Near-time-optimal control for quantum systems

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Near Time-Optimal Control for Quantum Systems

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For a quantum system controlled by an external field, time-optimal control is referred to as the shortest time duration control that can still permit maximizing an objective function J, which is especially a desirable goal for engineering quantum dynamics against decoherence effects. However, since rigorously finding a time-optimal control is usually very difficult, and in many circumstances the control is only required to be sufficiently short and precise, one can design algorithms seeking such suboptimal control solutions for much reduced computational effort. In this paper, we propose an iterative algorithm for finding near time-optimal control in a high level-set (i.e., the set of controls that achieves the same value of J) that can be arbitrarily close to the global optima. The algorithm proceeds seeking to decrease the time duration T with the value of J remains invariant, until J leaves level-set value; the deviation of J due to numerical errors is corrected by gradient climbing that brings the search back to the level-set J value. Since the level-set is very close to the maximum value of J, the resulting control solution is nearly time-optimal with manageable precision. Numerical examples demonstrate the effectiveness and general applicability of the algorithm.

PACS numbers:

I. INTRODUCTION

When quantum systems are complex, or when they are exposed to unwanted environments, control theory provides powerful tools for improving the performance of quantum operations [1]. Over the past few decades, considerable successes have been achieved in the control of atomic, molecular, optical, and solid-state quantum systems [2–6]. Since quantum operations are only effective within the coherence time, the control needs to either prolong the coherent dynamics via dynamical decoupling [7, 8] or feedback [9] strategies, or be performed as rapid as possible [10–12]; the latter circumstance poses the quantum time-optimal control problem. Based on Pontryagin's Maximum Principle [13–16], geometric analysis shows that the minimal time is mainly determined by the evolution speed of the drift Hamiltonian when the controls are unbounded. Such time-optimal gate control solutions have been found for 1-qubit, 2-qubit, and some special 3-qubit systems [17, 18]. Cases with bounded controls are far more complex, and only for several special cases have analytical [19–27] or partially analytical [28, 29] solutions been found.

Under most circumstances, quantum time-optimal control problems can be numerically solved by minimizing the time duration while maintaining the objective function J at the maximum value (e.g., gate fidelity). To first maximize the objective function J with fixed T, the genetic algorithm [30], the monotonic iterative algorithm [31], the Krotov algorithm [32], the gradient algorithm [18], and the hybrid algorithm [33] are introduced for the search of optimal controls. To further shorten the control time, a natural approach is to gradually decrease T and apply the algorithm maximises J for each fixed T until the desired control precision can no longer be attained [18, 34]. One can also take the time duration as a control variable and design 'free-time and fixed-endpoint' algorithms, by which the time duration and the control error can be decreased [35–37] in presence of trade-offs with other penalty functions (e.g., field fluence).

Although the optimization of J itself with fixed T is generally very efficient [38–41], the search for a precise time-optimal control is much more expensive

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due to its bi-objective nature and potential existence of traps at reduced value of J [33, 34]. However, as will be shown in this paper, the search for minimum-time solutions is relatively easy if J is allowed to be slightly lower than its maximal value. Such a control is nearly time-optimal because both J and the corresponding optimal time are very close to their ideal optimal values. From an engineering point of view, this solution is likely acceptable because control precision is usually limited by the tomography and pulse shaping techniques (e.g., the fidelity of tomography experiments is seldom above 99%), and it makes no substantial difference when the control time is slightly prolonged. Therefore, it is worth designing algorithms for finding such control protocols that can be computationally much cheaper.

This paper will present a two-stage level-set based algorithm (LS Algorithm) seeking near time-optimal control solutions. The algorithm will first climb to a level-set, which is referred to as the set of control functions corresponding to a fixed value of J, then find a highly efficient path toward minimum-time control in this level-set until a satisfactory solution is found. The paper is organized as follows. In Sec. II, we define the time-optimal and near time-optimal control problems for quantum systems. In Sec. III, we present the strategy and details of the algorithm, which is then illustrated by examples in Sec. IV. Finally, we draw conclusions in Sec. V.

