Time-optimal bang-bang control for the driven spin-boson system

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In this paper we investigate the application of optimal control of a single qubit coupled to an ohmic heat bath. For the weak bath coupling regime, we derive a Bloch-Redfield master equation describing the evolution of the qubit state parametrized by vectors in the Bloch sphere. By use of the optimal control methodology we determine the field that generates an arbitrary single qubit rotation in minimum time. In particular we develop an efficient method for solving the time-optimal control problem, namely the implementation of X gate, which consists of a rotation about the $\vec{ox}$ axis through angle π. The time-optimal control problem requires a bounded control. If upper and lower bounds are imposed for the external control, the optimal solution is of bang-bang type and switches from the upper to the lower values of the control bounds. We compare our results using the techniques of automatic differentiation to compute the gradient for the cost functional with some known results using Pontryagin's minimum principle. We use an alternative numerical approach for the optimization strategy.

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I. INTRODUCTION

Given a physical quantum device, the study of how to efficiently generate a target unitary gate is important for both fundamental theory and quantum technology [1]. A powerful approach to this task is to use a time-varying Hamiltonian [2]. From the point of numerical optimization methods, finding accurate time-optimal protocols is difficult because it is a two-objective optimization problem: one must maximize the gate fidelity and simultaneously minimize the transition time between the identity and the target gate. To overcome this difficulty, we employ the penalty approach involving a Lagrangian multiplier [3].

Since real systems experience noise from their environment which induces decoherence (decay of the off-diagonal elements of the reduced density matrix) and dissipation (change of population of the reduced density matrix). In the weak system-bath coupling limit, the two-level system (TLS) Hamiltonian is not diagonal and one must solve the time-dependent Schrödinger equation to compute the coherent propagator. Then master equations derived in the weak system-bath coupling will generally involve nontrivial propagations of the coherent system. In this case, the application of Pontryagin's minimum principle (PMP) [4] to the optimal control problem is less easy. However, the automatic differentiation (AD) [5] allows us to compute the gradient for the cost functional with high precision. AD is a powerful tool that allows calculating derivatives of implemented algorithms with respect to all of their parameters up to machine precision, without the need to explicitly add any additional functions [6].

Thus AD has great potential in optimal control theory, where gradients are omnipresent but also difficult to obtain. The automatic differentiation method has been successfully applied to coherent destruction of tunneling [7] and driving-induced tunneling oscillation [8]. We also applied AD to optimal generation of a single-qubit rotation at fixed target time [9].

A theory of optimal control is a well developed field and finds numerous applications to the optimization of nonlinear and highly complex dynamic systems [10]. This approach has the great advantage that the decoherence control can be achieved [11,12] without making radical approximations such as rotating wave approximation or short time approximation usually used for time-ordering manipulations [13]. Optimal control theory provides a systematic and flexible formalism that can be used to find the time-optimal pulse sequence for the manipulation of multiqubit dissipative systems and for the implementation of the quantum logical gates (see Ref. [14] for a recent review, and references therein)

In the present paper we consider the numerical solution of the minimum time-optimal control problem. We try to implement the X gate by minimizing the cost functional involving the resolvent of the master equation. An important property of our cost functional is its independence of the initial state. The dissipative effect was described by the so-called driven spin-boson model [15,16] in which a quantum TLS is modeled by a spin, the environmental heat bath by quantum oscillators, and the spin subjected to an external control field is coupled to each bath oscillator independently. The spin-boson model is a widely used model system. It can be mapped to a number of physical situations [17]. In the theory of open quantum systems, the spin-boson model is actually one of the most popular models and has gained recent practical importance in the field of quantum computation [1]. A special variant of it, in which the interlevel coupling is absent, is known as the independent–boson model [18].

These models have been used to study the role of the electron-phonon interaction in point defects and quantum dots, interacting many-body systems, magnetic molecules, bath assisted cooling of spins, and a two level Josephson

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junction [19–24]. It has also been applied to the dissipative Landau-Zener problem [25].

The dynamics of a generic quantum XOR gate operation involving two interacting qubits being coupled to a bath of harmonic was explored [26]. The quantization of such a system was done using the double path integrals methodology [15,27].

In the case of bounded control and in the absence of dissipation, the optimal solution is of bang-bang type. It switches from the upper to the lower values of the control bounds. In the presence of dissipation the numerical results show that the optimal solution is of bang-bang type too. Then we conjecture that the driven spin-boson model in weak-system bath coupling is controllable.

The remainder of the paper is organized as follows. In Sec. II we present a derivation of Born-Markov master equations for dissipative N-level quantum systems in the presence of the time-dependent external control field. The master equation is written as a set of Bloch-Redfield equations. The latter is the starting point for the derivation of the kinetic equation for the driven spin-boson model as outlined in Sec. III. In Sec. IV we introduce the concept of the resolvent. In Sec. V we define a single qubit rotation. We define the time-optimal control problem in Sec. VI. In Sec. VII we describe the techniques of AD. In Sec. VIII we present our numerical results. Summary and conclusion are given in Sec. IX.

II. BLOCH-REDFIELD FORMALISM

We begin by reviewing some basic facts about the Bloch-Redfield formalism for general driven dissipative systems in the weak system-coupling limit. We consider a physical system S embedded in a dissipative environment B and interacting with a time-dependent classical external control field. Note that we take $\hbar = k_B = 1$ throughout this paper. The Hilbert space of the total system $\mathcal{H}_{\text{tot}} = \mathcal{H}_S \otimes \mathcal{H}_B$ is expressed as the tensor product of the system Hilbert space $\mathcal{H}_S$ and the environment Hilbert space $\mathcal{H}_B$. Here, we suppose that $\mathcal{H}_S$ is N dimensional with some time-independent orthonormal basis $\{|i\rangle\}$, $i = 1, 2 \ldots N$. The total Hamiltonian has the general form

$$H_{\text{tot}} = H_c(t) + H_b + H_{\text{int}}, \tag{2.1}$$

where $H_c(t)$ is the system part of the Hamiltonian, H_b describes the bath, and H_{int} is the system-bath interaction that is responsible for decoherence. The operators $H_c(t)$ and H_b act on $\mathcal{H}_S$ and $\mathcal{H}_B$, respectively. The system Hamiltonian $H_c(t)$ is explicitly time dependent through the external control field.

