Time Scaling Transformation in Quantum Optimal Control Computation

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Abstract: The optimal control problem of the closed quantum systems can be equivalent to the parameters optimization problem of bilinear control systems. Numerical optimization techniques such as time scaling transformation are introduced to the Gradient Ascent Pulse Engineering (GRAPE) algorithm. The modified scheme can improve the fidelity, reduce the optimal evolutionary time and errors caused by the nonlinear hardware as illustrated in the numerical simulation of homonuclear optimal control.

Key Words: time scaling transfromation, GRAPE, quantum optimal control

1 Introduction

Quantum optimal control is widely used in the quantum systems, such as superconducting quantum systems [1], nuclear magnetic resonance (NMR) [2, 3], Bose-Einstein condensates [4], etc. The closed quantum systems are earlier studied, followed by the open quantum systems [5-7] which are generally complicated. The reason is that the interactions with the environment, such as the quantum decoherence, are usually required to be taken into consideration. Although time scaling transformation can be applied to the open quantum systems, this paper focuses on the optimal control of the closed quantum systems.

The modeling and controllability of the closed quantum systems are introduced in [8] which regards the dynamic quantum systems as bilinear control systems. The analytical solution can be found for the time optimal problem of the single spin systems by Pontryagin maximum principle [9]. However, only approximate numerical solutions can be found for the two-objective optimization problem of systems with multiple quantum bits, especially for the homonuclear systems [7, 10-12]. A great variety of methods have been developed for the problem. Firstly, the most widely adopted algorithm is Gradient-Ascent-Pulse-Engineering (GRAPE) algorithm [13]. The smoothness, robustness and amplitude constraints of the sequences are discussed in [14]. In the second place, the numerical problem can also be analyzed geometrically. The time optimal control problem can be transformed into a geodesic problem in finding a shortest path on a manifold [15, 16]. Quantum brachistochrone equation (QBE) is proposed in [17, 18], which is related to the geodesic problem. As the computational complexity grows exponentially with the number of the quantum bits, the dimension of QBE can be reduced by the relationship for further calculations [11, 19]. In addition, the pseudospectral method is proposed for optimal pulse design of both the closed and open quantum systems [20, 21]. There are also many other approaches, for example, the Krotov method [22] and dynamic programming algorithm are also applied to solve the problem [23].

Besides the aforementioned schemes, there exist still some other skills to improve the performance of the pulse sequence both theoretically and in practice. On the one hand, the numerical methods represented by GRAPE need to discretize the time horizon to obtain the optimal pulse sequence. In the procedure, the time horizon T is divided into M subintervals, and the controls are regarded as piecewise-constant. When the time slice is short enough, or M is sufficiently large, the discretized system approximates the original continuous system with little errors. Meanwhile, it is also time-consuming, especially when the number of quantum bits are considerably large. On the other hand, the theoretical $fidelity = 1$ pulse sequences have relatively poor performance [12] in practice owing to some practical factors. Quantum decoherence certainly contributes to the poor performance. At the same time, nonlinear classical environmental disturbance and devices are also the culprits. The errors are systematically analyzed in [24], among which Pulse Length Errors (PLEs) and Off Resonance Errors (OREs) are the most common, caused by the inhomogeneity and variations across the sample respectively. Finite rise time resulting in nonstandard square input pulse and crosstalk giving rise to the interference of different control channels, are another two reasons.

The closed quantum systems can be considered to be the bilinear control systems. The systematic illustration and analysis are given in [25]. Time scaling transformation is introduced to the quantum optimal control. The adaptive switching points can reduce the subdivision number of time horizon, which are able to save more computation time. The switching points are optimized by gradients. Moreover, the switching points can be deliberately set during the rising and declining intervals of the square input signal to reduce the errors caused by the finite rise time. Introduction of time scaling transformation and more optimization techniques is available in [26-29].

The paper is organized as follows: Section 2 formulates the optimal control of the closed quantum systems and Section 3 introduces time scaling transformation to the conventional GRAPE algorithm. Section 4.1 shows how the gradi-

This work was supported by the National Natural Science Foundation of China (Grant No. 61473253) and the Science Fund for Creative Research Group of China (Grant No. 61621002). It was also supported by the Fundamental Research Funds for the Central Universities

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ent method with time scaling transformation applies to the time optimal control of homonuclear spins in liquid NMR. The simulation results are given in Section 4.2. Potential effects on error reduction by the gradient method with time scaling transformation are briefly discussed in Section 4.3. Finally, the strengths and drawbacks are concluded in Section 5.

