hamiltonian given by equation (28).

of which is depicted in figure 4. We observe that with the decrease of the coupling strength $J$, the change of entanglement $E_p(t)$ tends to be a linear curve. In addition, we observe that there is an approximate center symmetry about $t = 0.5T$, indicating a fast initial rise and final relaxation but a steady transition between.

Case 2, we consider a two-qubit model with the following Hamiltonian

$$H = \sum_{L,m} B_{m}^{(L)} \sigma_{m}^{(L)} + J \sum_{m} \sigma_{m}^{(1)} \sigma_{m}^{(2)},$$

where $\sigma_{m}^{(l)}$ with $(m = x, y, z, l = 1, 2)$ are the Pauli matrices for the $l$th qubit. The initial and final spin states are the same as in section 5.2 and the coupling constant $J = 1$. The results obtained with our method
Figure 5. The evolution and the convergence with the Hamiltonian given by equation (30). The evolution of the measurement \( \langle \sigma(t) \rangle \) (a) and the control magnetic field \( B(t) \) (b), where \( \langle \sigma(t) \rangle = \langle \psi(t) | \sigma(t) | \psi(t) \rangle \) \((m = x, y, z; l = 1, 2)\) represents the observed value of the spin in the \( m \)-direction of the \( l \)th bit. (c) The convergence of our method (scheme I), the Krotov algorithm (scheme II) and the Grape algorithm (scheme III), where error \( d = \| \psi_{\text{true}} - \psi(T) \| \), \( N \) is the number of iteration steps and \( J = 1, L = 1, T = 1.5211 \). (d) The evolution of the control magnetic field intensity \( |B(t)| \) obtained by our method (scheme I), the Krotov algorithm (scheme II) and the Grape algorithm (scheme III).

are portrayed in figures 5(a) and (b), where (a) depicts the components of the observable and (b) shows that the control magnetic field \( B(t) \). In this case, \( N_u = 6, N_{x} = 9, N_{y} = N_{z} = 8, N_{\lambda} = 1 \), the number of QBEs that we solve is 23 both in the reference [31] and in our method.

Next, we make a comparison of the efficiency of finding such a connecting wavefunction among different methods with the same initial conditions. The convergence of different methods is compared in figure 5(c). Our method (scheme I, red points), which though oscillates at the initial stage (in the first dozen iteration), converges much more quickly (within less than 30 iterations) and displays good stability as well. Scheme II and III denote the Krotov algorithm [13–16] and the Grape algorithm [12, 13], respectively. The error of these two algorithms are always monotonously decreasing. For the Krotov algorithm, the error drops very fast at the beginning (the Krotov scheme shows better convergence for short times), but the decrease slows down after 10 iterations and hence takes long to reach a small value. For the Grape algorithm, we clearly see that the convergence is quite slow (with more than 500 iterations), and the rapid convergence is not achieved until the iteration proceeds many steps. From the perspective of energy, as shown in figure 5(d), our method ensure that the strength of the magnetic field remains constant \( |B(t)| = 2.23607 \) (red line) during the evolution, while in the Krotov algorithm (black line) and the Grape algorithm (blue line) the magnitude of the magnetic field changes over time. The optimal time is computed as \( T = \frac{\sqrt{2\pi}}{\omega \hbar} \) for a quantum state evolving between two end states of a diameter on the Bloch sphere, which is consistent with the lower bound computed by Margolus and Levitin [34, 35]. The Fubini–Study distance to the target state seems to decrease linearly with time as shown in figure 6, and we note that with the decrease of the energy \( \omega \), the traveling time \( T \) increases. Therefore, because the initial state \( \psi_0 \) and target state \( \psi_{\text{target}} \) are given, the total Fubini–Study distance of the two states is consistent. Our method ensures that the energy of the system is constant in the process of evolution. Larger energy corresponds to faster movement, so the larger the energy, the faster the \( F(t) \) decreases. The linear dependence of \( F(t) \) on time indicates a uniform approach to the target state on the optimal path.
Figure 6. The Fubini–Study distance $F(t)$ between $\psi(t)$ and $\psi_{\text{target}}$ with $\omega = 2.8284, 2.7803, 2.6926, 2.5554, 2.3601$ and the Hamiltonian given by equation (30). The distance between neighboring states along a trajectory is defined by using the Fubini–Study line element $d_{\psi} = \sqrt{\langle d\psi | (1-P)| d\psi \rangle}$, where $d\psi$ is the change of the state along the path and $P = |\psi \rangle \langle \psi |$ is a projection operator.