The system-environment interaction is assumed to be of bilinear form $H_{\text{int}} = A \otimes B$ with A and B Hermitian operators of the system and the environment, respectively.

In order to investigate decoherence in the limit of weak system-bath coupling, the Bloch-Redfield formalism can be used to derive a set of master equations for the reduced density matrix $\rho_s(t) = \text{tr}_{\text{B}}\{\rho_{\text{tot}}(t)\}$ describing the system dynamics, where ρ_{tot} is the total density matrix for both the system and the bath. Starting from the Liouville–von Neumann equation $i\dot{\rho}_{\text{tot}}(t) = [H_{\text{tot}}, \rho_{\text{tot}}(t)]$ for the total density operator and after performing Born and Markov approximations, one obtains the Bloch-Redfield master equation for $\rho_s(t)$ in the basis $\{|i\rangle\}$ [28,29]

$$\dot{\rho}_{s,ij}(t) = -i \sum_{kl} [H_{s,ik}(t)\delta_{lj} - \delta_{ik} H_{s,lj}(t)]\rho_{s,kl}(t) - \sum_{kl} \mathcal{D}_{ijkl}(t)\, \rho_{s,kl}(t), \tag{2.2}$$

where the first term on the right-hand side represents the unitary part of the dynamics generated by the system Hamiltonian $H_s(t)$ and the second term accounts for dissipative effects of the coupling to the environment. The Redfield relaxation tensor $\mathcal{D}_{ijkl}(t)$ is given by

$$\mathcal{D}_{ijkl}(t) = \delta_{lj} \sum_r \Gamma^+_{irrk}(t) + \delta_{ik} \sum_r \Gamma^-_{lrrj}(t) - \Gamma^+_{ljik}(t) - \Gamma^-_{ljik}(t), \tag{2.3}$$

where the time-dependent rates $\Gamma^\pm_{ijkl}(t)$ are evaluated as

$$\Gamma^+_{lj,ik}(t) = \int_0^t dt' \langle B(t-t')B(0)\rangle_B \times A_{lj} \sum_{m,n} U^c_{im}(t,t') A_{mn} U^{c*}_{kn}(t,t'),$$
$$\Gamma^-_{lj,ik}(t) = \int_0^t dt' \langle B(0)B(t-t')\rangle_B \times \sum_{m,n} U^c_{lm}(t,t') A_{mn} U^{c*}_{jn}(t,t')\, A_{ik}, \tag{2.4}$$

with

$$U^c(t,t') = \mathcal{T}\left\{\exp\left[-i\int_{t'}^t d\tau\, H_c(\tau)\right]\right\} \tag{2.5}$$

being the propagator of the coherent system dynamics satisfying the Schrödinger equation

$$i\frac{\partial}{\partial t} U^c(t,t') = H_c(t) U^c(t,t'), \quad U^c(t',t') = \mathcal{I}. \tag{2.6}$$

In Eqs. (2.4), the environment correlation functions read

$$\langle B(\tau)B(0)\rangle_B = \text{tr}_{\text{B}}\{B(\tau)B(0)\rho_B\}, \tag{2.7}$$

where $\rho_{\text{B}} = \exp(-\beta H_B)/Z_B$ is the thermal equilibrium density matrix of the bath with the inverse temperature $\beta = 1/T$ and the partition function $Z_B = \text{tr}_{\text{B}}\{\rho_{\text{B}}\}$. Equation (2.2) was obtained under the assumption that

$$\langle B(\tau)\rangle_B = \text{tr}_{\text{B}}\{B(\tau)\rho_B\} = 0, \tag{2.8}$$

which states that the reservoir averages of $B(\tau)$ vanish. Note that the time-dependent control field which enters $H_c(t)$ is treated nonperturbatively in the derivation of the master equation. Note also that the time-dependent control field enters the dissipative part of the evolution as well through the field-dependent relaxation rates $\Gamma^\pm_{ijkl}(t)$ via $U^c(t,t')$, which is a consequence of quantum interference between the system-bath coupling and the external coupling to the control field. This allows for an external control of dissipation [28,30].

In the next section, we will apply the foregoing formalism to a TLS coupled to a boson bath via weak diagonal TLS-bath coupling, and derive the corresponding Bloch equations satisfied by the Bloch vector of the TLS.

III. MODEL AND MASTER EQUATION

The driven spin-boson Hamiltonian in which the qubit is described as a spin-1/2 coupled to a bosonic bath and subjected to a time-dependent external force can be written as $H_{\text{tot}}(t) = H_{\text{s}} + H_{\text{c}}(t) + H_{\text{b}} + H_{\text{sb}}$, where

$$H_{\text{s}} = -\varepsilon_0\sigma_z/2, \quad H_{\text{c}}(t) = -\varepsilon(t)\sigma_x/2, \tag{3.1}$$

$$H_{\text{b}} = \sum_i \omega_i b_i^\dagger b_i, \quad H_{\text{sb}} = \sigma_z \sum_i c_i(b_i^\dagger + b_i)/2. \tag{3.2}$$

Here H_{s} is the bare qubit Hamiltonian, in which $\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$ and $\sigma_x = |0\rangle\langle 1| + |1\rangle\langle 0|$, where $|0\rangle$ and $|1\rangle$ denote the computational basis states. H_{c} specifies the coupling between the σ_x qubit operator and the control field $\varepsilon(t)$. H_{b} is the free Hamiltonian of the heat bath and H_{sb} represents the Hamiltonian interaction between the qubit and the heat bath. This situation is relevant to many experimental systems, from nuclear and electronic spin resonance to atomic systems and superconducting qubits.

