Exact quantum dynamics for two-level systems with time-dependent driving

Zhi-Cheng He,1 Yi-Xuan Wu,1 and Zheng-Yuan Xue1,2,3,∗

1Key Laboratory of Atomic and Subatomic Structure and Quantum Control (Ministry of Education), and School of Physics, South China Normal University, Guangzhou 510006, China
2Guangdong Provincial Key Laboratory of Quantum Engineering and Quantum Materials, Guangdong-Hong Kong Joint Laboratory of Quantum Matter, and Frontier Research Institute for Physics, South China Normal University, Guangzhou 510006, China
3Hefei National Laboratory, Hefei 230088, China

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It is well-known that time-dependent Schrödinger equation can only be exactly solvable in very rare cases, even for two-level quantum systems. Therefore, finding exact quantum dynamics under time-dependent Hamiltonian is not only of fundamental importance in quantum physics but also can facilitate active quantum manipulations for quantum information processing. Here, we present a method which could generate a near infinite number of analytical-assisted solutions of the Schrödinger equation for a qubit with time-dependent driving. This analytical-assisted solution has free parameters with only boundary restrictions, and thus can find many applications in precise quantum manipulations. Due to the general form of the time-dependent Hamiltonian in our scheme, it can be readily implemented in various experimental setups of qubits. Therefore, our scheme provides new solutions for Schrödinger equation, thus provides an alternative and analytical-based routine for precise control over qubits.

I. INTRODUCTION

Searching exact solutions for the time-dependent Schrödinger equation has attracted many interests right after the birth of quantum mechanics. Nowadays, it plays an important role in many quantum tasks that need precise quantum control. Especially, the exact evolution of two-level systems receives much attention as it facilitates precise qubit control in quantum information processing. As a time-dependent Hamiltonian is non-commutative in different time, obtaining an arbitrary target evolution for a qubit is challenging. Therefore, exact solutions are only found for special cases, such as Landau-Zener Transition [1,2], Rabi problems [3], hyperbolic secant pulse [4], etc.

Recently, different schemes for exact quantum dynamics were proposed [5,17]. Especially, an exactly solvable model for a two-level quantum system under single-axis driving field was proposed [18], which allows one to design certain types of quantum manipulation [19–22]. However, an analytical solution for general cases are still unknown. Meanwhile, previous solutions have limitations on the systematic parameters, e.g., the initial condition of the pulse shape leads to difficulty in designing of evolution operators. In addition, the exact dynamics is hardly obtained when the time-dependent phase of driving pulse in off diagonal term, making it difficult to extend to the case of large-scale and long-time controlling.

Here, for the general time-dependent Hamiltonian of a qubit under driving, we present an analytically obtained scheme, which could generate a near infinite number of analytical solutions for its exactly arbitrary dynamics. The desired evolution driven by non-commutative Hamiltonian can be obtained as long as these Hamiltonian can be expressed as functional of a dimensionless auxiliary function. We also find that the analytically-assisted solutions can reduce to well-known analytical solutions, such as Rabi driving and the Landau-Zener transition, under specific choices of the auxiliary functions. Moreover, we apply our solution in two typical problems and present them in detail. Firstly, exact quantum dynamics with smooth pulses can be obtained when manipulating a singlet-triplet (ST) qubit for semiconductor quantum dot systems [23], avoiding discontinuous points in pulse shapes in previous schemes. Secondly, we implement individual control in multi-level quantum systems with nearby transitions [24]. We find that the analytical-assisted solution allows us to design the Rabi rate without the constraint of pulse area, thus making it possible to get the two wanted evolution in both two subspaces with only one pulse. Therefore, our scheme provides an analytical-based routine for precise quantum manipulation.

II. ANALYTICAL-ASSISTED SOLUTIONS

In this section, we present our scheme for exactly arbitrary dynamics of qubit system under different driving directions.