II. TIME-OPTIMAL CONTROL PROBLEMS

Consider an N-dimensional quantum control system whose unitary propagator $U(t)$ obeys the following Schrödinger equation

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}U(t) &= -i\left[H_0 + \sum_{k=1}^{m} u_k(t)H_k\right]U(t), \\ U(0) &= I,\ t \in [0,T], \end{aligned} \tag{1}$$

where the free Hamiltonian H_0 and the control Hamiltonians H_k's are Hermitian operators in the underlying Hilbert space (the common constant $\hbar$ has been absorbed into the Hamiltonians), and the system is manipulated by the multiple control functions $u_1(t), u_2(t), \cdots, u_m(t)$ that act during the time interval $t \in [0,T]$.

Time-optimal control problems are always associated with an objective J as a function of the controls. For example, in quantum information processing, we have

$$J_1 \ = \ N^{-1}Re\mathrm{Tr}\left[W^{\dagger}U(T)\right], \tag{2}$$

where $Re(\cdot)$ denotes the real part of a complex number, for implementing a target unitary evolution W at time T; or

$$J_2 \ = \ \mathrm{Tr}[U(T)\rho_0 U^{\dagger}(T)O] \tag{3}$$

for maximizing the expectation value of the quantum observable O, where ρ_0 is the initial density matrix.

In numerical simulations, we discretize the whole time interval $[0,T]$ into M steps at points

$$t_j = T\cdot\frac{j}{M},\ j = 1,\cdots,M,$$

and take the values of $u_{kj} \triangleq u_k(t_j)$ at these time instances as the control variables:

$$\mathbf{u} \triangleq [u_{11},\cdots,u_{1M},\cdots,u_{m1},\cdots,u_{mM}]. \tag{4}$$

Considering T as an additional control variable, the objective J is a function of the $(mM+1)$-dimensional vector $\mathbf{x} = [T,\mathbf{u}]$.

For convenience, we denote the set of control vectors

$$\mathcal{L}(J = J_0) = \{\mathbf{x} :\ J(\mathbf{x}) = J_0,\ T \geq 0\}$$

that achieve the same value of J, and term it as the level-set at $J = J_0$. Then, a control vector $\mathbf{x}$ is said to be time-optimal if it is in the highest level-set $\mathcal{L}(J = J_{\max})$, where $J_{\max}$ is the maximal value of J, and its corresponding T is minimal among all control vectors in $\mathcal{L}(J = J_{\max})$; a control vector $\mathbf{x}$ is near time-optimal if it belongs to a slightly lower level-set $\mathcal{L}(J = J_H)$, where $J_H \lesssim J_{\max}$, and its corresponding T is minimal among all control vectors in $\mathcal{L}(J = J_H)$.

III. THE ALGORITHM FOR SEARCHING NEAR TIME-OPTIMAL CONTROLS

In this section, we present the two-stage iterative algorithm for seeking a near time-optimal control vector.

A. Basic concepts

Since the objective function J depends on both T and $\mathbf{u}$, one could follow the gradient $\mathrm{d}J/\mathrm{d}\mathbf{x}$ to maximize J, during which T and $\mathbf{u}$ are simultaneously updated. However, there is no guarantee that T will always decrease in this process (i.e., $\partial J/\partial T < 0$); even if T can be decreased, the search may be trapped at a non-time-optimal solution (i.e., especially in the regime when near minimal value of T becomes a limiting resource), or the search may cease at a negative value of T that is physically unacceptable.