Figure 7. The evolution of the wave function $\psi(t)$ with $J = 0.2, L = 1, T = 2.8216$ and the Hamiltonian given by equation (31). $\text{Re}(\psi(t))$ and $\text{Im}(\psi(t))$ represent real part (a) and imaginary part (b) of wave function $\psi(t)$ respectively. The notation $|000\rangle \sim |111\rangle$ in the legend represents the eight components of $\psi(t)$.

Case 3, we study a model with three qubits for which the Hamiltonian is

$$H = \sum_{Lm} B_m^{(L)} \sigma_m^{(L)} + J_1 \sigma_1^{(1)} \sigma_2^{(2)} + \sigma_2^{(2)} \sigma_3^{(3)},$$

(31)

where $\sigma_m^{(L)}$ with $(m = x, y, z, L = 1, 2, 3)$ are the Pauli matrices for the $L$th qubit. We choose the initial state $|+x(1)\rangle \otimes |+y(2)\rangle \otimes |+x(3)\rangle$ and the final state $|-x(1)\rangle \otimes |-y(2)\rangle \otimes |-x(3)\rangle$. The obtained optimal wavefunction $\psi(t)$ connecting them with the interaction strength $J = 0.2$ and $L = 1$ is depicted in figure 7. Figure 7(a) depicts the real and (b) the imaginary part of $\psi(t)$. In this case, $N_u = 9, N_{x'} = 54$, $N_{\phi} = N_{\psi} = 16, N_z = 1$, the number of quantum Brachistochrone equations that have to be solved is 79 with the method in reference [31], however, the number is only 42 for our method. At this time, it is obvious that the number of equations we need to solve is much less, especially with the increase of the qubit number.

5.4. A symmetry operation

In this section, we check a symmetry operation of the Hamiltonian equation (28) and ferret out possible mechanism underlying the phenomenon discussed in section 5.3 above. It is interesting to observe a discrete symmetry operation in Hamiltonian (28) associated with

$$F = \begin{bmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix},$$

(32)
with the transformed Hamiltonian which connects the initial state $B$ evolution of those in figures 9(g) and (h) respectively up to a minus sign in the relevant component. In addition, the $\psi$ figures 9(a)–(d)). When we overlap graphs figures 9(a) and (c), we find that they are axisymmetric with respect to (0.5, 0), or vice versa. All the above indicates that the maximum of $t$ respect to $t_0$. On the other hand, under the discrete symmetry operation $L = 2$ and figures 9(e) and (f) ($L = 3$) depict the time course of $B(t)$ from $\psi_0$ to $\psi_f$ while figures 9(c) and (d) ($L = 2$) and figures 9(g) and (h) ($L = 3$) plot the time course of $B(t)$ from $\psi_0 = F\psi_0$ to $\psi_f' = F\psi_f$ with the transformed Hamiltonian $H' = F^2HF$. Apparently, the curves in figures 9(e) and (f) coincide with those in figures 9(g) and (h) respectively up to a minus sign in the relevant component. In addition, the evolution of $B_{z1}^{(1)}$ and $B_{z2}^{(1)}$ have a reflection symmetry with respect to $t = 0.5$ and $B_{y1}^{(1)}$ and $B_{y2}^{(1)}$ have a center symmetry with respect to (0.5, 0), or vice versa. All the above indicates that the maximum of $E_p$ is associated with a fixed point of the operation $F$ for the case $L = 3$.