A. The σz control

It is widely known that the dipole-interacting Hamiltonian for a two-level quantum system with time-dependent driving can be generally expressed as,

$$H_z = \begin{pmatrix}
\Delta(t) & \Omega(t) e^{-i\varphi(t)} \\
\Omega(t) e^{i\varphi(t)} & -\Delta(t)
\end{pmatrix},$$  \hspace{1cm} (1)

and its time evolution operator, respected to the unitary condition, can be written as,

$$U_0 = \begin{pmatrix}
u_{11} & u_{21} \\
u_{21} & u_{11}
\end{pmatrix},$$  \hspace{1cm} (2)
where $|u_{11}|^2 + |u_{21}|^2 = 1$.

First, we rotate the entire system into a special reference frame, yielding the Schrödinger equation for the evolution operator as,

$$i \frac{\partial}{\partial t} (S^\dagger U_0) = \left( S^\dagger H_2 S + i \frac{\partial S^\dagger}{\partial \tau} S \right) (S^\dagger U_0),$$

where the transformation operator $S(t)$ is defined as,

$$S(t) = \exp \left[ -i \int_0^t \Delta(t') dt' \sigma_z \right].$$

Note that this Schrödinger equation remains in matrix form. We rewrite it as two algebraic equations as follows,

$$\dot{v}_{11} = i\Omega e^{i\alpha} v_{21}, \quad \dot{v}_{21} = i\Omega e^{i\alpha} v_{11},$$

where $\alpha(t) = 2 \int_0^t \Omega(t') dt' - \varphi + \pi$, $\dot{v}_{11}$ and $\dot{v}_{21}$ represent the time derivative of $v_{11}$ and $v_{21}$. Here, $v_{11}$ and $v_{21}$ are defined as functional of $u_{11}$ and $u_{21}$, the matrix elements in Eq. (2). The detailed forms of $v_{11}$ and $v_{21}$ can be written as,

$$v_{11} = \exp \left( i \int_0^t \Delta(t') dt' \right) u_{11},$$

$$v_{21} = \exp \left( -i \int_0^t \Delta(t') dt' \right) u_{21}. \tag{6a}$$

Combining two equations in Eq. (5), once get

$$(\dot{v}_{11}/v_{11})(\dot{v}_{21}/v_{21}) = -\Omega^2.$$ Next, we separate this equation into two distinct equations as follows,

$$\dot{v}_{11}/v_{11} = -i\Omega e^{\kappa(t)}, \quad \dot{v}_{21}/v_{21} = -i\Omega e^{-\kappa(t)}, \tag{7}$$

where $\kappa(t)$ is an unknown complex parameter introduced to satisfy the combined equation. Then, we obtain a general solution for $v_{11}$ and $v_{21}$ as,

$$v_{11} = \exp \left[ i\theta_1 - i \int_0^t \Omega(t') e^{\kappa(t')} dt' \right],$$

$$v_{21} = \exp \left[ i\theta_2 - i \int_0^t \Omega(t') e^{-\kappa(t')} dt' \right]. \tag{8a}$$

where $\theta_1$ and $\theta_2$ are constant phase. These phases arise from the derivation operation and are currently unknown. Substituting Eq. (8) into Eq. (5), we can express $\alpha(t)$ in terms of $\kappa(t)$ as,

$$\alpha(t) = -i\kappa(t) + \theta - 2 \int_0^t \Omega(t') \sinh \kappa(t') dt' \tag{9}$$

where $\theta = \theta_1 - \theta_2$.

Since $\Delta$ and $\varphi$ need to be real, $\alpha(t)$, defined in terms of them, also needs to be real. This restriction ensures that the imaginary part of right side of Eq. (9) to be zero. Thus, we get,

$$\kappa_R(t) = -2 \int_0^t \Omega(t') \sin \kappa_I(t') \cos \kappa_I(t') dt', \tag{10}$$

where we have already separated the complex function $\kappa(t)$ to the real and imaginary parts and labeled them as $\kappa_R(t)$ and $\kappa_I(t)$. Furthermore, we can obtain the derivative form of this equation as follows,

$$\frac{\kappa_R(t)}{\cosh \kappa_R(t)} = -2\Omega \sin \kappa_I(t). \tag{11}$$

Generally, this parametric equation cannot be solved analytically. However, it is not necessary to do so if the goal is to obtain the evolution operator. By defining a dimensionless function $\chi(t) = \int_0^t \Omega(t') dt$ in $\kappa_I(t)$, we aim to establish the relationship between the Hamiltonian and its evolution operator by parameterizing them as functions of $\chi(t)$.