The correlation environment reads

$$\langle B(\tau)B(0)\rangle_B = \sum_{ij} c_i c_j \langle [b_i^\dagger(\tau) + b_i(\tau)][b_j^\dagger(0) + b_j(0)]\rangle_B \tag{3.3}$$

$$= \int \frac{d\omega}{\pi} J(\omega) \times [\cos(\omega\tau)\coth(\beta\omega/2) - i\,\sin(\omega\tau)], \tag{3.4}$$

where the spectral density of the environment

$$J(\omega) = \pi \sum_i c_i^2 \delta(\omega - \omega_i) = 2\pi\alpha\omega\, e^{-\omega/\omega_c} \tag{3.5}$$

is assumed to be Ohmic with exponential cutoff ω_c and dimensionless system-bath coupling α chosen to be weak.

The quantum state of the qubit will be characterized by the Bloch vector defined by

$$\mathbf{p}(t) = \text{Tr}(\sigma \cdot \rho_{\text{s}}(\text{t})), \tag{3.6}$$

where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is the vector composed of the three Pauli matrices with the components

$$p_x(t) = \rho_{s12}(t) + \rho_{s21}(t),$$
$$p_y(t) = i[\rho_{s12}(t) - \rho_{s21}(t)],$$
$$p_z(t) = \rho_{s11}(t) - \rho_{s22}(t). \tag{3.7}$$

By combining Eq. (2.2) with Eq. (3.7) we obtain the following set of Bloch equations:

$$\dot{\mathbf{p}}(t) = \mathcal{M}(t)\mathbf{p}(t) + \mathcal{R}(t), \tag{3.8}$$

with

$$\mathcal{M}(t) = \begin{pmatrix} -\Gamma_{xx}(t) & \varepsilon_0 & -\Gamma_{xz}(t) \\ -\varepsilon_0 & -\Gamma_{yy}(t) & -[-\varepsilon(t) + \Gamma_{yz}(t)] \\ 0 & -\varepsilon(t) & 0 \end{pmatrix},$$
$$\mathcal{R}(t) = [-A_x(t), -A_y(t), 0]^T. \tag{3.9}$$

Following the notation used in [29], the fluctuating terms in the inhomogeneous part $\mathcal{R}(t)$ are given by

$$A_x(t) = 2\int_0^t dt' M''(t - t')\text{Im}[U_{11}(t, t')U_{12}(t, t')],$$
$$A_y(t) = 2\int_0^t dt\, M''(t - t')\text{Re}[U_{11}(t, t')U_{12}(t, t')], \tag{3.10}$$

and the temperature-dependent relaxation rates are determined by

$$\Gamma_{ij}(t) = \int_0^t dt' M'(t - t')b_{ij}(t, t'), \tag{3.11}$$

with $\Gamma_{xx}(t) = \Gamma_{yy}(t)$.

In Eqs. (3.11) and (3.12), the functions M' and M'' are the real part and imaginary part, respectively, of the bath correlation function (3.4), which can be written in the following form:

$$M(t) = \frac{1}{\pi}\int_0^\infty d\omega\, J(\omega)\frac{\cosh\left(\frac{\beta\omega}{2} - i\omega t\right)}{\sinh\left(\frac{\beta\omega}{2}\right)}. \tag{3.12}$$

The functions $b_{ij}(t, t')$ read

$$b_{xx}(t, t') = \text{Im}[U_{11}^2(t, t') - U_{12}^2(t, t')],$$
$$b_{xz}(t, t') = 2\,\text{Re}[U_{11}(t, t')U_{12}(t, t')],$$
$$b_{yz}(t, t') = -2\,\text{Im}[U_{11}(t, t')U_{12}(t, t')], \tag{3.13}$$

where $U(t, t')$ is the nondissipative time evolution operator for the spin system with $U_{11}(t, t') = \langle 0|U(t, t')|0\rangle$ and $U_{12}(t, t') = \langle 0|U(t, t')|1\rangle$, and satisfies the Schrödinger equation

$$\dot{U}(t) = \frac{i}{2}[\varepsilon_0\sigma_z + \varepsilon(t)\sigma_x]\, U(t). \tag{3.14}$$

In the case of a driven spin-boson model, it has been shown that the Bloch-Redfield master equation (3.8), which was obtained without using the so-called secular or rotating wave approximation, is equivalent to the double path-integral formulation [29].

In the undriven case the analytical expression for the coherent propagator is trivial and reads

$$U_{11}(t) = \cos(\varepsilon_0 t/2) + i\,\sin(\varepsilon_0 t/2), \tag{3.15}$$

$$U_{12}(t) = 0, \tag{3.16}$$

which leads to the following analytical expressions of the free decay rates:

$$\Gamma_{xx} = \Gamma_{yy} = \tfrac{1}{2}S(\varepsilon_0), \tag{3.17}$$

$$\Gamma_{xz} = 0, \tag{3.18}$$

$$\Gamma_{yz} = 0, \tag{3.19}$$

$$A_x = 0, \tag{3.20}$$

$$A_y = 0, \tag{3.21}$$

$$S(\varepsilon_0) = J(\varepsilon_0)\coth\,(\varepsilon_0/2T), \tag{3.22}$$

where

$$S(\varepsilon_0) = J(\varepsilon_0)\coth(\varepsilon_0/2T). \tag{3.23}$$

IV. RESOLVENT

The formal solution of the master equation (3.8) is given in terms of the resolvent $\mathcal{G}(t)$,

$$\mathbf{p}(t) = \mathcal{G}(t)\mathbf{p}(0) + \int_0^t d\tau\, \mathcal{G}(t,\tau)\mathcal{R}(\tau), \tag{4.1}$$

with $\mathcal{G}(t,\tau) = \mathcal{G}(t,0)\mathcal{G}(0,\tau) = \mathcal{G}^{-1}(t)\mathcal{G}(\tau)$ and satisfies the following equation of motion:

$$\dot{\mathcal{G}}(t) = \mathcal{M}(t)\mathcal{G}(t), \quad \mathcal{G}(0) = \mathbb{1}_{3\times 3}, \tag{4.2}$$

where $\mathcal{M}(t)$ is given by Eq. (3.9).

