Research Article Vol. 15, No. 3 / 1 Mar 2025 / Optical Materials Express 578
Optical Materials EXPRESS

Optimizing state transfer in a three-qubit array via quantum brachistochrone method [Invited]

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Abstract: The quantum brachistochrone method has recently emerged as a technique that allows one to implement the desired unitary evolution operator in a physical system within a minimal time. Here, we apply this approach to the problem of time-optimal quantum state transfer in an array of three qubits with time-varying nearest-neighbor couplings and analytically derive the fastest protocol.

1. Introduction

The development of quantum technologies requires preparing and processing quantum states within the minimal possible time while maintaining reasonably high fidelity. The elementary building blocks of such systems are qubits – two-level systems – which can be implemented in a variety of material platforms ranging from superconducting circuits and cold atoms to trapped ions, quantum dots and photonic systems [1]. While decoherence and dissipation inevitably degrade the performance of quantum systems, recent advances suggest the possibility of correcting occurring errors [2] and achieving long coherence times up to 1 ms in the superconducting architecture [3], allowing for multiple operations with qubits.

On the other hand, the speed of the quantum state evolution is restricted by the quantum speed limit [4,5], which is intrinsically connected to the time-energy uncertainty relation. This motivates interest in *quantum optimal control theory* [6], which aims to tailor the time-varying Hamiltonian of the system to achieve the desired quantum state within the minimal possible time, given the constraints on the Hamiltonian.

The most straightforward approach to this problem is the adiabatic evolution of the Hamiltonian, which transforms the initial set of eigenstates into the desired one. In particular, adiabatic evolution allows the transfer of a particle in the array via the so-called Thouless pump [7]. However, this requires an extremely slow variation of the Hamiltonian, which is impractical.

This limitation can be overcome using advanced methods such as conter-adiabatic driving, also known as shortcuts to adiabaticity [8–10], and the Pontryagin maximum principle [6]. These techniques allow one to approach the quantum speed limit through numerical optimization. While being powerful numerical tools, these techniques are restricted by the chosen form of the control and do not provide straightforward access to analytical solutions.

A recently suggested alternative is the quantum brachistochrone method [11], which recasts a bi-parametric search of the minimum evolution time along with the maximum fidelity as a variational problem. Originally formulated by Carlini *et al* [11], the variational problem to find the time-optional evolution of quantum states and the Hamiltonian for given initial and final conditions has been further generalized to the operator form to determine the time-optimal realization of a target unitary operation [12]. Using this technique, one can derive the control protocol for the systems with the Hermitian Hamiltonian, converting the optimization task into a boundary value problem. In some cases, this can be solved analytically, providing insights into the optimal control of the simplest quantum systems.

#547936 https://doi.org/10.1364/OME.547936
Journal © 2025 Received 13 Nov 2024; revised 27 Jan 2025; accepted 12 Feb 2025; published 26 Feb 2025

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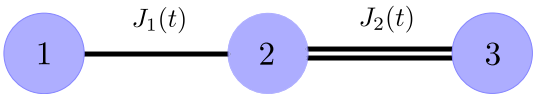

Fig. 1. Sketch of a three-qubit array with the controllable and time-varying nearest-neighbor couplings $J_1(t)$, $J_2(t)$.

In addition, the problem of finding a time-optimal solution can be presented as a quantum geodesic search [13,14] providing a geometric interpretation of the quantum brachistochrone technique. While this approach has proven to be successful in several specific types of problems [15–20], obtaining such solutions remains challenging, especially in large-scale systems with multiple degrees of freedom and many control parameters.

In this Article, we illustrate the quantum brachistochrone technique with a simple but instructive example. Specifically, we study the time-optimal transfer of a single-particle excitation in an array of three nearest-neighbor coupled qubits, shown schematically in Fig. 1. We assume that the excitation is initially launched in the leftmost qubit of the array. By varying the couplings $J_{1,2}$ in time such that $J_1^2 + J_2^2 = J_0^2 = \text{const}$, we aim to achieve the fastest possible transfer of the excitation to the rightmost qubit. Technically, time-varying couplings in superconducting architecture can be implemented by inserting auxiliary qubits with controlled eigenfrequency [21]. Other prospective platforms also allow real-time coupling control. For simplicity, we assume that the eigenfrequencies of the qubits are fixed. While the quantum brachistochrone method can be generalized to the dissipative case [22,23], here we discuss the Hermitian situation, which is more transparent from a physical perspective.