2 Problem Formulation

According to the Schrödinger equation, the closed quantum systems can be formulated as the bilinear control systems. In the absence of relaxation, the bilinear systems can be defined as:

$$\left|\dot{\psi}(t)\right\rangle = -i\left(H_d + \sum_{l=1}^{m} u_l(t)H_l\right)|\psi(t)\rangle$$
$$\dot{U}(t) = -i\left(H_d + \sum_{l=1}^{m} u_l(t)H_l\right)U(t)$$

where the wave function represents the state such as spin state, energy level state, etc. In the absence of relaxation, the evolution matrix $U(t)$ should be $2^N - D$ unitary matrix, and N is the number of quantum bits. The Hamiltonians H_d and H_l represent the drift Hamiltonians and the l-th external control Hamiltonians respectively. The goal is to drive the system to implement the designated quantum gate U_f within admissible control. Total evolutionary time T should be as short as possible; meanwhile, the sufficiently large fidelity should be guaranteed. Given time T and U_f, the problem is to maximize following objective function where control amplitude is required to satisfy the physical constraints($\Re(\cdot)$ denotes the real part of a complex number, and $tr(\cdot)$ denotes the trace of the matrix):

$$J(\boldsymbol{u}(t)) = 2^{-N}\Re(tr\{U_f^{\dagger}U(T)\})$$
$$\boldsymbol{u}(t) = [u_1(t), u_2(t), \cdots, u_m(t)]$$
$$s.t.\,|u_l(t)| \le u_{lmax}, \forall l = 1, 2, \cdots, m$$

Every unitary gate can be implemented provided that the control amplitudes or the total evolutionary time are unbounded. However, the control amplitudes are often limited in practice, and time optimal control is expected in case of quantum decoherence. Time scaling skills are coordinated with the conventional GRAPE algorithm in which time horizon is often uniformly discretized. The new optimal parameter selection scheme can outperform the conventional GRAPE method.

3 Optimal Control Computation

3.1 Piecewise-Constant Parameterization

The control parameterization method is introduced in [27, 28], the continuous control can be discretized by the approximation below, where $t_k, k = 0, \cdots, M$ are knot points or switching times which satisfy:

$$u(t) \approx u^M(t) = \sum_{k=1}^{M} \sigma^k \chi_{[t_{k-1},t_k)}(t)$$
$$\chi_{[t_{k-1},t_k)}(t) = \begin{cases} 1, \text{if } t \in [t_{k-1}, t_k) \\ 0, \text{otherwise} \end{cases}$$
$$0 = t_0 < t_1 < \cdots < t_{M-1} < t_M = T$$

In the traditional parameterization method, the switching times are fixed, or, the time horizon is subdivided into M isometric subintervals. After the parameterization, the original Schrödinger equation with initial condition becomes:

$$\dot{U}(t) = \sum_{k=1}^{M} -i\left(H_d + \sum_{l=1}^{m} \sigma_l^k H_l\right)U(t)\chi_{[t_{k-1},t_k)}$$
$$U(0) = I_{2^N \times 2^N}$$

The $m * M + M - 1$ variables are shown below in the procedure of control parameterization with variable switching times. The solution can be expressed as $U(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu})$, where

$$\boldsymbol{\sigma} = [\boldsymbol{\sigma^1}; \boldsymbol{\sigma^2}; \cdots; \boldsymbol{\sigma^M}] \in \mathbb{R}^{Mm}; \boldsymbol{\sigma^k} = [\sigma_1^k, \sigma_2^k, \cdots, \sigma_m^k]^{\mathrm{T}}$$
$$s.t.\,\left|\sigma_l^k\right| \le \sigma_{l\max}, \forall l = 1, 2, \cdots, m, \forall k = 1, 2, \cdots, M$$
$$\boldsymbol{\nu} = [t_1, \cdots, t_{M-1}] \in \mathbb{R}^{M-1}$$
$$s.t. 0 = t_0 < t_1 < \cdots < t_{M-1} < t_M = T$$

Note that the objective function is related to $U(T)$ which is determined by $\boldsymbol{\sigma}, \boldsymbol{\nu}$, therefore, the objective function can be expressed as

$$J(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu}) = 2^{-N}\Re(tr\{U_f^{\dagger}U(T)\})$$
$$= 2^{-N}\Re(tr\{U_f^{\dagger}U_M(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu})U_{M-1}(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu}) \cdots U_1(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu})\})$$