To achieve the above goal, we need to parameterize $\kappa(t)$ as the function of $\chi(t)$. Since $\kappa_I(t)$ has already parameterized, we only need to deal with $\kappa_R(t)$. This parameterization is achieved by treating Eq. (11) as a differential equation for $\kappa_R(t)$ and $\kappa_I(t)$. Finally, they are parameterized as,

$$\kappa_R(t) = \ln \left[ -\tan \left( \chi + C \right) \right], \tag{12a}$$

$$\kappa_I(t) = \arcsin \frac{\chi}{\Omega}, \tag{12b}$$

where $C$ is a undetermined constant came from the integral operation of Eq. (11), which will be discussed and determined later. Since we have parameterized $\kappa(t)$ as a function of $\chi$, the only unknown parameter in the $u_{11}$ and $u_{21}$ is $\chi$. Introducing $\zeta(t) = \chi(t) + C$ for clarity, the elements of the evolution operator, $u_{11}$ and $u_{21}$, can be calculated and expressed as functions of $\zeta(t)$,

$$u_{11} = \exp \left\{ i[\theta_1 + \xi - \frac{1}{2}(\theta - \varphi - \pi)] \right\} \cos \zeta, \tag{13a}$$

$$u_{21} = \exp \left\{ i[\theta_2 + \xi + \frac{1}{2}(\theta + \varphi + \pi)] \right\} \sin \zeta, \tag{13b}$$

where the parameter $\xi(t) = \int_0^t \Omega(t') \sinh(\kappa(t')) dt' \pm \frac{1}{2} \arcsin(\chi/\Omega)$. In the above derivation, we have used two identities, i.e., $\sinh \left[ \ln \left( -\tan z \right) \right] = \cot 2x$ and $\sinh \left( \ln \left( -\tan z \right) \right) = \csc 2x$. Then, the evolution operator can be written as,

$$U_0 = \begin{pmatrix} e^{i\theta_1} e^{i\xi_C} \cos \zeta & -e^{-i\theta_2} e^{-i\xi_C} \sin \zeta \\ e^{i\theta_2} e^{i\xi_C} \sin \zeta & e^{-i\theta_1} e^{-i\xi_C} \cos \zeta \end{pmatrix}, \tag{14}$$

where $\xi_C(t) = \xi_L + [\theta + (\varphi + \pi)]/2$. Next, we address the integral constant $C$. Considering an integral constant can be arbitrary, the function $\zeta(t)$ should allow a non-zero value when $t = 0$. However, this setting appears to conflict with the initial condition stipulated in Eq. (14), which requires $\zeta(0) = 0$ to ensure that the evolution operator is the identity when $t = 0$. To resolve this contradiction, we modify the evolution operator to satisfy both the arbitrary choice of $C$ and the initial condition. It is given by,

$$U(t) = U_0(t) \cdot U_0^\dagger(0). \tag{15}$$
is generally more challenging than controlling the longitudinal $\sigma_z$ term. Hence, we present the analytical-assisted solution under $\sigma_{xy}$ control. In this case, to distinguish from Eq. (14), we denote the general Hamiltonian as

$$H_{xy} = \left( \frac{\Delta'(t)}{\Omega'(t)} e^{-i\varphi(t)} - \Delta'(t) \right),$$  