Interestingly, the problem under study is analogous to the time-optimal population transfer in a three-level system, where the direct transition between the first and third levels is prohibited. Although the solution to this problem was proposed long ago [24], its optimality was proven only much later using a different technique [25].

2. Summary of quantum brachistochrone method

To derive the time-optimal evolution of a quantum system with zero-trace $N \times N$ Hermitian Hamiltonian, we introduce a set of $N \times N$ traceless Hermitian matrices $\hat{A}_i$ and $\hat{B}_j$, spanning the subspaces $\mathbb{A}$ and $\mathbb{B}$ and normalized by the relations $\mathrm{Tr}(\hat{A}_i\hat{A}_j) = \delta_{ij}, \mathrm{Tr}(\hat{B}_i\hat{B}_j) = \delta_{ij}, \mathrm{Tr}(\hat{A}_i\hat{B}_j) = 0$. We assume that the Hamiltonian can only contain the matrices from $\mathbb{A}$ subspace, while the $\hat{B}_j$ matrices are unavailable due to the physical constraints on the system:

$$\hat{H} = \sum_i \alpha_i \hat{A}_i \,. \tag{1}$$

Also, we assume that the norm of the Hamiltonian is bounded $||\hat{H}(t)|| = \sqrt{\mathrm{Tr}\hat{H}^2(t)} \le \Delta E$. Our goal is to find such a temporal variation of the Hamiltonian $\hat{H}(t)$ that the initial state $|\psi(0)\rangle$ is transferred to the final state $|\psi(\tau)\rangle = \hat{U}(\tau)|\psi(0)\rangle$ within the minimal possible time τ, where $\hat{U}(t)$ is the unitary evolution operator satisfying Shrödinger equation $i\partial\hat{U}/\partial t = \hat{H}\hat{U}$. If the evolution operator is known, the Hamiltonian can be readily expressed as

$$\hat{H} = i\frac{\partial\hat{U}}{\partial t}\hat{U}^\dagger \,. \tag{2}$$

Obviously, the transfer time τ is inversely proportional to the bound ΔE, while their product $\Delta E\,\tau$ is a dimensionless coefficient dependent on the chosen $\hat{H}(t)$ protocol. Therefore, the original problem of finding the minimal possible transfer time τ for a fixed constraint ΔE is equivalent to

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finding the minimal possible ΔE for the prescribed transfer time $\tau = 1$. This motivates the choice of the functional [26]

$$S = \int_0^\tau ||\hat{H}(t)||\, dt + \int_0^\tau \sum_k \lambda_k \mathrm{Tr}\left(\hat{B}_k \hat{H}\right) dt\,, \tag{3}$$

where the first term aims to minimize the norm of the Hamiltonian (i.e. ΔE), while the second set of terms constrains the form of the Hamiltonian, excluding the contribution from $\hat{B}_k$ matrices. The coefficients λ_k are time-dependent Lagrange multipliers.

Making use of Eq. (2), we present the target functional S in the form

$$S = S_1 + S_2 = \int_0^\tau L_T^0\, dt + i \int_0^\tau \sum_k \lambda_k \mathrm{Tr}\left(\hat{B}_k \frac{\partial \hat{U}(t)}{\partial t} \hat{U}^\dagger(t)\right) dt \tag{4}$$

with $L_T^0 = ||\hat{H}(t)|| = \sqrt{\mathrm{Tr}\left(\partial \hat{U}^\dagger/\partial t \cdot \partial \hat{U}/\partial t\right)}$. Thus, the target functional only depends on the evolution operator $\hat{U}(t)$ and its time derivative.