In the cases $L = 2$, 4, the symmetry in $\psi(t)$ and $B(t)$ discussed previously disappear. Taking $L = 2$ for an example, figures 9(a) and (b) do not coincide with figures 9(c) and (d) and the maximum value of $E_p$ is not at $t = 0.5$. On the other hand, under the discrete symmetry operation $F$, we have $B_{y1}^{(1)} = FB_{y1}^{(1)}F^T = -B_{y2}^{(1)}$, $B_{y2}^{(1)} = FB_{y2}^{(1)}F^T = B_{y1}^{(1)}$, $B_{z1}^{(2)} = FB_{z1}^{(2)}F^T = B_{z2}^{(2)}$, $B_{z2}^{(2)} = FB_{z2}^{(2)}F^T = -B_{z1}^{(2)}$. It’s still true for $L = 2$, 4 (see figures 9(a)–(d)). When we overlap graphs figures 9(a) and (c), we find that they are axisymmetric with respect to $t = 0.5$. As the symmetry partner $\psi'_f$ of the wave function $\psi_f$ is obtained with the symmetry operation $F$, even if the entanglement evolution of $\psi'(t)$ or $\psi(t)$ (see figure 10(a)) itself is asymmetric, they are axially symmetric with respect to each other about $t = 0.5$, which also indirectly reflects the symmetry of the corresponding Hamiltonian equation (28).

In the case that $\psi_0$ and $\psi_f$ do not flip to each other, e.g. the angle between $\psi_0$ and $\psi_f$ is less than $\pi$, we then have $F\psi_0 \neq -\psi_f$ (take the case $L = 1$ as an example), which indicates that the entanglement evolution cannot be symmetric (shown in figure 10(b)). However, the maximum entanglement still exists which is
6. Summary and discussion

In this work, we derive a general set of differential equations (equation (23)) for the optimal quantum control of single or multiple qubits with or without interaction. In the derivation and application of equation (23), we discussed the following aspects: first, previous numerical methods conventionally involve a large number of physically irrelevant variables derived from the commutation relation with system Hamiltonians. We thus introduce a new set of observables to eliminate the physically irrelevant part, whereby an accelerated computation becomes possible. As a result, the efficiency of computation are boosted significantly. With the help of a ‘relaxation’ idea, the drawback of the shooting method, of requiring a good initial guess, is surpassed by slowly pushing the trial solution to the correct one with a gradual restoration of the interaction. Second, we discussed symmetries of the Lagrangian formalism of the

unique but not at $t = 0.5$, and also from the figure we see that this maximum increases with the angle between the initial and the final state.
QBE. In the numerical calculation, these entail unwanted degenerate directions in the Jacobian matrix, which may cause serious trouble in the solution of the resulting boundary value problem. Finally, groups of analytic solutions are given as rotations of qubits on Bloch spheres in the absence of interaction, which may be used as the starting point of the above relaxation scheme.

In an application of the new scheme to the case of two qubits with interaction, the solution to the QBE displays a unimodal evolution profile of the entanglement. If the initial and final state transform to each other under a symmetry operation of the Hamiltonian. The evolution of the optimal path either bears a related symmetry or has a symmetry partner. More explicitly, the solutions with even number of oscillations in the profile are asymmetric and the symmetry operation gives another optimal path—the symmetry partner of the original solution.

With the current formalism, we are able to design optimal control strategy for multi-qubits with possibly complex interaction. However, the evolution is not unique and many local optimal paths exist which could be indexed by the number of oscillations of the paths in simple cases. It could be interesting to classify these paths and check their bifurcation routes when system parameters change. On the other hand, this work may provide experimental researchers a practical computation tool for quantum information regulation, since an optimal control strategy of the magnetic field is readily designed based on our scheme.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. The demonstration of equation (5)

The variation of the Hamiltonian $H$ could now be taken as multivariate change with respect to $\{\xi_j\}_{j=1,2,\ldots,m}$. Let’s respectively check different parts of the action integral equation (2). First, check one term of the integrand

$$I = \langle \phi | H | \psi \rangle + \text{c.c.}$$

$$= \sum_j \langle \phi | A_j | \psi \rangle \xi_j(t) + \text{c.c.}$$

$$= \sum_j \xi_j(t) D_j, \quad (A1)$$

where $D_j = \langle \phi | A_j | \psi \rangle + \text{c.c.}$ are real numbers, thus the Hamiltonian variation of the term I is

$$\delta I = \sum_j D_j \delta \xi_j(t). \quad (A2)$$

Next, let’s consider the second part

$$II = g(\xi, \lambda, \lambda') = \lambda \left( \frac{1}{2} \sum_{j=1}^{m} \xi_j^2 - \omega^2 \right) + \sum_{j=n+1}^{m} \lambda'_j (\xi_j - Q_j).$$