(17)

here the off-diagonal part of the Hamiltonian can be designed arbitrarily, the diagonal part cannot. To address this, we introduce a transformation to convert this off-diagonal controllable Hamiltonian into a diagonal controllable one, which is solvable as shown in the previous section. The transformation is

$$U_R(t) = \exp \left[ -\frac{\pi}{4} \left( \begin{array}{cc} 0 & e^{-i(\varphi(t)+\frac{\pi}{4})} \\ e^{i(\varphi(t)+\frac{\pi}{4})} & 0 \end{array} \right) \right],$$

(18)

then the Hamiltonian in Eq. (17) is changed to

$$H' = i \frac{\partial U_R^\dagger}{\partial t} U_R + U_R^\dagger H_{xy} U_R
$$

\begin{align*}
\left( \frac{\Omega'}{2} + \frac{1}{2} \dot{\varphi} \right) e^{i\varphi} & \quad \left( \frac{-\Delta' + \frac{1}{2} \dot{\varphi} e^{-i\varphi}}{1} \right),
\end{align*}

(19)

Now, since $\Omega'(t)$ is arbitrary, comparing with the Hamiltonian in Eq. (14), the evolution operator can be obtained by treating $(\Omega'(t) + \dot{\varphi}/2)$ as the new parameter of the $\sigma_z$ term in Eq. (14). As a result, the evolution operator can be written as

$$U(t) = U_R(t) U'(t) U_R^\dagger(0).$$

(20)

where $U'(t)$ is the evolution operator respect to the Hamiltonian in Eq. (19), which can be obtained according to the $\sigma_z$ control case. And, the controllable off diagonal part in Eq. (17) can be expressed as,

$$\Omega'(t) = \frac{\dot{\varphi} - \frac{\Delta''}{2} \frac{\dot{\varphi}}{\Omega''} \csc (\zeta) - \frac{\dot{\varphi}}{2}},$$

(21)

where $\Delta'' = -\Delta'(t) + \frac{1}{2} \dot{\varphi}(t)$. Furthermore, this analytical quantum dynamics enables the use of phase modulation, in addition to conventional amplitude shaping, in designing the pulse. As a simple case, we design a Hadamard gate when existing a harmful constant detuning $\Delta' = 2\pi$ MHz and the time-dependent phase $\varphi(t) = \sin(2\pi t/T)$, as shown in Fig. 2. The parameters of $\zeta(t)$ is $\{A_0, A_1, A_2, A_3\} = \{\pi/8, 0.26, 1\}$ and $T = 0.69 \mu s$. The fidelity of the state $|\psi(t)\rangle$ is defined as $F(t) = |\langle \Psi | \psi(t) \rangle|^2$, where $|\Psi\rangle$ labels the ideal target state.

C. Dynamics

Now we write the evolution operator in Eq. (15),

$$U(t) = \left( \begin{array}{cc} U_{11} & -U_{21}^* \\ U_{21} & U_{11} \end{array} \right),$$

(22)

where
Notice that the evolution depends on various parameters and ultimately depends on the time-independent term of the Hamiltonian and the auxiliary function \( \zeta(t) \). Such as the parameter \( \xi(t) \), which mainly depend on the integral of \( \zeta(t) \), and, the parameters \( \zeta(0) \) or \( \zeta(T) \) are the boundary conditions of \( \zeta(t) \). Therefore, a near infinite number of analytical solutions can be obtained since the auxiliary function \( \zeta(t) \) can be arbitrarily set.

Then, we will demonstrate that analytically-assisted solutions can reduce to well-known analytical solutions of Schrödinger equation. The dynamics for Landau-Zener transition, such as a ground state is driven through the anti-crossing produced if we set the auxiliary function \( \zeta(0) \) or \( \zeta(T) \) are the boundary conditions of \( \zeta(t) \). Therefore, a near infinite number of analytical solutions can be obtained since the auxiliary function \( \zeta(t) \) can be arbitrarily set.

In this section, we demonstrate that the analytical solution can be utilized to implement universal gates with smooth pulses, which are well-suited for experimental setups.