3.2 Time Scaling Transformation

Time scaling transformation can effectively solve the computational difficulties caused by the variable switching times [28, 29]. The key is to transform the approximate problem with variable switching times into a new one with fixed knot points. New time variable and time-related decision parameters are introduced respectively as $s \in [0, M]$ and

$$\boldsymbol{\theta} = [\theta_1, \theta_2, \cdots, \theta_M]$$
$$\theta_k = t_k - t_{k-1}, \forall k = 1, 2, \cdots, M$$
$$s.t.\,\theta_k \ge 0, \sum_{k=1}^{M} \theta_i = T$$

Since the designed pulse is piecewise-constant, the following equality holds

$$t(s) = \theta_k \cdot s, s \in [k-1, k), \forall k = 1, 2, \cdots, M$$

Hence, the original Schrödinger equation can be rewritten as

$$\dot{\tilde{U}}(s) = -i\left(H_d + \sum_{l=1}^{m} \sigma_l^k H_l\right)\tilde{U}(s)\theta_k$$
$$s \in [k-1, k), \forall k = 1, 2, \cdots, M$$
$$\tilde{U}(0) = I_{2^N \times 2^N}$$

3.3 Gradient Ascent Pulse Engineering

During the k-th subinterval, the solution of the matrix ODE can be written as

$$\tilde{U}_k(s) = \Gamma_k \exp\left(-i\theta_k\left(H_d + \sum_{l=1}^{m} \sigma_l^k H_l\right)\right)$$

In fact, the unitary matrix is constant during the subinterval. Ignoring the Dyson time-ordering operator since the

global phase does not matter, the unitary evolutionary matrix is shown below:

$$U_k = \exp\left(-i\theta_k\left(H_d + \sum_{l=1}^{m}\sigma_l^k H_l\right)\right) \tag{1}$$

As is shown in [13], the gradient can be calculated accurately, though time-consuming. On the assumption that θ_k is small enough, or rather

$$\theta_k \ll \left\| H_d + \sum_{l=1}^{m}\sigma_l^k H_l \right\|^{-1}$$

the gradients of evolutionary matrix over the control can be approximated as follows:

$$\begin{aligned}
\frac{\partial U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \sigma_l^k} &\approx -i\theta_k H_l U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu}) \\
\frac{\partial U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \theta_k} &= -i\left(H_d + \sum_{l=1}^{m}\sigma_l^k H_l\right) U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu}) \\
\frac{\partial J(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \sigma_l^k} &= 2^{-N}\Re(tr\{\Lambda_{M+1:j+1}^{\dagger}\frac{\partial U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \sigma_l^k}X_{j-1:0}\}) \\
\frac{\partial J(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \theta_k} &= 2^{-N}\Re(tr\{\Lambda_{M+1:j+1}^{\dagger}\frac{\partial U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \theta_k}X_{j-1:0}\})
\end{aligned} \tag{2}$$

There are two common gradient methods for solving the optimal control problem: GRAPE and Krotov algorithms. The gradient method with time scaling transformation is briefly introduced as follows:

1) Initialize the counters.
2) Outer loop: Initialize $\boldsymbol{\sigma}, \boldsymbol{\nu}$ randomly within admissible sets.
3) Inner loop: Given initial control parameters, calculate the exponent as formula (1), forward propagation, backward propagation, and the objective function, or fidelity as below.

$$\begin{aligned}
X_{j:0} &= U_j U_{j-1}, \cdots, U_2 U_1 \\
\Lambda_{M+1:j+1}^{\dagger} &= U_f^{\dagger} U_M U_{M-1}, \cdots U_{j+1} \\
\Phi &= 2^{-N}\Re\{tr(\Lambda_{M+1:j+1}^{\dagger} X_{j:0})\}
\end{aligned}$$

4) If target fidelity is not reached, update the control parameters according to the gradients as formula (2) or the exact gradients. Other options are numerical gradients including Newton, Quasi-Newton, L-BFGS, etc.
5) If target fidelity is still not reached after multiple iterations, finish the inner loop, then choose another initial guess of parameters and restart the inner loop.
6) If target fidelity is reached, finish the outer loop, and smooth the pulse sequence.