Let $G_j = \frac{\partial g(\xi, \lambda)}{\partial \xi_j}$ and we obtain the variation of II

$$\delta II = \sum_j G_j \delta \xi_j. \quad (A3)$$
Third, before treating first term of the equation (2), we need to do some preparation. Here, we define:

\[ F_{jk} = \langle A_j A_k + A_k A_j \rangle - 2 \langle A_j \rangle \langle A_k \rangle, \quad (A4) \]

which is a symmetric tensor, and the energy variance could be written as:

\[ \Delta E^2 = \langle H^2 \rangle - \langle H \rangle^2 \]
\[ = \sum \xi_k \xi_k \langle A_j A_k \rangle - \xi_k \xi_k \langle A_j A_k \rangle \]
\[ = \frac{1}{2} \sum \xi_k \xi_k, \quad (A5) \]

leading to

\[ \delta \Delta E^2 = \frac{\delta \xi \cdot F \cdot \xi}{2} = \sum F_{jk} \xi_k \delta \xi_j, \quad (A6) \]

which gives

\[ \frac{\delta \Delta E}{\Delta E} = - \frac{\Delta E}{2 \Delta E} \delta \Delta E^2 \]
\[ = - \frac{1}{2 \Delta E^2} \sum \xi_k F_{jk} \delta \xi_j. \quad (A7) \]

So, the variation with respect to \( \xi_j \) of the first term of equation (2) gives

\[ \delta \sqrt{\langle \psi (1 - P) | \psi \rangle} \frac{1}{\Delta E} = \delta \sqrt{\langle \psi (1 - P) | \psi \rangle} \frac{1}{\Delta E} + \sqrt{\langle \psi | (1 - P) H | \psi \rangle} \frac{1}{\Delta E} \]
\[ = \sqrt{\langle \psi | (1 - P) | \psi \rangle} \frac{1}{\Delta E} \delta \frac{1}{\Delta E}, \quad (A8) \]

where \( \delta \sqrt{\langle \psi | (1 - P) | \psi \rangle} = 0 \), because here we only take the variation with respect to \( \xi_j \), and \( \sqrt{\langle \psi | (1 - P) | \psi \rangle} \) does not contain \( \xi_j \). Then, substituting equations (3) and (A7) into the above equation (A8) gives

\[ \sqrt{\langle \psi | (1 - P) | \psi \rangle} \frac{1}{\Delta E} = \sqrt{\langle \psi | H(1 - P) H | \psi \rangle} \frac{1}{\Delta E} \]
\[ = \Delta E \delta \frac{1}{\Delta E} \]
\[ = - \frac{1}{2 \Delta E^2} \sum \xi_k F_{jk} \delta \xi_j, \]

where \( (A5) \) has been used. With equation (A2), (A3) and (A9), the variation with respect to \( \xi_j \) gives

\[ - \frac{1}{2 \Delta E^2} \sum \xi_k F_{jk} + D_j + G_j = 0, \quad (A10) \]

where

\[ G_j = \begin{cases} \lambda \xi_j, & (j \leq n), \\ \lambda \xi_j - \lambda_j', & (n < j \leq m). \end{cases} \quad (A11) \]

Appendix B. The demonstration of \( \frac{d}{dt} D \cdot \xi = 0 \)

\[ \frac{d}{dt} D \cdot \xi = D \cdot \frac{d \xi}{dt} + \frac{d D}{dt} \cdot \xi \]
\[ = \sum \xi_j D_j + \frac{\xi_j}{2 \Delta E^2} \left( \sum \xi_k F_{jk} - \frac{\tilde{F} \cdot \xi}{\Delta E^2} \right) + \sum \xi_j C_{jk} D_k \]
\[ \dot{\xi} \cdot D + \frac{1}{2\Delta E^2} (\ddot{F} \cdot \dot{\xi} - \dot{F} \cdot \ddot{\xi}) + \xi \cdot C \cdot D = 0 \]

where \( \ddot{F} \cdot \xi = 2\Delta E^2 \). As \( D_j = \frac{1}{2\Delta E^2} \sum_k F_{jk} \xi_k = \lambda \xi_j - \lambda'_j \), which gives

\[ \frac{d}{dr} D \cdot \xi = \frac{\ddot{F} \cdot \dot{\xi} - \dot{F} \cdot \ddot{\xi}}{2\Delta E^2} + \xi \cdot C \cdot D = 0 \]

with \( \xi \cdot \dot{\xi} = 0, \lambda' \cdot \dot{\xi} = \lambda' \cdot \dot{u} = 0 \) and \( \xi \cdot C = 0 \) (see appendix C).