**III. APPLICATIONS**

In this section, we demonstrate that the analytical solution can be utilized to implement universal gates with smooth pulses, which are well-suited for experimental setups.

**A. Gate operation in semiconductor qubits**

The Hamiltonian for ST qubit in semiconductor double quantum dot systems \([23, 28, 29]\) is

\[
H_{ST}(t) = \hbar \sigma_x + J(t) \sigma_z,
\]

with the qubit basis being defined as \( |0\rangle = |T\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2} \) and \( |1\rangle = |S\rangle = (|\uparrow\rangle - |\downarrow\rangle)/\sqrt{2} \), where \( |\uparrow\rangle \) / \( |\downarrow\rangle \) indicates the spin up/down of an existed electron in left or right dot. \( \hbar = g \mu_B \Delta \) and \( J(t) \) is the exchange interaction of two dots. Considering the randomized benchmarking (RB) \([30, 32]\) would choose different quantum gates randomly in Clifford gate series to test the quality of gate implementation, these 24 Clifford gate \([33]\) need to be implemented by the Hamiltonian Eq. (25). In the single-transmon (ST) qubit system, the Hamiltonian comprises only the \( \sigma_x \) and \( \sigma_z \) terms, which are used for implementing quantum gates. Typically, the value in the \( \sigma_x \) term remains time-independent. Previously, to implement quantum gates, it was necessary to keep the time-dependent parameter \( J(t) \) constant throughout the evolution, as the dynamics could not be solved if \( J(t) \) is time-dependent. Therefore, this manipulation can result in unwanted discontinuities in the pulse profile at the beginning and
end of each gate when randomized benchmarking (RB) is performing. These discontinuities can lead to infidelities in the RB process, as it is challenging to achieve exact realization in experiments. Therefore, we prefer smooth pulse schemes without such breaking points.

We demonstrate that these smooth pulses can be achieved using the analytical-assisted solution. The Hamiltonian in Eq. (25) and Eq. (16) suggests that the time-dependent control scheme is suitable for the ST qubit system. Since $\hbar$ is time-independent and $\varphi = 0$, we obtain the expression of $J(t)$ as a functional of $\zeta(t)$ as

$$J(t) = \frac{\dot{\zeta}(t)}{2\hbar\sqrt{1 - \frac{\dot{\zeta}(t)^2}{\hbar^2}}} - \hbar \sqrt{1 - \frac{\dot{\zeta}(t)^2}{\hbar^2}} \cot [2\zeta(t)].$$

Note that, the evolution operator in Eq. (14) does not depend on $\zeta(t)$ directly. Therefore, it is possible to design the suitable $\zeta(0)$ and $\dot{\zeta}(T)$ ensure that the value of $J(t)$ at the start and end points can be a fixed constant (usually zero) in the implementation of all the 24 Clifford gate operations. As the result, a RB process with smooth pulse is obtained.

As demonstrations, we show how to construct Hadamard gate and S gate, which are the generators of the group of 24 Clifford gate operations. To achieve smooth pulses, we set the value of the time-dependent $J(t)$ to be zero at the start and end points for both gates. For H gate, the $\pi$ rotation around the axis $x + z$, we choose the boundary condition of $\zeta(0) = \zeta(t) = 3\pi/8$, numerically solve equations to ensure $\xi_{\pm} = \pi/2$. As a specific example, we choose the trigonometric series of $\zeta(t)$ in Eq. (24) as

$$\zeta(t) = A_0 + A_2 \cdot \sin^2 \left(\frac{a_2 \pi t}{T}\right) + A_3 \cdot \sin^3 \left(\frac{a_3 \pi t}{T}\right),$$

with parameters $\{A_0, A_1, A_2, a_2, A_3, a_3\} = \{3\pi/8, 0, -0.22, 4, 0.18, 1\}$. Under these settings, a H gate is implemented. The pulse shape of $J(t)/\hbar$, the corresponding state population and the gate-fidelity dynamics of this case are shown in Fig. 3.