Varying the functional S with respect to the evolution operator, we recover

$$\begin{aligned} \delta S_1 =& \frac{1}{2} \int_0^\tau \frac{1}{L_T^0} \mathrm{Tr}\left(\frac{\partial \hat{U}^\dagger}{\partial t} \frac{\partial \delta \hat{U}}{\partial t} + \frac{\partial \delta \hat{U}^\dagger}{\partial t} \frac{\partial \hat{U}}{\partial t}\right) dt \\ =& \frac{1}{L_T^0} \mathrm{Tr}\left(\frac{\partial \hat{U}^\dagger}{\partial t} \delta \hat{U}\right)\Big|_0^\tau + \frac{1}{L_T^0} \int_0^\tau \mathrm{Tr}\left(\left(\hat{U}^\dagger \frac{\partial^2 \hat{U}}{\partial t^2} \hat{U}^\dagger + \hat{U}^\dagger \frac{\partial \hat{U}}{\partial t} \frac{\partial \hat{U}^\dagger}{\partial t}\right) \delta \hat{U}\right) dt\,, \end{aligned} \tag{5}$$

where we used the identity $\delta \hat{U}^\dagger = -\hat{U}^\dagger \delta \hat{U} \hat{U}^\dagger$. Similarly, we compute the variation of S_2:

$$\begin{aligned} \delta S_2 =& i\, \mathrm{Tr} \sum_k (\hat{U}^\dagger \hat{B}_k \lambda_k \delta \hat{U})\Big|_0^\tau \\ & - i \int_0^\tau \mathrm{Tr}\left(\sum_k \left(\lambda_k \hat{U}^\dagger \hat{B}_k \frac{\partial \hat{U}}{\partial t} \hat{U}^\dagger + \hat{U}^\dagger \hat{B}_k \frac{\partial \lambda_k}{\partial t} + \frac{\partial \hat{U}^\dagger}{\partial t} \hat{B}_k \lambda_k\right) \delta \hat{U}\right) dt\,, \end{aligned} \tag{6}$$

where we used full derivative $\frac{\partial}{\partial t}(\lambda_k \delta \hat{U} \hat{U}^\dagger) = \frac{\partial \lambda_k}{\partial t} \delta \hat{U} \hat{U}^\dagger + \lambda_k \frac{\partial \delta \hat{U}}{\partial t} \hat{U}^\dagger + \lambda_k \delta \hat{U} \frac{\partial \hat{U}^\dagger}{\partial t}$.

Since the initial and final states of the quantum system are fixed, $\delta \hat{U}(0) = \delta \hat{U}(1) = 0$. Moreover, $L_T^0 = \Delta E$ along the trajectory, and thus we can rescale $L_T^0 \lambda_k \to \lambda_k$. Requiring the extremum of the functional $\delta S = \delta S_1 + \delta S_2 = 0$, we obtain *quantum brachistochrone equation* [12]:

$$\frac{d\hat{F}}{dt} + i\left[\hat{H}, \hat{F}\right] = 0\,, \tag{7}$$

where $\hat{F} = \hat{H} + \sum_k \lambda_k \hat{B}_k$. Projecting this equation onto the matrices $\hat{A}_m$ and $\hat{B}_n$ and taking into account their orthogonality, we recover the system

$$\frac{d\alpha_m}{dt} = i \sum_k \lambda_k \mathrm{Tr}\left([\hat{A}_m, \hat{B}_k]\hat{H}\right), \tag{8}$$

$$\frac{d\lambda_n}{dt} = i \sum_k \lambda_k \mathrm{Tr}\left([\hat{B}_n, \hat{B}_k]\hat{H}\right). \tag{9}$$

Equations (8) define the evolution of the control parameters α_m in the optimal scenario, while the complementary Eqs. (9) determine the change of the Lagrange multipliers λ_n in time. Notably,

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the initial conditions for λ_n are unknown, which makes quantum brachistochrone equations hard to solve. Furthermore, the existence and uniqueness of the solution is generally not guaranteed.

Note also that in the absence of the constraints on the Hamiltonian (i.e. when $\hat{B}$ matrices are absent), the time-optimal strategy is straightforward. Equation (7) suggests that the Hamiltonian should be time-independent and should directly couple the initial and final states of the quantum system.