**Appendix C. The demonstration of \( C \cdot \xi = \xi \cdot C = 0 \)**

Here we demonstrate that \( C \cdot \xi = \xi \cdot C = 0 \) is universally valid with respect to spin algebra. In the case of \( H \in \mathcal{A} \) i.e. \( \xi = u \), it yields \( C \cdot u = u \cdot C = 0 \).

**C.1. One qubit**

Consider \( A_1, A_2 \) in a qubit and suppose that \( \{A_j\}_{j=1,\ldots,M} \) satisfy the spin algebra

\[ [A_n, A_j] = \sum_k \frac{1}{\sqrt{\text{Tr} I}} \epsilon_{njk} A_k, \]

and \( I \) is 2\( q \) dimensional unit matrix \((q \text{ is the number of qubits})\) and \( A_k = \frac{1}{\sqrt{\text{Tr} I}} \epsilon_{njk} \) for \( q = 1 \). Hence

\[ \sum_k C_{jk} A_k = i[H, A_j] = \sum_n i \epsilon_{jn}[A_n, A_j] = \sum_{n,k} \frac{1}{\sqrt{\text{Tr} I}} \epsilon_{njk} \xi_n A_k \]

which yields \( C_{jk} = \sum_n \frac{1}{\sqrt{\text{Tr} I}} \epsilon_{njk} \xi_n \). Thus \( \xi \cdot C = -C \cdot \xi = 0 \).

**C.2. Many qubits with and without entanglement**

We will prove that \( \xi \cdot C = C \cdot \xi = 0 \) remains valid. Below, we denote the unit matrix \( I_0 \) with \( \sigma_0 \) and extend our index to include 0.

**Lemma.** \( C_{jk} = \sum \Gamma_{ijk} \xi_n \), where \( \Gamma \) is an antisymmetric tensor.

**Proof.** First let us check some properties of Pauli matrices. With the commutation and anti-commutation relations \( \{\sigma_i, \sigma_j\} = 2\delta_{ij}I, i, j = 1, 2, 3 \), it is easy to check even if \( i, j = 0, 1, 2, 3 \)

\[ \sigma_i^{(\alpha)} \sigma_j^{(\beta)} = \sum_k (\delta^{(\alpha)}_{ijk} + i\epsilon^{(\alpha)}_{ijk}) \sigma_k^{(\beta)}, \]

where \( \sigma_0 = I_0 \) which is two-dimensional unit matrix and \( \alpha \) is the order index of qubits,

\[ \epsilon^{(\alpha)}_{ijk} = \begin{cases} 1, & ijk \in \{123, 231, 312\} \\ -1, & ijk \in \{321, 213, 132\}, \\ 0, & \text{otherwise} \end{cases} \]

and

\[ \delta^{(\alpha)}_{ijk} = \begin{cases} 1, & \text{one index is 0, the other two equal} \\ 0, & \text{otherwise} \end{cases} \]

which is totally symmetric with respect to any permutation of its subscripts. Now consider the commutator of \( N \)-fold entanglement \( [A_{\mu}, A_{\nu}] = \frac{1}{\sqrt{\text{Tr} I^{\mu\nu}}} \sum_{j=1}^{M} \Gamma_{\mu\nu\gamma}^{(j)} A_{(j)}^{\gamma} [A_{\mu}, A_{\nu}] \). Here the factor \( \frac{1}{\sqrt{\text{Tr} I^{\mu\nu}}} \) is introduced to guarantee that \( \text{Tr} A_j^2 = 1 \) and \( \{\mu_j, \nu_j, \gamma_j\}_{j=1,\ldots,N} = \{0, 1, 2, 3\} \). Without loss of generality,