The procedure can be easily found in the relevant papers [13, 30]. The optimization result is heavily dependent on the initial guess. Therefore, varies of initial parameters are required to obtain a high-fidelity pulse sequence. Except for the traditional line search method for the control update, Matlab package $fmincon$ includes four algorithms for optimization problems with constraints, among which trust-region-reflective is efficient and tends not to be trapped in the local minimum. However, only constraints in the form of lower and upper bounds can be applied. The modular programming framework DYNAMO package [30] is a time-saving tool for the unbounded parameter optimization. Also, it is a good platform for benchmarking and comparing the performance of the new algorithms.

4 Application

4.1 Optimal Control for the Homonuclear Spins

The Spin Hamiltonian Hypothesis holds for almost all systems at the ordinary temperature[31]. Then the homonuclear spins in the liquid nuclear magnetic resonance (*lNMR*) can be formulated in the rotating frame as below [12]:

$$\begin{aligned}
\dot{U}(t) &= -i\left(H_Z + H_J + H_{RF}\right)U(t) \\
H_z &= -\sum_{i=1}^{N}[(1-\delta_i)\omega_0 - \omega_{rf}]S_z^{\otimes i} \\
H_J &= 2\pi J_{ij}\sum_{i<j}(S_x^i S_x^j + S_y^i S_y^j + S_z^i S_z^j)^{\otimes} \\
H_{RF} &= -\sum_{i=1}^{N}(1-\delta_i)[u_x(t)S_x^{\otimes i} - u_y(t)S_y^{\otimes i}] \\
S_k^{\otimes i} &= I_k^1 \otimes \cdots \otimes I_k^{i-1} \otimes S_k^i \otimes I_k^{i+1} \otimes \cdots \otimes I_k^N \\
(S_k^i S_k^j)^{\otimes} &= I_k^1 \otimes \cdots \otimes S_k^i \otimes I_k^{i+1} \otimes \cdots \otimes S_k^j \otimes \cdots \otimes I_k^N
\end{aligned}$$

where $k = x, y, z$ and the Hamiltonians are respectively the Hamiltonians of the static magnetic field, J-coupling, the radio frequency magnetic field. For N homonuclear spins, the spins can be separated by the minor difference of the Larmor frequency under the magnetic field. Taking for example the 4^{th} and 5^{th} carbon atoms in the L-Histidine molecule in Fig. 1, their chemical shifts are respectively $\delta_1\omega = -22562Hz$ and $\delta_2\omega = -20657Hz$ under the $600MHz$ NMR. The two quantum bits system is control by the 2-channels radio frequency magnetic field marked as x and y.

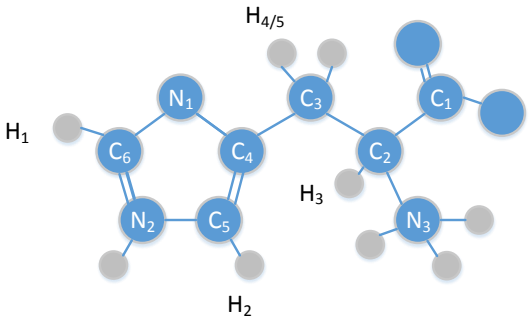

Fig. 1: L-Histidine Structure Diagram.

Set the target quantum gate to be $R_x(\pi/2)\otimes I_{2\times 2}$, that is

$$U_{1f} = R_x(\pi/2) = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix}, U_{2f} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The minimum can be estimated by the geodesic distant [12]:

$$T_{\text{minimum}} \gtrapprox T_{\text{geodesic}} = \frac{\left\|\log(U_{1f}^{\dagger}U_{2f})\right\|}{\|(\delta_1-\delta_2)\omega_0 S_z\|} = 132\mu s$$

4.2 Numerical Simulation

The simulation model is illustrated in Section 4.1. In the simulation, maximum control power is $\Omega_{\max}$,

$$N=2, m=2, M=50, \omega=150MHz, \delta_1\omega=-22562Hz,$$
$$\delta_2\omega=-20657Hz, \sqrt{u_x^2+u_y^2} \le \Omega_{\max}=12.5kHz$$

In the first simulation, we suppose that total evolutionary time T is a constant. If $T=150\mu s > T_{\text{minimum}}$, for example, high fidelity can be reached. The improved DYNAMO package with bounded constraints can work out the pulse sequence, where the fidelity reached $1-5.95078\times10^{-5} \approx 0.9999$, and the CPU time is $18.0337s$. Since the quantum gate is unitary, the state is separable. Hence, the evolution of individual spin can be plotted on their own Bloch spheres respectively. On condition that the initial states are both at the North Pole, the evolutions are drawn in Fig. 2. The Larmor frequency has been turned up a little for the convenience of the Bloch sphere display.