3. Derivation of the time-optimal evolution

Next, we apply the quantum brachistochrone approach to the specific system – an array of 3 qubits depicted in Fig. 1. Overall, the dimensionality of the Hilbert space for such a system is $2^3 = 8$. However, since the Hamiltonian conserves the number of excitations and we focus on a single-particle sector, the dynamics of interest occurs in the 3-dimensional subspace spanned by the three single-particle basis states. In turn, the Hamiltonian is parametrized by the two variables, which are the nearest-neighbor couplings J_1 and J_2.

In these conventions, $\hat{A}$ and $\hat{B}$ are expressed in terms of the Gell-Mann matrices and read

$$\hat{A}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{A}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{10}$$

$$\hat{B}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{B}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \hat{B}_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \tag{11}$$

$$\hat{B}_4 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \hat{B}_5 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{B}_6 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \tag{12}$$

while the Hamiltonian of the system is presented as:

$$\hat{H} = \sum_{m=1}^{2} \alpha_m \hat{A}_m = \begin{pmatrix} 0 & J_1 & 0 \\ J_1 & 0 & J_2 \\ 0 & J_2 & 0 \end{pmatrix} \tag{13}$$

with $J_1 = \alpha_1/\sqrt{2}, J_2 = \alpha_2/\sqrt{2}$. Starting from the general brachistochrone Eqs. (8)–(9), we derive the control equations for our case:

$$\begin{cases} \frac{dJ_1}{dt} = -\lambda_3 J_2(t)/\sqrt{2}, \\ \frac{dJ_2}{dt} = \lambda_3 J_1(t)/\sqrt{2}, \\ \frac{d\lambda_3}{dt} = 0\,. \end{cases} \tag{14}$$

Interestingly, the equations for J_1, J_2 and λ_3 decouple from the rest of the system, which strongly simplifies the solution. Taking into account the constraint $J_1^2 + J_2^2 = J_0^2$, we derive an

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analytical solution:

$$\lambda_3 = \Omega\sqrt{2} = \text{const}\,, \tag{15}$$

$$J_1(t) = J_0 \cos(\Omega t + \varphi)\,, \tag{16}$$

$$J_2(t) = J_0 \sin(\Omega t + \varphi)\,, \tag{17}$$

where φ is a constant phase that depends on the initial conditions. Using the obtained couplings and solving the Shrödinger equation analytically, we compute the components of the wave function $|\psi\rangle = (\psi_1, \psi_2, \psi_3)^T$:

$$\psi_1(t) = -\frac{iJ_2}{\Omega}A + \frac{\omega J_1 + iJ_2\Omega}{J_0^2}B_+e^{-i\omega t} - \frac{\omega J_1 - iJ_2\Omega}{J_0^2}B_-e^{i\omega t}, \tag{18}$$

$$\psi_2(t) = A + B_+e^{-i\omega t} + B_-e^{i\omega t}, \tag{19}$$

$$\psi_3(t) = \frac{iJ_1}{\Omega}A + \frac{\omega J_2 - iJ_1\Omega}{J_0^2}B_+e^{-i\omega t} - \frac{\omega J_2 + iJ_1\Omega}{J_0^2}B_-e^{i\omega t}, \tag{20}$$

where $J_{1,2}$ are given by Eqs. (16),(17) above and $\omega = \sqrt{\Omega^2 + J_0^2}$. Unknown integration constants $A, B_+, B_-, \Omega, \varphi$ and the transfer time τ are determined from the initial and boundary conditions.

Due to the choice of the initial and target state, we have the set of conditions for the wave function:

$$\psi_1(0) = 1\,,\ \psi_2(0) = 0\,,\ \psi_3(0) = 0\,, \tag{21}$$

$$\psi_1(\tau) = 0\,,\ \psi_2(\tau) = 0\,, \tag{22}$$

while the phase of $\psi_3(\tau)$ is unknown. However, these five requirements are insufficient to determine six unknowns above. Therefore, we additionally request that

$$J_2(0) = 0\,. \tag{23}$$

Physically, this requirement is easy to understand. Since the initial excitation is localized in the first qubit, only the first coupling $J_1(0)$ should be maximized, and hence $J_2(0)$ should be set to zero.