\[ \text{Tr} I[A_{\mu}, A_{\nu}] = \prod_j \sigma_{\mu_j}^{(0)} \sigma_{\nu_j}^{(0)} - \prod_j \sigma_{\gamma_j}^{(0)} \sigma_{\nu_j}^{(0)} = \prod_j \sum_{\gamma_j} (\theta_{\mu_j\nu_j\gamma_j}^{(0)} + i\epsilon_{\mu_j\nu_j\gamma_j}^{(0)}) \sigma_{\gamma_j}^{(0)} - \prod_j \sum_{\gamma_j} (\theta_{\mu_j\nu_j\gamma_j}^{(0)} + i\epsilon_{\mu_j\nu_j\gamma_j}^{(0)}) \sigma_{\gamma_j}^{(0)}. \]
Define the polynomial coefficient of the kth power of $\epsilon$ as $c_k(\mu, \nu, \gamma)$, which satisfies
\[ \sum_k c_k p_k(\mu, \nu, \gamma) = \prod_j \left( \theta_{jj}^{(i)} + i \epsilon_{jj}^{(i)} \gamma_j \right) - \prod_j \left( \theta_{jj}^{(i)} - i \epsilon_{jj}^{(i)} \gamma_j \right), \]

where $p_k(\mu, \nu, \gamma)$ is the polynomial function of $\epsilon$ and $A_\gamma = \frac{1}{\sqrt{2\pi}} \prod_j c_{ij}^{(i)}$, $P_{\mu\nu\gamma} = \frac{1}{\sqrt{2\pi}} \sum_k c_k p_k(\mu, \nu, \gamma)$ is a pure imaginary number and holds the series of odd powers of $\epsilon$ (it is easy to check that $c_{2k} = 1 - (-1)^k \equiv 0, k \in \mathbb{N}$). Here we have utilized the symmetry of $\theta$ and the anti-symmetry of $\epsilon$.

Now commutate two of the indices $\mu, \nu, \gamma$ of $P$. Notice that $P$ is written as series of odd powers of $\epsilon$ and each pair of $\{\mu, \nu\}$ anti-commutes. Hence $P$ has the same anti-symmetry as $\epsilon$. Given the definition of $C$
\[ \sum_\gamma C_{\gamma\gamma} A_\gamma = i[H, A_\nu], \] (C7)
we have $C_{jk} = \sum_n iP_{njk} e_n$.

According to the lemma, $C \cdot \xi = \sum \sum \sum iP_{njk} \xi_n \xi_k = - \sum \sum \sum iP_{njk} \xi_n \xi_k = - C \cdot \xi$. Thus $C \cdot \xi = 0$.

Furthermore, $C$ is anti-symmetric in consistency with $P$. Hence $\xi \cdot C = \sum_j \xi_j C_{jk} = - \sum_j \xi_j C_{jk} = - C \cdot \xi = 0$.

Appendix D. The detailed derivation of equation (8),

Multiplying $\langle \psi | A_j$ on both sides of equation (4) results in
\[ \frac{i}{2 \Delta E} (\langle A_j | \dot{H} \rangle - \langle A_j | H \rangle) + i(\langle A_j | H \rangle - \langle A_j | \dot{H} \rangle) \frac{d}{dt} \frac{1}{2 \Delta E^2} - i \frac{d}{dt} \langle \psi | A_j | \phi \rangle + \langle \psi | [A_j, H] | \phi \rangle = 0. \] (D1)

The derivative of $\frac{1}{\Delta E}$ is
\[ \frac{d}{dt} \frac{1}{2 \Delta E} = - \frac{1}{\Delta E} \frac{1}{2 \Delta E} \frac{d}{dt} \Delta E^2. \] (D2)

Therefore, with equations (A4) and (A5) and using $\xi \cdot \dot{F} \cdot \xi = 0$, we have
\[ \frac{d}{dt} \Delta E^2 = \xi \cdot F \cdot \dot{\xi} = \dot{F} \cdot \xi, \] (D3)

where $\dot{F} = \xi \cdot F$. And the equation (D2) can be rewritten as
\[ \frac{d}{dt} \frac{1}{2 \Delta E} = - \frac{1}{2 \Delta E^2} \Delta E^2. \] (D4)