V. SINGLE QUBIT ROTATION

A general single qubit gate corresponds to a unitary evolution operator that acts on single qubit and is represented in the basis $\{|0\rangle, |1\rangle\}$ by the two-dimensional unitary matrices $\hat{O}(\vec{n},\delta) = e^{-i\frac{\delta}{2}\vec{n}\cdot\vec{\sigma}} \in \mathrm{SU}(2)$, which acts on the qubit as a rotation about the unit real vector $\vec{n} \in \mathbb{R}^3$ through the angle δ [1]. In the coherence vector representation, $\vec{\mathbf{p}}(t) = \mathrm{tr}_s(\vec{\boldsymbol{\sigma}}\rho_s(t))$, the unitary transformation $\hat{O}(\vec{n},\delta) \in \mathrm{SU}(2)$ is equivalent to a real rotation matrix $\hat{R} \in \mathrm{SO}(3)$. Since any qubit unitary transformation $\hat{O}$ is associated with a rotation $\hat{R}(\vec{n},\delta)$, we have $\hat{O}\rho(t)\hat{O}\dagger = [\mathbb{1} + \hat{R}\,\vec{\mathbf{p}}(t)\cdot\vec{\boldsymbol{\sigma}}]/2$. An element $\hat{R}(\vec{n},\delta)$ of the group SO(3) is given by the following expression [31]:

$$\hat{R}_{jk} = \cos\delta\,\delta_{jk} + (1-\cos\delta)n_j n_k - \sin\delta\sum_{l=1}^{3}\epsilon_{jkl}n_l, \tag{5.1}$$

with

$$\cos\delta = \frac{1}{2}(\mathrm{Tr}\hat{R} - 1), \tag{5.2}$$

and

$$n_l = \frac{-1}{2\,\sin\delta}\sum_{j,k=1}\epsilon_{jkl}\hat{R}_{jk}. \tag{5.3}$$

The tensor ϵ_{jkl} is defined by

$$\epsilon_{jkl} = \begin{cases} +1 & \text{if } (j,k,l) \text{is an even permutation of 1,2,3,} \\ -1 & \text{if } (j,k,l) \text{ is an odd permutation of 1,2,3,} \\ 0 & \text{otherwise.} \end{cases} \tag{5.4}$$

VI. TIME-OPTIMAL CONTROL PROBLEM

Now we formulate the problem of implementing a single qubit rotation at a free final time as an optimal control problem [10–12].

Let $\mathcal{G}(t)$ be the resolvent at time t. Its time evolution is governed by Eq. (4.2) with the initial condition $\mathcal{G}(0) = \mathbb{1}$. The objective is to compute an appropriate time-dependent control function $\varepsilon(t)$ steering the time evolution operator $\mathcal{G}(t)$ from the identity $\mathcal{G}(0) = \mathbb{1}$ into a desired quantum logical gate $\mathcal{G}(t_F) = \mathcal{G}_D = \hat{R}(\vec{n},\delta) \in \mathrm{SO}(3)$ at minimal time t_F. The following bounds are imposed for the control function $|\varepsilon(t)| \leqslant M$ for all $t \in [0, t_F]$. Here the final time is free but the control energy is fixed. Indeed, this goal leads to the following optimal control problem: determine a piecewise continuous control function $\varepsilon(t)$, $0 \leqslant t \leqslant t_F$, that minimizes

$$J = t_F, \tag{6.1}$$

subject to constraint control

$$|\varepsilon(t)| \leqslant M, \tag{6.2}$$

system dynamics

$$\dot{\mathcal{G}}(t) = \mathcal{M}(t)\mathcal{G}(t), \tag{6.3}$$

$$i\dot{U}(t) = [H_s + H_c(t)]U(t), \tag{6.4}$$

initial conditions

$$\mathcal{G}(0) = \mathbb{1}_{3\times 3}, \tag{6.5}$$

$$U(0) = \mathbb{1}_{2\times 2}, \tag{6.6}$$

and final condition

$$\mathcal{G}(t_F) = \mathcal{G}_D. \tag{6.7}$$

Since the final condition is given, we solve this problem using a penalty approach [3]. At step k we consider the following augmented cost function given by

$$\overline{J} = t_F + \frac{p}{2}||\mathcal{G}(t_F) - \mathcal{G}_D||_F^2 + \mathrm{Tr}\{\mu_k[\mathcal{G}(t_F) - \mathcal{G}_D]\}, \tag{6.8}$$

with the 3×3 matrix Lagrange multiplier μ and a constant penalty factor p. At step $k+1$ μ is updated by

$$\mu_{k+1} = \mu_k + p[\mathcal{G}(t_F) - \mathcal{G}_D]. \tag{6.9}$$

Note that μ_0 is given. Here $||.||_F^2$ is the Frobenius norm defined by $\|A\|_F^2 = \sum_{ij}a_{ij}^2 = \sum_{ij}a_{ij}a_{ij} = \mathrm{Tr}(AA^T)$.

By penalty approach, we solve the optimal control problem Eq. (6.1) by recursively calling the L-BFGS-B routine [32], each iteration involved in updating the value of μ. The program will stop when the value $||\mathcal{G}(t_F) - \mathcal{G}_D||_F$ is no longer decreasing. The L-BFGS-B routine is based on a bound constraint quasi-Newton method with the BFGS update rule. This routine is appropriate and efficient for solving constrained problems, i.e., Eq. (6.2).

VII. TECHNIQUES OF AUTOMATIC DIFFERENTIATION

In order to implement a single qubit rotation using the algorithm given in Sec. VI, we have to compute the gradient for the cost function (6.8), namely

$$\nabla\overline{J} = \left(\frac{\partial\overline{J}}{\partial\varepsilon(t)}, \frac{\partial\overline{J}}{\partial t_F}\right)^T. \tag{7.1}$$

In principle one can use Pontryagin's minimum principle to treat our optimal control problem and derive the gradient for the cost function $\overline{J}(\varepsilon, t_F)$ [10]. However, for a driven spin-boson model studied here, the response of the system to the variation of the control $\varepsilon(t)$ is determined by the master equation (3.8) and the equation of motion for the propagator of the coherent system dynamics Eq. (3.15). As a result, the application of Pontryagin's minimum principle is less straightforward since two operators' Lagrange multipliers have to be introduced to implement these two dynamical constraints.