To reconcile the desires of increasing J and decreasing T, one can start from some sufficiently large T and look for the solution that maximizes J, then design an algorithm to only decrease T without lowering J. Due to the vanishing of gradient vector, full realization of this procedure requires that the Hessian of J be calculated at the achieved maximum value, which can be computationally expensive. However, the search for a near time-optimal control in a slightly lower level-set can be much more efficient because one can make use of the gradient vector that is still dominant. In this regard, we propose the following two-stage iteration strategy:

Stage 1 Fix T and use the gradient vector $\mathrm{d}J/\mathrm{d}\mathbf{u}$ to increase J with an arbitrary gradient-based algorithm (possibly with constrains on the control field), until J reaches a prescribed high value $J = J_H$.

Stage 2 Choose a direction $\Delta\mathbf{x}$ to update $\mathbf{x}$, along which T decreases most rapidly in the level-set $\mathcal{L}(J = J_H)$. Considering the inevitable numerical errors in executing the algorithm, we return to **Stage 1** to bring the search back to the level-set $\mathcal{L}(J = J_H)$ when J drops to a prescribed lower bound $J = J_L$.

As schematically illustrated in Fig. 1, we keep shortening the time duration T by iteratively repeating the above two-stage processes. The procedure continues until the objective J can no longer be maintained at $J = J_H$. Then the resulting T is the minimal time required for reaching the level-set $\mathcal{L}(J = J_H)$, and the corresponding $\mathbf{u}$ is called a near time-optimal control vector. If one wishes to find the control in a very high level-set, the Hessian may need to be taken into account, whose null space can be used to refine $\mathbf{x}$ further; the present paper does not take this last step.

Note that since the gradient-based algorithm is local, there is no guarantee that searches from any initial guesses will lead to the desired near time-optimal solutions (i.e., shrinking T may significantly constrain the search when $\mathbf{x}$ enters a regime where the action of the drift Hamiltonian is encroached). Nevertheless, as shown later in examples, near time-optimal solutions can usually be found. Even if a less than best $T_{\min}$ is obtained, the resulting control solution is still useful in practice since it can effectively reduce the time for control.

B. Optimal choice of $\triangle\mathbf{x}$

Suppose that the current value of the control vector is $\mathbf{x} = \mathbf{c} \in \mathcal{L}(J = J_H)$, and we look for the direction along which T decreases most rapidly and $J = J_H$ remains invariant. Let $\nabla J(\mathbf{c})$ be the gradient vector of J with respect to $\mathbf{x}$ at $\mathbf{c}$, whose explicit expressions are given in Appendix A. To keep the search in the level-set $\mathcal{L}(J = J_H)$, the algorithm should iterate along a direction $\triangle\mathbf{x}$ that is orthogonal to $\nabla J(\mathbf{c})$. The first-order Taylor expansion in a small neighborhood of $\mathbf{c}$ gives

$$J(\mathbf{c} + \triangle\mathbf{x}) \approx J(\mathbf{c}) + (\nabla J(\mathbf{c}))^{\intercal} \triangle\mathbf{x}. \tag{5}$$

Let $\mathbb{S}$ be must the mM-dimensional hyperplane that is orthogonal to $\nabla J(\mathbf{c})$ and denote by

$$\mathrm{P} = \mathrm{I} - (\nabla J(\mathbf{c}))(\nabla J(\mathbf{c}))^{\intercal} / \| \nabla J(\mathbf{c} \|^2 \tag{6}$$