Substituting equation (D4) into equation (D1), we arrive at
\[ \frac{d}{dt} D_j = \frac{1}{2 \Delta E^2} \left( \sum_k F_{jk} \dot{\xi}_k - \frac{\dot{F} \cdot \xi}{\Delta E^2} \dot{\xi}_j \right) + \sum_k C_{jk} D_k, \] (D5)

where $C_{jk}$ is a real number and satisfies
\[ [H, A_j] = -i \sum_k C_{jk} A_k. \] (D6)

Appendix E. The demonstration of $\dot{F} = C \cdot F + F \cdot C^T$

According to the equation (A4):
\[ F_{jk} = \langle A_j A_k + A_k A_j \rangle - 2 \langle A_j \rangle \langle A_k \rangle, \] (E1)
we have
\[ \dot{F}_{jk} = i \langle HA_k A_j + HA_j A_k - A_j A_k H - A_k A_j H \rangle - 2i \langle HA_j - A_j H \rangle \langle A_k \rangle - 2i \langle A_j \rangle \langle HA_k - A_k H \rangle \]
\[ = i \langle [H, A_j] A_k + A_k [H, A_j] + A_j [H, A_k] + [H, A_k] A_j \rangle - 2i \langle [H, A_j] \rangle \langle A_k \rangle - 2i \langle A_j \rangle \langle [H, A_k] \rangle \]
irrelevant symmetry directions. The constraint to cope with this problem, our strategy is to totally ignore this eigen-direction since it corresponds to

The shooting method aims to implement the multidimensional Newton–Raphson method to locate zeros of \( N \) target functions with \( N \) target unknowns, which are obtained by integrating \( N \) differential equations in our examples.

For a general dynamical system described by the ordinary differential equation

\[ \dot{x} = v(x(t)), \]  

(F1)

where \( x \in \mathbb{R}^d, t \in \mathbb{R} \), the solution obtained by integrating equation (F1) is \( x(t) = f(t)(x) \). The corresponding Jacobian matrix is \( J(x, t) = \frac{\partial v_i(x)}{\partial x_j(t)} \), obtained by integrating

\[ \frac{dJ}{dt} = AJ, \quad A_{ij} = \frac{\partial v_i}{\partial x_j}, \quad \text{with} \quad J(x, 0) = I \]  

(F2)

which give the displacement \( \delta x(T) \) at time \( T \)

\[ \delta x(T) = J(x, T) \cdot \delta x(0) \]  

(F3)

in terms of the initial value \( \delta x(0) \). Define a discrepancy vector \( \Delta = x(T) - x_{\text{target}} \), which could be minimized to give the correction \( \Delta x_0 \) with the Newton descent

\[ J \cdot \Delta x_0 = -\Delta \]  

thus reaching a better approximation

\[ x_{0,\text{new}} = x_{0,\text{old}} + \Delta x_0. \]  

(F4)

Typically, the Jacobian matrix \( J \) is numerically evaluated by

\[ J_j \equiv \frac{X_j(x_{0,1}, \ldots, x_{0,j} + \Delta x_{0,j}, \ldots, T) - X_j(x_{0,1}, \ldots, x_{0,j}, \ldots, T)}{\Delta x_{0,j}}. \]  

(F5)

In the current case, the adjustable part is the free parameter \( \phi \) and the discrepancy is \( \psi(T) - \psi_{\text{target}} \).

Let’s slow down here and have a discussion on possible additional constraints and the treatment of the symmetries mentioned earlier. Firstly, based on equation (I1), \( \Re(\langle \delta \phi | \psi \rangle) = 0 \), which with the help of the symmetry transformation \( U_1 \) could always be satisfied by taking the difference \( \phi_{\text{new}} - i\psi \), where \( i\psi = |\psi\rangle\langle\psi|\phi_{\text{new}} \). The unitary evolution of \( \psi \) will produce a singularity for the Jacobian matrix \( J \). To cope with this problem, our strategy is to totally ignore this eigen-direction since it corresponds to irrelevant symmetry directions. The constraint \( \sum_{j=1}^{n+1} \epsilon_j^2 = \omega_2^2 \) could be guaranteed by the symmetry \( U_2 \) since \( \lambda_2 \) and thus \( b \) could be obtained by substituting \( \phi_{\text{new}} \) into equation (20) with \( j \leq n \) when starting a new iteration.