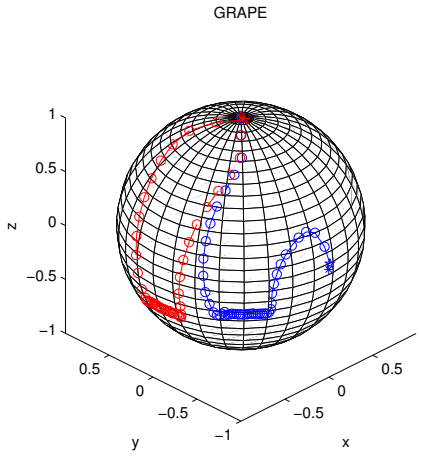

Fig. 2: The blue line denotes the evolution of the first bit on the Bloch sphere, while the red line denotes the second bit.

In another situation, for example, if $T = 120\mu s < T_{\text{minimum}}$, the fidelity cannot reach 1 theoretically. The simulation is organized as follows:

1) Initial sequence. The initial sequence is obtained by the improved DYNAMO package. It is almost Bang-bang control with fidelity $1-0.0252847 \approx 0.9747$, and CPU time for the initial sequence computation is $36.239s$. The $x-y$ control sequences can be seen in Fig. 3. The fidelity differences between multiple simulations are less than 10^{-6}, and every individual simulation contains a lot of randomized initial guess. The initial sequence is almost global optimal, therefore, it is a good initial guess for the subsequent optimization.
2) The traditional GRAPE cannot enhance the fidelity of the aforementioned initial sequence. More control parameters can be added for further optimization. Two possible methods are respectively increasing the number of the subintervals M and the gradient method with time scaling transformation. The former method with $M=75$ and the latter with $M=50$ both have 150 independent variables. The average results are in Table 1. The control amplitude and phase are drawn in Fig. 4 and Fig. 5. It is obviously that the gradient method gives higher fidelity with fewer parameters.

Table 1: Simulation Results

No.	Algorithm	Fidelity	No. of Parameters
$T=120\mu s < T_{\text{minimum}}$			
1	Initial Sequence	0.9747153	100
2	M=75 GRAPE	0.9748384	150
3	M=100 GRAPE	0.9749424	200
4	M=50 Time Scaling	0.9749855	150
$T=150\mu s > T_{\text{minimum}}$			
5	Initial Sequence	0.9999405	100

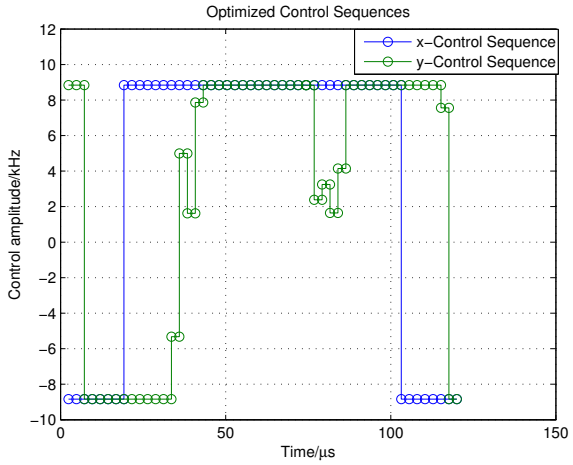

Fig. 3: The optimal control sequence calculated by DYNAMO when $T < T_{minimum}$. Time horizon is uniformly divided.

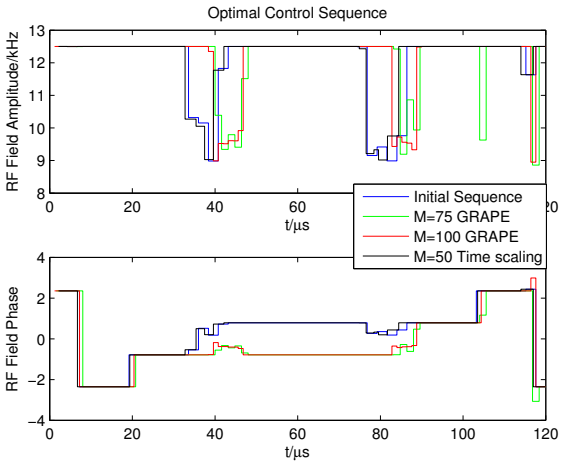

Fig. 4: The amplitudes and phases of four simulations, the black one has the maximum fidelity. Plotted in stairs.