An alternative to this approach is the technique of automatic differentiation [5], which in principle amounts to doing calculus on the fully discretized form of the optimal control problem. For this purpose, we first discretize the time interval $I = [0, t_F]$ into N equal-sized subintervals ΔI_k with $I = \bigcup_{k=1}^{N} \Delta I_k$ and then approximate $\varepsilon(t)$ as $\varepsilon(t) \to \varepsilon(t_k) = \varepsilon_k$, $k = 1 \dots N$. Thus the problem becomes that of finding $\vec{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_N)^T \in \mathbb{R}^N$ and the minimum time t_N such that $\overline{J}(\vec{\varepsilon}, t_N) = \inf\{\overline{J}(\vec{\zeta}) : \vec{\zeta} \in \mathbb{R}^{N+1}\}$. Automatic differentiation tools can be viewed as black boxes taking as input a program computing the cost function $\overline{J}(\vec{\varepsilon}, t_N) : \mathbb{R}^{N+1} \longrightarrow \mathbb{R}$ and giving as output another program computing the gradient $\nabla\overline{J} = (\frac{\partial \overline{J}}{\partial \varepsilon_1}, \dots, \frac{\partial \overline{J}}{\partial \varepsilon_N}, \frac{\partial \overline{J}}{\partial t_N})^T \in \mathbb{R}^{N+1}$.

Two approaches to automatic differentiation are possible: the forward (or tangent) mode and backward (or adjoint) mode which is similar to the adjoint method [5]. In this work, we employ the latter since it is theoretically more efficient in computing the gradient of a scalar value function. With the gradient obtained from the adjoint mode of automatic differentiation, the optimization of the cost function $\overline{J}(\vec{\varepsilon}, t_N)$ is then performed by using the L-BFGS-B routine [32].

VIII. NUMERICAL RESULTS

A. Nondissipative qubit

In the absence of dissipation, the resolvent $\mathcal{G}$ of the system (2.2) satisfies the following equation of motion:

$$\dot{\mathcal{G}}(t) = \mathcal{M}(t)\mathcal{G}(t), \quad \mathcal{G}(0) = \mathbb{1}_{3\times 3}, \tag{8.1}$$

where $\mathcal{M}(t)$ is given by

$$\mathcal{M}(t) = \begin{pmatrix} 0 & \varepsilon_0 & 0 \\ -\varepsilon_0 & 0 & \varepsilon(t) \\ 0 & -\varepsilon(t) & 0 \end{pmatrix}. \tag{8.2}$$

Our application is to generate in minimum time t_F X-gate $\mathcal{G}_D = \hat{R}(\vec{n}, \delta)$ with $\vec{n} = (1, 0, 0)^T$ and $\delta = \pi$. The time-optimal control problem defined in Sec. VI leads to

$$\begin{aligned} &\min \overline{J} = t_F + \frac{p}{2}||\mathcal{G}(t_F) - \mathcal{G}_D||_F^2 + \mathrm{Tr}\{\mu_k[\mathcal{G}(t_F) - \mathcal{G}_D]\} \\ &\text{subject to} \\ &\dot{\mathcal{G}}(t) = \mathcal{M}(t)\mathcal{G}(t), \quad \mathcal{G}(0) = \mathbb{1}_{3\times 3}, \\ &|\varepsilon(t)| \leqslant M, \quad \mathcal{G}(t_F) = \mathcal{G}_D. \end{aligned} \tag{8.3}$$

In order to test our algorithm we compare our results with some known results using Pontryagin's minimum principle [33]. In Fig. 1 we plot the minimum time t_F versus the amplitude M of the optimal control field. The comparison with the analytic calculation $T_{\min} = \pi^2/2M$ [33] is also shown. The agreement between the two different methods is remarkable.

For the amplitude $M = 1.5$ (arb. units) and the energy splitting $\varepsilon_0 = 5$ (arb. units) the optimal control is shown in Fig. 2. It switches back and forth between the two extremal values $-M$ and M. This is the so-called bang-bang control. The optimal control has six as the minimum number of switches. The optimal time t_F versus the number of iterations is displayed in Fig. 3 with minimum time convergence $t_F = 3.4311372908111$ (arb. units). Figure 4 shows the time evolution of the Bloch vector for two initial conditions. In Fig. 4(a) $\vec{\mathbf{p}}_I = (0, 0, 1)^T$ and Fig. 4(b) $\vec{\mathbf{p}}_I = (0, 0, -1)^T$. So the realization of the X gate is perfect. The gate fidelity $\mathrm{Tr}\{\mathcal{G}(\mathrm{t_F})\mathcal{G}_\mathrm{D}\}$ is equal to the unity.

Figure 5 displays the power spectrum of the selected optimal control field showing several pronounced peaks at near equidistant frequencies. Here $\nu = \varepsilon_0/2\pi \simeq 0.8$ (arb. units) is the fundamental frequency corresponding to the first peak of the power spectrum in Fig. 5. The remaining higher frequency peaks are located at about $(2n + 1)\nu$, where n is an integer.

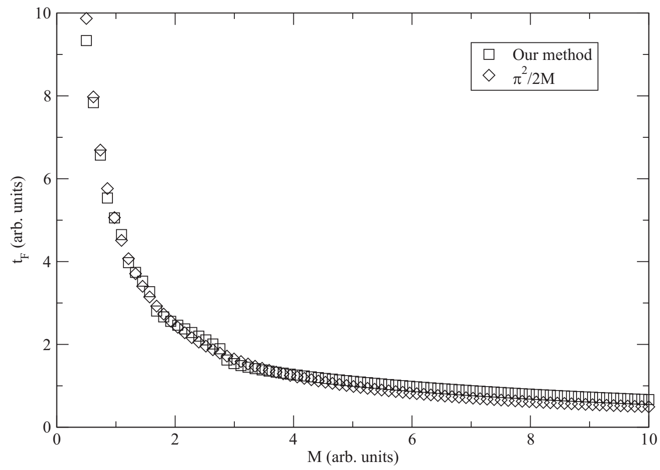

FIG. 1. Implementation of the X gate in the absence of dissipation. Depicted is the minimum time vs the amplitude of the optimal control field. The comparison with PMP is also shown. The energy splitting is set as $\varepsilon_0 = 5$ (arb. units). The number of mesh points, i.e., the dimension of the optimal control problem, is set as $N = 1000$.