the projector onto $\mathbb{S}$. Then, $\triangle\mathbf{x}$ can be written as

$$\triangle\mathbf{x} = \mathrm{P}\mathbf{k}, \tag{7}$$

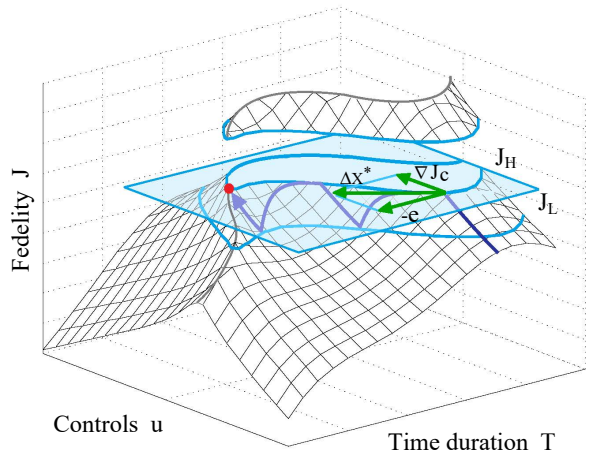


FIG. 1: (Color online) (a) Schematic of the proposed algorithm. The search is initially guided in **Stage 1** by a standard gradient algorithm with a fixed T to reach the level-set $\mathcal{L}(J = J_H)$. Then, T is changed in **Stage 2** along an optimal direction aiming to decrease T as fast as possible while staying in the level-set $\mathcal{L}(J \approx J_H)$. When J decreases to the lower limit J_L due to numerical errors, the standard gradient algorithm is restarted to bring the search back to $\mathcal{L}(J = J_H)$.

where $\mathbf{k}$ is an arbitrary vector to be determined below.

Since the first entry of $\triangle\mathbf{x}$ represents the decreasing speed of T, $\triangle\mathbf{x}^*$ should be chosen such that

$$\mathbf{e}^\intercal \triangle\mathbf{x}^* = \min_{\mathbf{k}}(\mathbf{e}^\intercal \triangle\mathbf{x}) = \min_{\mathbf{k}}\Big((\mathbf{Pe})^\intercal \mathbf{k}\Big), \tag{8}$$

where $\mathbf{e} = [1, 0, \cdots, 0]^T$. Thus

$$\triangle\mathbf{x}^* \propto \mathrm{P}(-\mathbf{Pe}) = -\mathbf{Pe}, \tag{9}$$

which means $\mathbf{k}$ must be antiparallel with $\mathbf{Pe}$. Substituting (6) into (9), we obtain the optimal direction

$$\triangle\mathbf{x}^* \propto -\mathbf{e} + \frac{\mathbf{e}^\intercal \nabla J(\mathbf{c})}{\| \nabla J(\mathbf{c}) \|^2} \cdot \nabla J(\mathbf{c}). \tag{10}$$

As indicated in Fig. 1, the expression (10) reveals that the optimal direction $\triangle\mathbf{x}^*$ is a weighted linear combination of $-\mathbf{e}$ and the gradient $\nabla J(\mathbf{c})$. The component $-\mathbf{e}$ is responsible for reducing the time duration T towards a near time-optimal control vector, but merely along this direction the iteration will be steered off the level-set $\mathcal{L}(J = J_H)$. The combination with the component $\nabla J(\mathbf{c})$ compensates to keep $J = J_H$ in the level-set; the compensation will be more effective if the Hessian can be taken into account of (we will not consider it in this paper). Thus, the search following this direction shortens T and maintains J at the same time, and hence is expected to be more efficient than merely reducing T or climbing along the gradient direction.

	C_1	C_2	C_3	C_4	C_5	C_6
C_1	17662					
C_2	53.9	5382.4				
C_3	0.8	33.96	4006.7			
C_4	2.47	0	33.96	2435.8		
C_5	0	3.03	0	34.73	2216.6	
C_6	0	2.42	0	34.93	0	2105.8

TABLE I: The chemical shifts $\delta_k\omega_0/2\pi$ (diagonal elements, in unit of Hz) and coupling strengths J_{jk} (off-diagonal elements, in unit Hz) of the carbon spins in D-Norleucine (CAS NO: 327-56-0). The data are experimentally obtained and provided by University of Science and Technology of China (unpublished).

IV. NUMERICAL IMPLEMENTATION

In this section, we apply the algorithm to gate and state operations in nuclear magnetic resonance (NMR) systems that are often used for testing quantum control protocols [42, 43].