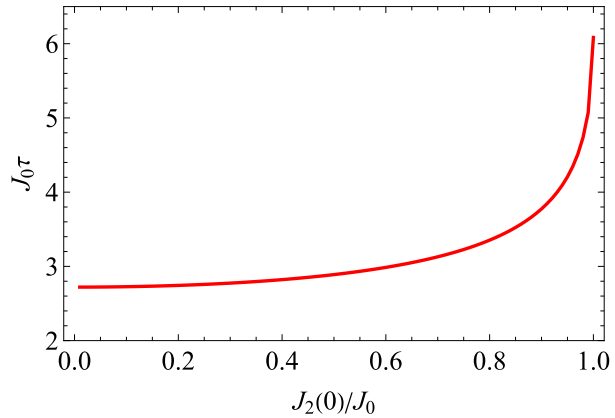

Fig. 2. Calculated transfer time of the excitation from the leftmost to the rightmost qubit versus the initial value $J_2(0)$ of the coupling constant. The minimal time is achieved when $J_2(0) = 0$.

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Equation (23) immediately yields $\varphi = 0$. Next, we analyze Eqs. (21) and recover $A = 0$, $B_+ = -B_- = J_0/(2\omega)$. Then we turn to Eqs. (22), which yield the requirements $\sin\omega\tau = 0$ and $\cos\Omega\tau = 0$, leading to $\omega = 2\Omega = \pi/\tau$. We thus recover $\Omega = \frac{J_0}{\sqrt{3}}$ and the transfer time

$$\tau = \frac{\sqrt{3}\pi}{2J_0} \approx 2.721/J_0\,. \tag{24}$$

This provides the fastest possible transfer protocol given the nearest-neighbor couplings and the constraint on the sum of their squares.

The dependence on the initial condition for J_2 can be further explored numerically by computing the transfer time for the same harmonic switching of the couplings, Eq. (16),(17), but with the different value of $J_2(0)$, sweeping the range from 0 to J_0. Interestingly, perfect transfer of the excitation occurs for any $J_2(0)$. However, the transfer time differs, as illustrated in Fig. 2. In particular, we observe that the minimal possible time is achieved when $J_2(0) = 0$, consistent with our reasoning above. Note that our initial condition for the coupling aligns with the initial and