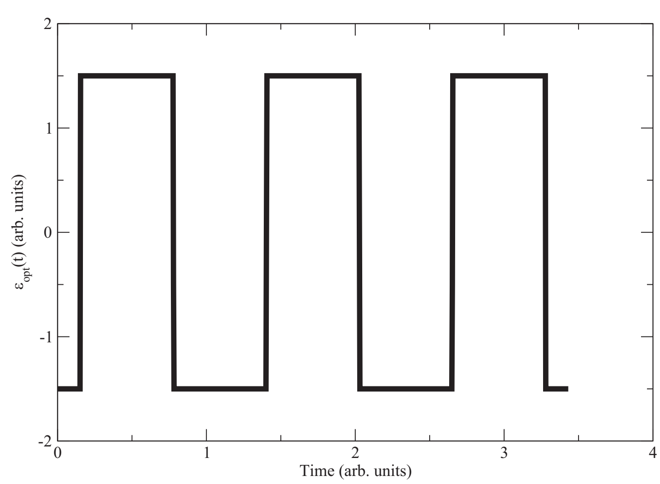

FIG. 2. Implementation of the X gate in the absence of dissipation. Depicted is the optimal control vs time. The energy splitting is set as $\varepsilon_0 = 5$ (arb. units) and the amplitude of the optimal control field is set as $M = 1.5$ (arb. units). The minimum time computed is $t_F = 3.43113729$ (arb. units). The number of mesh points, i.e., the dimension of the optimal control problem, is set as $N = 1000$.

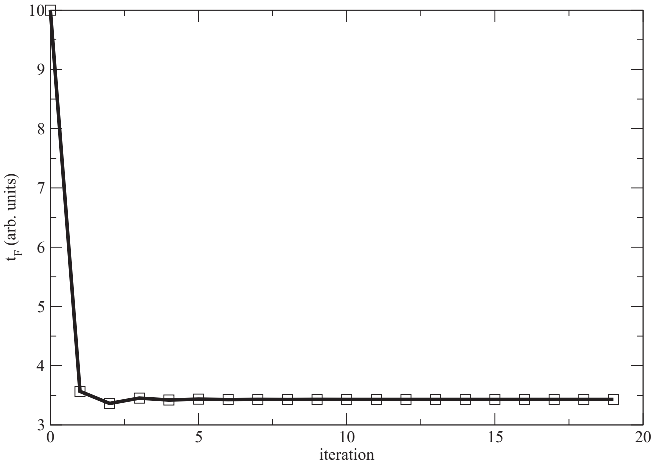

FIG. 3. Implementation of the X gate in the absence of dissipation. Depicted is the minimum time vs number of iterations. The energy splitting is set as $\varepsilon_0 = 5$ (arb. units); the amplitude of the optimal control field is set as $M = 1.5$ (arb. units). The number of mesh points, i.e., the dimension of the optimal control problem, is set as $N = 1000$.

The time-optimal trajectory is bang-bang and in particular the corresponding optimal control is periodic with frequency of the order of the resonance frequency $\nu = \varepsilon_0/2\pi$. For the example of X gate we set the penalty parameter as $p = 10$ and the optimal Lagrangian parameter μ is found to be

$$\mu_{(k=20)} = \begin{pmatrix} 8.04310837 & 5.02989022 & 5.32063140 \\ -5.02992534 & 1.01920957 & 0.63211306 \\ -4.60972806 & 1.31522137 & 0.94341099 \end{pmatrix}. \tag{8.4}$$

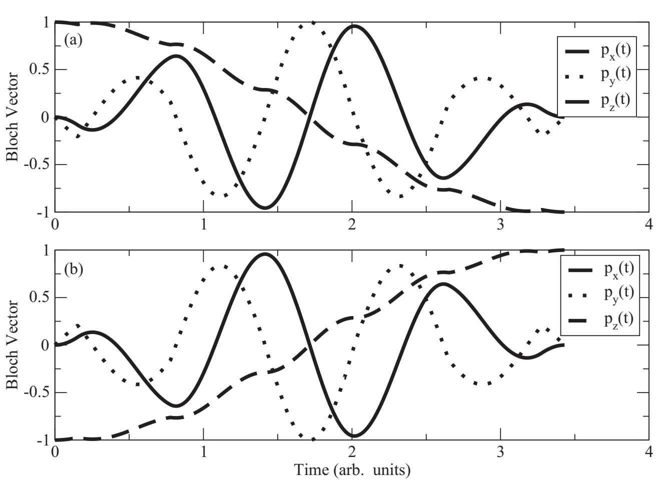

FIG. 4. Implementation of the X gate in the absence of dissipation. Depicted are the components of the Bloch vector vs time with an initial condition (a) $\vec{\mathbf{p}}_I = (0, 0, 1)^T$ and (b) $\vec{\mathbf{p}}_I = (0, 0, -1)^T$. The energy splitting is set as $\varepsilon_0 = 5$ (arb. units) and the amplitude of the optimal control field is given by $M = 1.5$ (arb. units). The minimum time computed is $t_F = 3.43113729$ (arb. units). The number of mesh points, i.e., the dimension of the optimal control problem, is set as $N = 1000$.

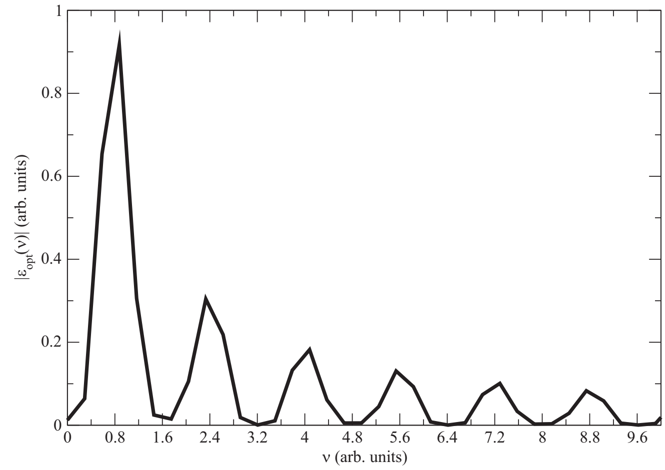

FIG. 5. Implementation of the X gate in the absence of dissipation. Depicted is the power spectrum of the optimal control field shown in Fig. 2. The parameters are the same as in Fig. 2.