A. System parameters

We pick several examples from the six homonuclear carbon spins in the D-Norleucine molecule, which are encoded as qubits for NMR quantum computation. The system's Hamiltonian reads [29]

$$H = H_0 + u_1(t)H_x + u_2(t)H_y, \tag{11}$$

where $u_1(t)$ and $u_2(t)$ are the controls implemented by radiofrequency magnetic fields, which satisfy $u_1^2(t) +$

$u_2^2(t) \leq 1$. Consider m spins of the six and ignore (or decouple) their couplings to the remaining spins. The drift and control Hamiltonians are as follows:

$$H_0 = \hbar \sum_{k=1}^{m} \delta_k \omega_0 S_z^k + 2\pi\hbar \sum_{1\leq j<k\leq m} J_{jk}(S_x^j S_x^k + S_y^j S_y^k + S_z^j S_z^k), \quad (12)$$

$$H_{x,y} = -\hbar\Omega \sum_{k=1}^{m} (1-\delta_k) S_{x,y}^k, \quad (13)$$

where

$$S_{x,y,z}^k = \frac{1}{2} I_2^{\otimes(k-1)} \otimes \sigma_{x,y,z} \otimes I_2^{\otimes(m-k)}$$

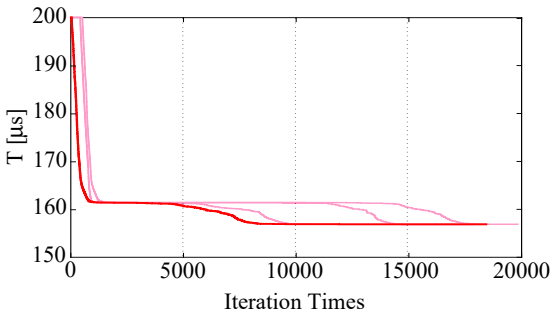
are spin operators act on the k-th spin, $\otimes$ represents the Kronecker product, $\sigma_{x,y,z}$ represent the standard Pauli operators. The chemical shift $\delta_k\omega_0$ of each spin and J-coupling constants J_{jk} between them are listed as the diagonal and off-diagonal elements in TABLE I. The parameter Ω is the bound on the amplitude of control fields.

B. Two-qubit and multiple-qubit gate optimization

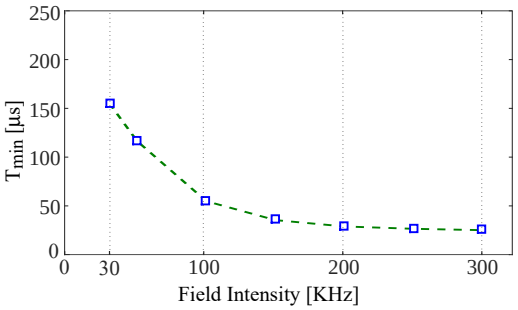
First, we consider $m = 2$ for a two-spin example with C_1 and C_2, and seek the time-optimal control for implementing a selective $\frac{\pi}{2}$ rotation on spin C_1, which corresponds to maximization of J_1 with $W = \exp(-i\frac{\pi}{2}S_x) \otimes I_2$.

We begin with $T_{initial} = 200\mu$s and divide it into $M = 250$ steps. Starting from a random field as the initial guess, we obtain the optimization result (the red line) shown in Fig. 2(a) with error thresholds $(1 - J_H) = 1 \times 10^{-4}$, $(1 - J_L) = 1.1 \times 10^{-4}$. The search ceases at $T_{\min} = 154.9\mu$s with error $(1 - J_1) = 1.07 \times 10^{-4}$ after about 8000 iterations.