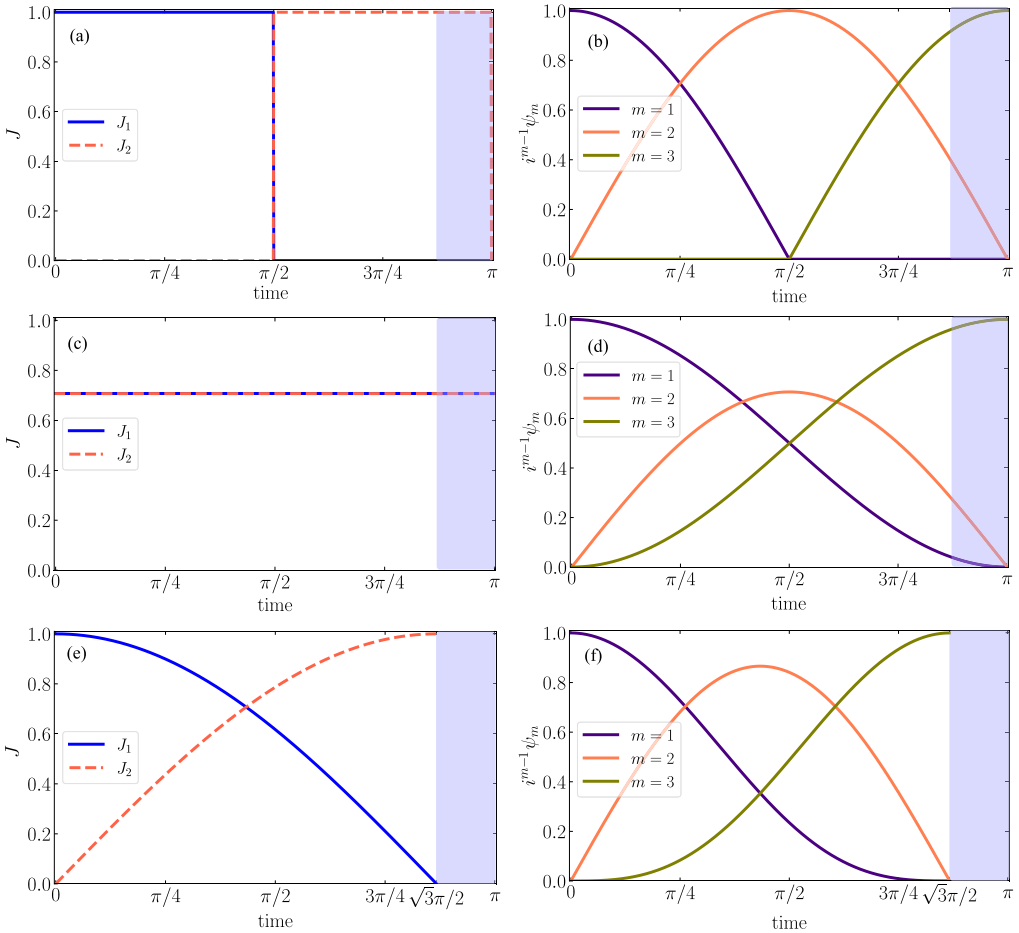

Fig. 3. Couplings J_1 and J_2 for the (a) stepwise switching, (c) perfect transfer, (e) time-optimal transport and the calculated wave functions $i^{m-1}\psi_m$ (b,d,f) for the respective scenarios. Transfer time in the time-optimal case is 13% less than in the two other examples. Horizontal axis shows the dimensionless values of $J_0\,t$.

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boundary conditions derived in quantum brachistochrone formulation with a movable endpoint [27].

To complete our analysis, we compare the derived protocol with two alternative strategies, also providing maximal fidelity. The first approach is a stepwise switching of the couplings [Fig. 3(a)]. In this case, $J_1(t) = J_0$ is switched on for some time until the excitation moves from the first qubit to the second one. Then, this coupling is turned off, and coupling J_2 is switched on instead. Straightforward analytical and numerical [28] calculation shows that this strategy indeed provides maximal fidelity of the transfer [Fig. 3(b)]. However, the timing in this case $\tau_{st} = \pi/J_0 \approx 3.142/J_0$ is non-optimal.

Another strategy, known as perfect transfer [29], suggests time-independent couplings, both equal to $J_0/\sqrt{2}$ [Fig. 3(c)]. In this case, the particle is perfectly transferred from the first to the third site [Fig. 3(d)]. However, the timing is also non-optimal $\tau_{pt} = \pi/J_0 \approx 3.142/J_0$.

These results should be compared with the calculated optimal control Eqs. (16)–(17), which assumes the change of the couplings according to cosine and sine functions, as shown in Fig. 3(e). Although the wave function's evolution shown in Fig. 3(f) strongly resembles the two previous scenarios, the transfer time is reduced by 13%.

In case of superconducting qubits, the couplings can realistically vary in the range from 1 to 100 MHz [3], yielding the characteristic transfer times in the range from 0.01 μs to 1 μs, shorter than the characteristic relaxation times. This justifies the Hermitian treatment of the problem.

4. Discussion and conclusions

In summary, the quantum brachistochrone method is a powerful tool that provides analytical insights into time-optimal control of relatively simple quantum systems. It offers an elegant solution to the two-factor optimization problems, such as finding the strategies that ensure both maximal fidelity of the transfer and the minimal transfer time.

However, optimal control of large quantum systems still poses a significant challenge, as the number of quantum brachistochrone equations grows rapidly with the system size, requiring extensive computations. Given current advances in the engineering of multi-qubit quantum processors, this provides an interesting topic for further research.

Funding. Russian Science Foundation (24-72-10069); State assignment within the framework of the national project "Science and Universities" (FSER-2025–0012); Foundation for the Advancement of Theoretical Physics and Mathematics "Basis".

Acknowledgments. Theoretical models were supported by the state assignment No. FSER-2025–0012 within the framework of the national project "Science and Universities". Numerical simulations were supported by the Russian Science Foundation, grant No. 24-72-10069. M.A.G. acknowledges partial support by the Foundation for the Advancement of Theoretical Physics and Mathematics "Basis".

Disclosures. The authors declare no conflicts of interest.

Data availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

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