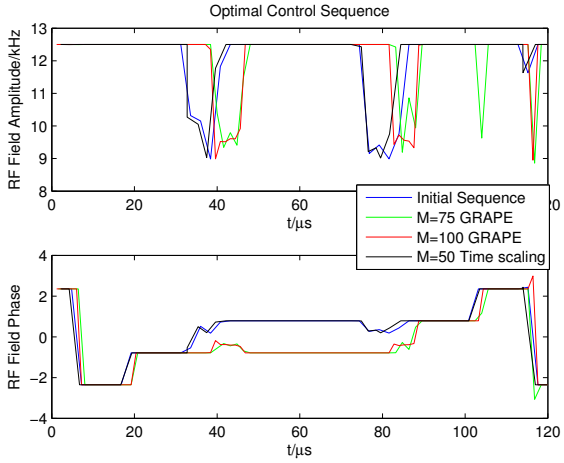

Fig. 5: The amplitudes and phases of four simulations, the black one has the maximum fidelity.

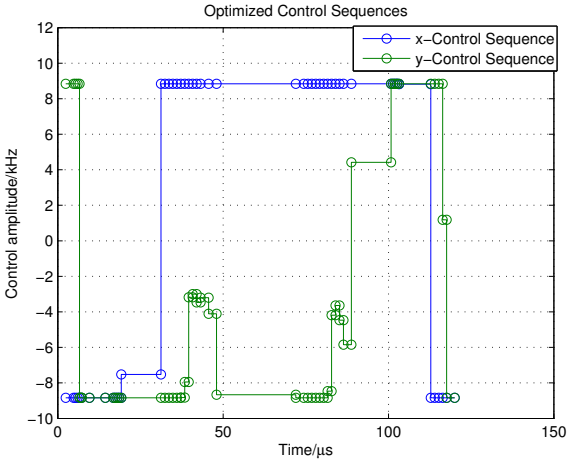

Fig. 6: Gradient method with time scaling transformation. The switching points are manually designated for the practical convenience. The method can be used in the error reduction.

4.3 Error Reduction

As previously mentioned, the square pulses cannot be implemented without errors [24]. The actual pulse will have trailing edge. Some typical methods are subdivision of the time intervals during which the pulse has a dramatic variation [32]. An alternative is to manually select the switching points using the time scaling transformation. The switching points on the time horizon can be adjusted to be concentrated when the pulse has a dramatic variation, and vice versa. Meanwhile, the total amount of the parameters stay unchanged, which can save much calculation. In this method, the switching points are not optimized since the minimal unit of the intervals is a quarter of the original length of time slice T/M. Therefore, the fidelity is 0.9749387, which is less than the former result in Section 4.2. The optimized sequences are shown in Fig. 6. The actual pulse can be modeled as the step response of a 2^{nd}-order filter [33]. The error is calculated as below, where ς is between 0 and 1, related to the response speed and overshoot.

$$e(t) = -e^{-\varsigma t/T}\sin(t\sqrt{1-\varsigma^2}/T + \arctan\sqrt{1-\varsigma^2})$$

This error can be proved to reduce when the time horizon of the rising or decline part is subdivided into more segments.

5 Conclusion

In summary, we propose the gradient method with time scaling transformation, which can theoretically enhance the fidelity with evolutionary time given. That means the gradient method with time scaling transformation can reach the designated fidelity in less time, which can be universally utilized in quantum optimal control problems. In addition, the method only adds M variables, which are independent of the number of external control channels m. The switching points are adaptive. Therefore, the method can also effectively reduce the error caused by the nonlinear hardware.

However, the bandwidth of the impulsator and other devices is limited. Arbitrary fractional switching times, that require high clock precision, cannot be accurately set, even with the state of the art hardware. Nevertheless, manually selecting switching times implement the nonuniform subdivision as the example shown in Section 4.3, which can improve the results to some extent. Experiments are expected to test the effect of the gradient method with time scaling transformation. The three theoretical pulse sequences, solved by GRAPE, the gradient method with time scaling transformation and the one taking hardware nonlinearity into consideration, can constitute a good comparison experiment, which is expected in the future work.

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