As displayed in Fig. 2(a), T decreases quickly in the first 500 iterations during which it is relatively easy to stay in the level-set $\mathcal{L}(J = J_H)$, then more and more iterations are required for corrections. To verify whether the $T_{\min}$ we obtained is the genuine minimum time duration, we test three other initial guesses (2 random fields and a null field), from which all of the



(a)



(b)

FIG. 2: (Color online) (a) The iterations for searching near time-optimal controls using the algorithm for the gate control over $C1$ and $C2$ spins with error thresholds $[1 \times 10^{-4}, 1.1 \times 10^{-4}]$. Starting from differential initial guesses, in all simulations T converges from $T_{initial} = 200\mu$s to $T_{\min} = 154.9\mu$s (pink). (b) The numerically solved $T_{\min}$ under different bounds on the field amplitude Ω (blue box) with fidelity above 0.9999, which approaches to $T_{geodesic} = 20.4\mu$s when Ω is larger.

searches converge to the same $T_{\min}$ but at different convergence rates. In particular, the case of null field takes more than twice the number of iterations of the first case (red) to reach $T_{\min}$.

To test how close our method can find a minimum time-optimal control, we raised the control amplitude Ω from 30kHz to 300kHz. As analyzed in [29], the theoretical minimal time $T_{\min}$ is supposed to approach to $T_{\text{geodesic}} = 20.4\mu$s calculated by Eq. (14) in [29] when Ω is sufficiently large. We apply the algorithm with different control bounds Ω and depict corresponding minimal times in Fig. 2(b). It shows that $T_{\min}$ does approach to the theoretical limit $T_{geodesic} =$

20.4μs when Ω goes to infinity (e.g., $T_{\min} = 25.1\mu$s when $\Omega = 300$kHz). This demonstrates that our algorithm is capable of finding the true time-optimal control fields in this case.

To explore more complex structures, we simulate a 4-spin example with spins C_1, C_2, C_3 and C_4, and seek time-optimal control for implementing a selective $\frac{\pi}{2}$ rotation $W = \exp(-i\frac{\pi}{2}S_x) \otimes I_8$ on spin C_1. We begin with $T_{initial} = 1000\mu s$ and divide it into $M = 1000$ steps. Starting from random fields as initial guesses, we obtain the optimization results (the blue and red lines) shown in Fig. 3 with error thresholds $(1 - J_H) = 1 \times 10^{-3}$, $(1 - J_L) = 1.1 \times 10^{-3}$. The search ceases at $T_{\min} = 474.1\mu s$ with error $(1 - J_1) = 1.04 \times 10^{-3}$ after about 10000 iterations. However, as shown in Fig. 3, the search appears less efficient when it starts from the other two randomly chosen initial guesses (the pink lines), which reveals the increasing complexity in the control Pareto behavior of large-number qubit systems. This shows that not only the dimensionality but also the potential traps for the search will increase the search effort as T is limited at a control resource. In such cases, one needs to more carefully choose the initial guess for T and $\mathbf{u}$, or develop better strategies for scanning over possible initial guesses [33].

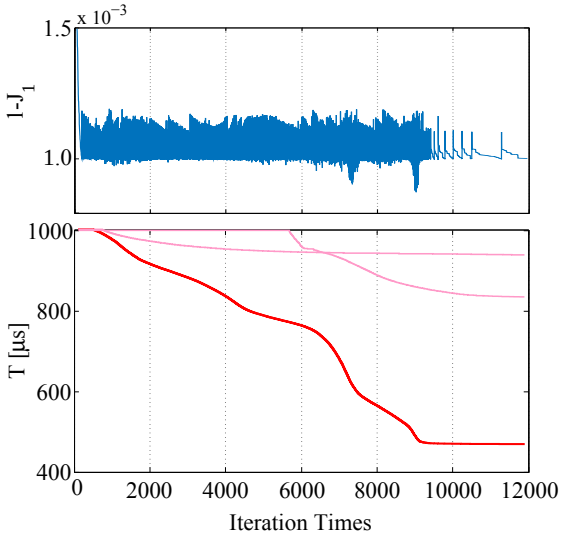


FIG. 3: (Color online) The searches for near time-optimal controls for the gate control over $C1$, $C2$, $C3$, and $C4$ spins with error thresholds with error thresholds $[1 \times 10^{-3}, 1.1 \times 10^{-3}]$. The three curves correspond to three different initial guesses, and in the best case T decreases from $T_{initial} = 1000\mu$s to $T_{\min} = 474.1\mu$s after 10000 iterations (blue/red).