Table I show the optimized time t_F versus the dimension of the optimal control problem (8.3). As one can see, t_F is independent of the dimension of the optimal control N. In order to integrate numerically the master equation I used a standard fourth-order Runge-Kutta scheme. The numerical error is of $O(h^4)$, where h is the time step given by t_F/N. In our numerical calculation $N = 1000$ and $t_F = 3.4311372908111$ (arb. units), which leads to $h = 0.0034311372908111$ (arb. units). As the time step h is small, the numerical fourth-order Rung-Kutta integration is employed with height precision. Note that AD does not work in the case of the variable time step h.

B. Dissipative qubit

Now we try again to implement the X gate $\mathcal{G}_D$ in the presence of dissipation. The quantum optimal control problem (6.1) becomes

$$\min \bar{J} = t_F + \frac{p}{2}||\mathcal{G}(t_F) - \mathcal{G}_D||_F^2 + \mathrm{Tr}\{\mu_k[\mathcal{G}(t_F) - \mathcal{G}_D]\}$$

TABLE I. Computed optimized time versus the dimension of time-optimal control problem. The bound control is set as $M = 1.5$ (arb. units) while the energy splitting is set as $\varepsilon_0 = 5$ (arb. units).

N	t_F (arb. units)
500	3.4316131619985
650	3.4312685775930
800	3.4311405965685
950	3.4311776820778
1100	3.4311063985436
1250	3.4310693331264
1400	3.4310884021711
1550	3.4310639761848
1700	3.4310488679574
1850	3.4310560403977
2000	3.4310422720740

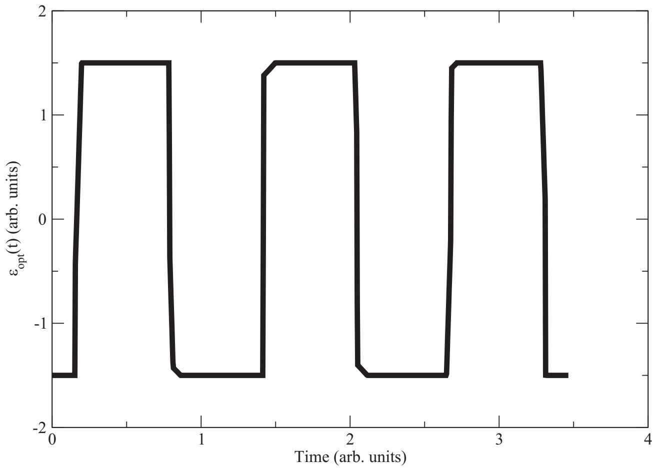

FIG. 6. Implementation of the X gate in the case of dissipative dynamics. Depicted is the optimal control vs time. The minimum time computed is $t_F = 3.46498957$ (arb. units). The parameters are the same as in Fig. 7.

subject to

$$\dot{\mathcal{G}}(t) = \mathcal{M}(t)\mathcal{G}(t), \quad \mathcal{G}(0) = \mathbb{1}_{3\times 3},$$
$$|\varepsilon(t)| \leqslant M, \quad \mathcal{G}(t_F) = \mathcal{G}_D,$$
$$\dot{U}(t) = \frac{i}{2}\big[\varepsilon_0\sigma_z + \varepsilon(t)\sigma_x\big]U(t),$$
$$U(0) = \mathbb{1}_{2\times 2}, \tag{8.5}$$

where the relaxation matrix $\mathcal{M}(t)$ is given by Eq. (3.9).

In numerical simulations we employ the following parameters: the cutoff frequency $\omega_c = 20$ (arb. units); the temperature $1/\beta = 0.5$ (arb. units); the system bath coupling $\alpha = 0.002$; the energy splitting $\varepsilon_0 = 5$ (arb. units); the amplitude of the optimal control field is set as $M = 1.5$ (arb. units). The penalty factor is set as $p = 10$ and the Lagrange multiplier $\mu_0 = 0$. In order to solve the problem (8.5) we use as a guess the optimal solution for the nondissipative case.

Figure 6 displays the time dependence of the optimal control. The optimal solution is again a bang-bang control. Figure 7 shows the time evolution of the Bloch vector for the initial condition, Fig. 7(a) $\vec{\mathbf{p}}_I = (0, 0, 1)^T$ and Fig. 7(b) $\vec{\mathbf{p}}_I = (0, 0, -1)^T$. The gate error $\|\mathcal{G}(t_F) - \mathcal{G}_D\|_F^2$ is small because the temperature $\beta^{-1} = 0.5$ (arb. units) is lower than the energy splitting $\varepsilon_0 = 5$ (arb. units) and the system bath coupling $\alpha = 0.002$ is weak. It is a regime where the Bloch-Redfield formalism is applicable.

Figure 8 and Fig. 9 display respectively the time dependence of the decay rates and the inhomogeneous terms appearing in the master equation (3.8). In contrast to the undriven case where the rates are constants the dynamics of these controlled rates reflects the temporal structure of the optimized control field. For the example of X gate we set the penalty parameter as $p = 10$ and the optimal Lagrangian parameter μ is found to be

$$\mu_{(k=5)} = \begin{pmatrix} 6.95793447 & 5.25331597 & 5.10706782 \\ -5.23693644 & 2.08138742 & 0.75639663 \\ -4.81875515 & 1.18759004 & 1.48704919 \end{pmatrix}. \tag{8.6}$$