Besides, to realize S gate, or any other phase gates, the decomposition in ST qubit system is

$$R(\sigma_z, \xi) = H R(\sigma_x, \xi) H,$$
Furthermore, another application of our solution is the ability to achieve precise control over both the target subspace and the nearby subspace. This allows for using one pulse to control two subspaces individually. Specifically, in the target subspace, a resonant Rabi process is implemented by designing the Rabi rate $\Omega(t)$ and the phase $\varphi$. The integral area of $\int_0^T \Omega(t) dt$ is then calculated to realize the desired quantum gates, where $T$ labels the operation duration. This Rabi process with different phase $\varphi$ could obtain universal control over the target resonant subspace. Notice the quantum gates in this resonant subspace do not restrict the pulse shape but only set the pulse integrals. Meanwhile, for the nearby detuned subspace, we can design the pulse shape to match the analytical-assisted solution and achieve universal quantum control over it, as long as we do not change the value of the pulse integral. As the result, an arbitrary individual control over two transitions can be obtained.

Now, we show the example to obtain individual controlling. The choice is $\zeta(0) = \zeta(T) = \pi/4$ with free $\varphi(t)$, it can implement arbitrary phase gates, as shown in Fig. 1. The corresponding evolution operator of the whole space at $t = T$ is

$$U_r = \begin{pmatrix}
\cos[\int \Omega dt] & -i\sin[\int \Omega dt]e^{-i\varphi} \\
-i\sin[\int \Omega dt]e^{i\varphi} & \cos[\int \Omega dt]
\end{pmatrix},$$

$$U_d = \begin{pmatrix}
e^{-i\zeta} & 0 \\
0 & e^{i\zeta}
\end{pmatrix}.$$  

(31a)  

(31b)

Since the phase $\xi$ depends on $\zeta(t)$, we can design $\zeta(t)$ to implement a desired phase gate. Such as, an identity gate can be obtained when $\xi = \pi$. We show numerical simulations of the case, which implementing an individual control consisted of a NOT gate in resonant subspace and a phase gate in the detuned subspace, described in Fig. 2. Moreover, for the situation $\varphi = 0$, another choice of $\zeta(t)$ can be used, it is $\zeta(0) = \zeta(T) = \pi/6$. It implements a rotation gate around the axis $\sigma_x$ in the resonant subspace and a gate determined by the value of $\xi$ in the nearby detuned subspace. The corresponding evolution operator is

$$U_r = \begin{pmatrix}
\cos[\int \Omega dt] & -i\sin[\int \Omega dt] \\
-i\sin[\int \Omega dt] & \cos[\int \Omega dt]
\end{pmatrix},$$

$$U_d = \begin{pmatrix}
\cos \xi + i\sqrt{3}/2 & \frac{i}{2}\sin \xi \\
\frac{i}{2}\sin \xi & \cos \xi - i\sqrt{3}/2 \sin \xi
\end{pmatrix}. $$

(32a)  

(32b)

If we design $\zeta(t)$ to satisfy $\zeta(T) = \pi$ and ensure $\int_0^T \Omega(t) dt = \pi$, we can realize an individual control gate consisting of a NOT gate in the resonant subspace and an identity gate in the detuned subspace. As known, a direct square pulse implementing the same individual control gate requires $\Omega = \Delta/\sqrt{3}$, which can be reproduced by this analytical solution case when setting $\zeta(t) = \pi/6$ for the whole time.

IV. CONCLUSION

In conclusion, we present an analytical-assisted solution of time-dependent Schrödinger equation for two level quantum system under driving, with few limitations. We show the details of the analytical progress and present some concrete examples to demonstrate its application in quantum control, i.e., deriving smooth pulse for the gate operation in ST qubit systems and individual control over two transitions with nearby frequencies. Further exploration in the field maybe the following. First, this solution could also take the gate robustness into account by choosing different free parameters. Second, it is also important to extend the study to higher level systems, e.g., three level system, which can be used to model superconducting transmon qubits.

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