C. Observable control optimization and comparison to other algorithms

In this case, we apply the algorithm to the objective function J_2 to maximize the expectation value of the observable O, and compare our algorithm with another time-optimal control procedure.

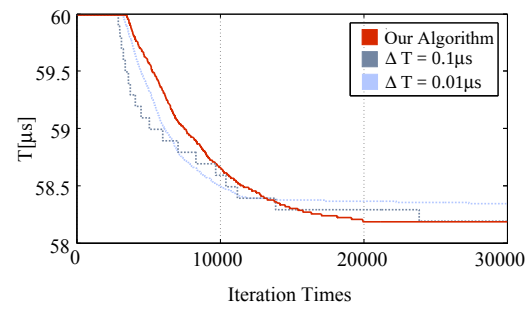
We simulate a two-spin example (C_1 and C_2) with the following initial state and observable:

$$\rho_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \; O = \begin{pmatrix} \frac{1-i}{2} & 0 & \frac{\sqrt{2}i}{2} & 0 \\ 0 & 0 & 0 & 0 \\ \frac{-\sqrt{2}i}{2} & 0 & \frac{1+i}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (14)$$

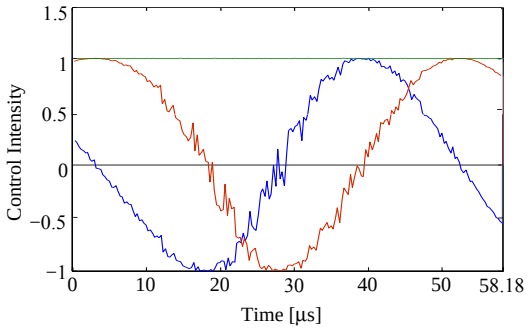
It can be verified that the maximal value of J_2 is $J_{\max} = 1$.

We begin with $T_{initial} = 60\mu$s and divide it into $M = 100$ steps. Starting from a random field as the initial guess, we obtain the optimization result (the red line) shown in Fig. 4(a) with error thresholds $(1-J_H) = 1 \times 10^{-6}$, $(1 - J_L) = 1.1 \times 10^{-6}$. The search ceases at $T_{\min} = 58.18\mu$s with error $(1 - J_2) = 1.00 \times 10^{-6}$ after about 20000 iterations. Fig. 4(b) shows the corresponding time-optimal control functions. The green line represents the constrain of the control amplitude, which is shown at highest level at all time. It could be taken as the feature of time-optimal solutions.

We then compare the proposed LS algorithm with an existing algorithm in the literature [18, 34], which decreases T step by step by a fixed size ΔT. Fig. 4(a) shows the results with step size $\Delta T = 0.01\mu$s and $\Delta T = 0.1\mu$s, respectively. For the bigger step size $\triangle T = 0.1\mu s$, T decreases faster than our algorithm in the first 5000 iterations, but slower in the last 25000 iterations, and finally ceases at $T = 58.2\mu s$ after 25000 iterations (light gray, lower); for the smaller step size



(a)



(b)

FIG. 4: (Color online) (a) The searches for near time-optimal controls for the observable control over $C1$ and $C2$ spins with error thresholds $[1 \times 10^{-6}, 1.1 \times 10^{-6}]$. T decreases from $T_{initial} = 60\mu$s to $T_{\min} = 58.18\mu$s after 20000 iterations (our algorithm; red); $T_{\min} = 58.20\mu$s after 25000 iterations ($\triangle T = 0.1\mu$; light grey); $T_{\min} = 58.35\mu$s after 30000 iterations ($\triangle T = 0.01\mu$; light blue). (b) The optimal control functions $u_1(t)$ (red, right), $u_2(t)$ (blue, left) in the 2-qubit observable control example. Each vertical line represents a value of control variable $u_k(t_j)$, and the green line shows the numerical result of $u_1^2(t_j) + u_2^2(t_j)$ at different t_j.