It is likely that the discrepancy may significantly fluctuate in the first few iterations. So it is important to properly choose the target hyperplane for the shooting on which the target state lies. The final state \( \psi(T) \) is adjusted to ‘hit’ the target state \( \psi_{\text{target}} \) by adjusting the initial position equation (F4) and the flight time \( T \).

Appendix G. The explanation of rotation matrix \( R(\phi, \theta, \Psi) \)

In this section, we’re going to elaborate on the rotation matrix \( R_{\Omega}(\theta) = R_{\gamma}^{-1}(\Psi)R_x(\theta)R_{\gamma}(\Psi) \) in the single qubit case. According to section 5.1, the \( \Omega \) lies in the \( z \) direction and perpendicular to the \( \omega_{\text{eff}} \), and \( R_{\Omega}(\theta) \) depicts the rotation of \( \psi(t) \) arounds a fixed axis with \( \Omega' = \omega_{\text{eff}} - \Omega \). Obviously, the \( \omega_{\text{eff}} \) lies on the \( x-y \) plane, and the direction of \( \omega_{\text{eff}} \) is taken as the \( -y \) axis for simplicity. Then the rotation \( R_{\Omega}(\theta) \) can be depicted as follow, first, rotating \( \psi \) around \( x \)-axis by \( \Psi \) to make \( \Omega' \) and \( y \)-axis coincide \( (R_{\gamma}(\Psi)) \), then, rotating \( \psi \) around \( y \)-axis by \( \theta(R_{\gamma}(\Psi)) \), finally, rotating \( \psi \) around \( x \)-axis back by \( \Psi \) \( (R_{\gamma}^{-1}(\Psi)) \), where \( \Psi \) is the angle between \( \Omega' \) and \( \omega_{\text{eff}} \) and \( \tan(\Psi) = \frac{\Omega'}{\omega_{\text{eff}}} \).
Appendix H. The geometric properties of spin vector evolution

Lemma. $D' \cdot \langle \sigma \rangle = 0$ for single qubit.

Proof. From equation (11) in the main text, we have $\text{Re}(\langle \phi' | \psi \rangle) = \text{Re}(\langle \phi | \psi \rangle) = 0$.

Considering the projection property of Pauli matrices

$$\sigma \cdot \hat{p} \equiv 2|\psi\rangle\langle\psi| - I,$$

where $|\psi\rangle$ is a normalized eigenvector of $\sigma$ in the direction of $\hat{p} = \langle \sigma \rangle$, and $I$ is the unit matrix, then we have that

$$D' \cdot \langle \sigma \rangle = 2\text{Re}(\langle \phi' | \sigma | \psi \rangle) \cdot \langle \sigma \rangle$$

$$= 2\text{Re}(\langle \phi' | \sigma \cdot \hat{p} | \psi \rangle)$$

$$= 2\text{Re}(2\langle \phi' | \psi \rangle \langle \psi | \psi \rangle - \langle \phi' | \psi \rangle)$$

$$= 0. \quad (H1)$$

Similarly, we can easily verify that

$$D \cdot \langle \sigma \rangle = 2\text{Re}(\langle \phi | \sigma | \psi \rangle) \cdot \langle \sigma \rangle = 0. \quad (H2)$$

Appendix I. A forbidden component of $\phi$

Based on equations (5) and (20) and the fact that $\text{Tr} H = 0$ (i.e. $\xi_0 = 0$), we immediately obtain

$$2\text{Re}(\langle \phi | \psi \rangle) = D_0 = \sum_j \frac{F_{0j}}{2\Delta} \xi_j - \lambda \xi_0 \equiv 0, \quad (I1)$$

$$\text{Re}(\langle \phi' | \psi \rangle) = D'_0 = -\lambda \xi_0 \equiv 0,$$

where $F_{0j} \equiv 0$ and $A_0 \equiv \sigma_0$, which is the unit matrix. Hence the component of $\phi$ or $\phi'$, being parallel to $\psi$, vanishes. Notice that $u$, in the absence of uncontrollable components, is parallel to $\text{Re}(\langle \phi' | \sigma | \psi \rangle)$ according to equation (20). So $u \cdot \langle \sigma \rangle \propto \text{Re}(\langle \phi' | \sigma | \psi \rangle) \cdot \langle \sigma \rangle = 0$ (proved in appendix I) for every qubit.

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