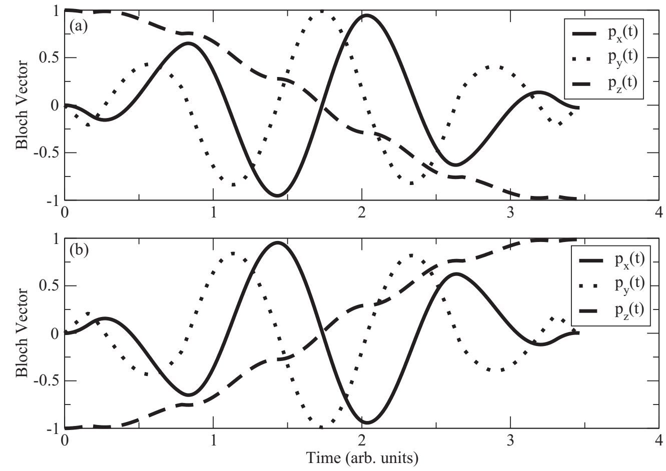

FIG. 7. Implementation of the X gate in the presence of dissipation. Depicted are the components of the Bloch vector vs time with an initial condition (a) $\vec{\mathbf{p}}_I = (0, 0, 1)^T$ and (b) $\vec{\mathbf{p}}_I = (0, 0, -1)^T$. The minimum time computed is $t_F = 3.46498957$ (arb. units). The spin-boson parameters are as follows: the cutoff frequency $\omega_c = 20$ (arb. units); the temperature $1/\beta = 0.5$ (arb. units); the system bath coupling $\alpha = 0.002$. The energy splitting $\varepsilon_0 = 5$ (arb. units) and the amplitude of the optimal control field is set as $M = 1.5$ (arb. units). The penalty factor is set as $p = 10$ and the Lagrange multiplier $\mu_0 = 0$. The number of mesh points, i.e., the dimension of the optimal control problem, is set as $N = 1000$.

C. Sensitivity analysis

Because of the external perturbations, practical devices are not capable of operating precisely either at the prescribed system parameters or at the computed control field. Then, it is of great importance to have information on the sensitivity of the optimal solution with respect to perturbations of any of the system parameters. For demonstration purposes, we consider the fluctuations of the initial conditions of the system. More

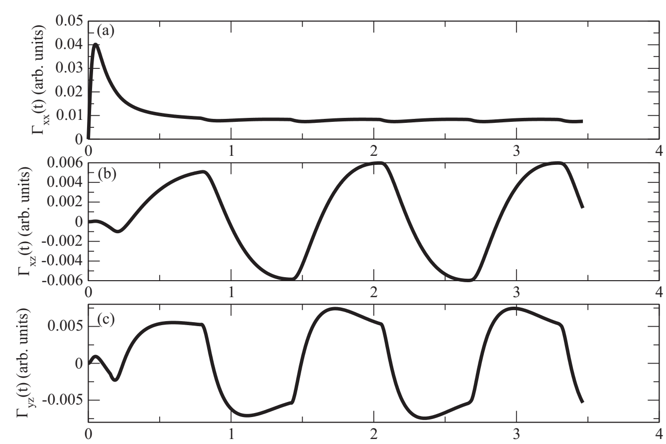

FIG. 8. Implementation of the X gate in the presence of dissipation. Depicted is the time evolution of the decay's rate under the influence of the optimal control field. The minimum time computed is $t_F = 3.46498957$ (arb. units). The parameters are the same as in Fig. 7.

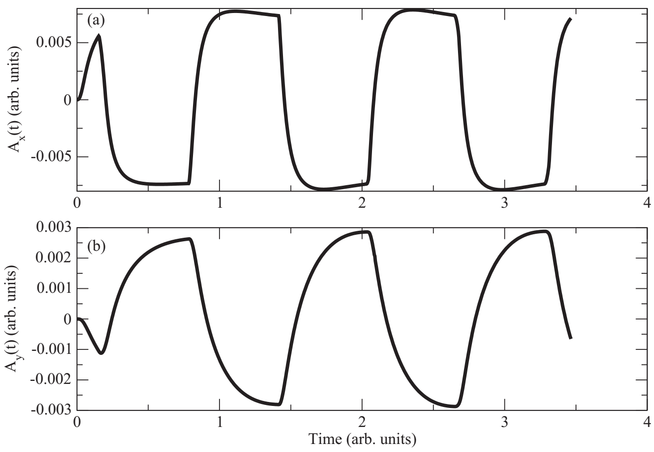

FIG. 9. Implementation of the X gate in the presence of dissipation. The time dependence of the inhomogeneous terms. The parameters are the same as in Fig. 7.

precisely we consider the average fidelity defined by

$$\overline{F} = \frac{1}{N}\sum_{j=1}^{N} \vec{\mathbf{p}}_j(t_F)\cdot \mathcal{G}_D \vec{\mathbf{p}}_j(0), \tag{8.7}$$

where

$$\vec{\mathbf{p}}_j(t_F) = \mathcal{G}(t_F)\vec{\mathbf{p}}_j(0) + \mathcal{G}^{-1}(t_F)\int_0^{t_F} d\tau\, \mathcal{G}(\tau)\mathcal{R}(\tau) \tag{8.8}$$

and $\vec{\mathbf{p}}_j(0) = (\cos\theta_j \sin\phi_j, \sin\theta_j \sin\phi_j, \cos\theta_j)^T$ is an input state. $\theta_j \in [0, \pi]$ and $\phi_j \in [0, 2\pi]$ are randomly chosen. We can calculate the average fidelity when the optimized control sequence is repeated N times assuming the initial condition $\vec{\mathbf{p}}_j(0)$ to be a random variable. In our numerical calculations, we get small statistical errors when N is about several thousand. For the quantum X gate, we find the following average fidelity $\overline{F} = 0.97945779$ and the standard deviation $\sigma_F = 0.01035038$. The overall high values of the average fidelity indicate that the optimal bang-bang control we obtained is indeed robust with random initial conditions.

IX. SUMMARY

In this work we investigated the realization of X gate in a driven spin-boson system. We use a bounded control. In the nondissipative case our numerical results agree with the results using the techniques of automatic differentiation with some known results using Pontryagin's minimum principle. The optimal control is bang-bang type for both the absence and presence of dissipation. Following our numerical results, we conjecture that the dissipative qubit is controllable. Our method works for an arbitrary single qubit rotation in minimum time. We also implemented the Hadamard gate which consists of a rotation about the $\vec{ox}$ or $\vec{oy}$ axis through angle $\pi/2$. It is not shown here for brevity. Our main objective is to extend this work to two qubits.

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