$\triangle T = 0.01\mu s$, T decreases so slow that no satisfying value can be obtained within 30000 iterations (light blue, upper). Thus, the LS algorithm achieves overall good performance with more rapid convergence, and higher final precision under the same computational burden.

V. CONCLUSION

To summarize, we present a level-set based iterative algorithm for searching near time-optimal controls of quantum systems. Operating near the prescribed level-set, the algorithm seeks high-quality time-optimal solutions by continuously updating the control functions and intermittently decreasing the time duration, in which the search are able to follow the optimal direction which takes care of both the fidelity J and the time duration T. Numerical examples show that the algorithm can quickly find near time-optimal solutions for both gate and observable control problems. The central idea of searching in high level-sets can be generalized with other local optimization algorithms with fixed T, and the control profiles can be further smoothed and optimized with advanced algorithms such as the hybrid procedure proposed in [33], so as the quality and robustness of the time-optimal control can be improved.

In principle, the proposed algorithm can also be applied to open quantum systems with non-unitary dynamics. However, it is not always easy to determine a proper high level-set that is reachable by admissible controls. Moreover, due to the complexity of the open system dynamics, we expect that the search will encounter more traps than the case of unitary dynamics. Nevertheless, since unitary dynamics is often a good approximation of open system dynamics within a short time interval, we can reasonably consider the unitary case under most circumstances. Even if the unitary approximation is not adequate, we can still use the obtained time-optimal control as an initial guess for optimization with non-unitary dynamics.

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Technology of China for useful discussions and the NMR data for simulations, as well as Wei Wang's work on the coding.

Appendix A: The Gradient formulas

For convenience, we denote

$$U_j = V_j V_{j-1} \cdots V_2 V_1, \quad j = 1, 2, \cdots, M,$$

where

$$V_j = \exp\left[-i\left(H_0 + \sum_{k=1}^{m} u_{kj} H_k\right)\frac{T}{M}\right].$$

When $\frac{T}{M}$ is sufficiently small, we have [18]

$$\begin{aligned}\frac{\partial V_j}{\partial u_{kj}} &\approx -\frac{iT}{M} H_k V_j,\\ \frac{\partial V_j}{\partial T} &= -\frac{i}{M}\left(H_0 + \sum_{k=1}^{m} u_{kj} H_k\right) V_j.\end{aligned}$$

Using the above results we obtain the total derivative of $U(T) = U_M$ with respect to $\mathbf{x}$

$$\begin{aligned}\frac{\partial U(T)}{\partial u_{kj}} &= -\frac{iT}{M} U(T) U_j^\dagger H_k U_j,\\ \frac{\partial U(T)}{\partial T} &= -\frac{i}{M}\sum_{j=1}^{M} U(T) U_j^\dagger \left(H_0 + \sum_{k=1}^{m} u_{kj} H_k\right) U_j.\end{aligned}$$

The above formulas can be directly applied to objective functions (2) and (3) to obtain the following gradient formula:

$$\begin{aligned}\frac{\partial J_i}{\partial u_{kj}} &= \frac{T}{M} Im\left(\mathrm{Tr}\left(D_i U_j^\dagger H_k U_j\right)\right),\\ \frac{\partial J_i}{\partial T} &= \frac{1}{M}\sum_{j=1}^{M} Im\left(\mathrm{Tr}\left(D_i U_j^\dagger \Big(H_0 + \sum_{k=1}^{m} u_{kj} H_k\Big) U_j\right)\right),\end{aligned}$$

where $Im(\cdot)$ denotes the imaginary part; $i = 1, 2$; $k = 2, \cdots, m$, and $j = 1, \cdots, M$ with

$$\begin{aligned}D_1 &= W^\dagger U_M,\\ D_2 &= [\rho_0, U_M^\dagger O U_M].\end{aligned}$$

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