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Realization of Quantum Hadamard Gate by Applying Optimal Control Fields to a Spin Qubit

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***Abstract*—In this paper, we study the manipulation of a two level quantum mechanical system which is the basic unit of representing data in quantum information science, a *qubit*. This research is motivated by the design of the quantum Hadamard gate for solid state spin qubits. We consider the problem of driving the initial state of a qubit into a desired final state in a specified time, while minimizing the energies of the control fields. Optimal control theory is employed to define optimum control fields which satisfy both dynamical constraints and optimality conditions. Time evolution of the system is calculated within the Schrödinger equation and a gradient method is used for tailoring optimal control fields.**

***Index terms*—solid state spin qubits; quantum Hadamard gate; optimal control theory; gradient methods.**

I. INTRODUCTION

The new emerging field of quantum computation has attracted much attention in the past two decades. The basic principle behind quantum computation is to utilize quantum mechanical systems as building blocks of a computing machine, a *quantum computer*. With the help of quantum mechanical principles, such as superposition and entanglement, quantum computers can efficiently perform certain computational tasks much faster than their classical counterparts [1].

In general, any two level quantum mechanical system can be used for the purpose of physical realization of quantum computers [2]. Several different schemes have been investigated to this aim, e.g. nuclear magnetic resonance quantum computer [3], quantized states of superconducting devices [4], trapped ions [5], etc. Although the knowledge acquired by these studies is so beneficial to our understanding of quantum computing systems, but the problem of scalability is one of their major obstacles. Large networks of various extremely small semiconductor devices are integrated on wafers nowadays. Therefore, solid state quantum computation is the most promising candidate that may overcome the challenging problem of scalability [6].

One of the most significant proposals for the physical realization of quantum computers is based on the spin states of single electrons confined to semiconductor quantum dots [6]. Quantum dots are small regions in semiconductors that can be filled with few electrons, up to zero, and confine their motions in all three dimensions. Quantum dots formed in semiconductor heterostructure based on GaAs technology have attracted much interest in recent years [7]. Different quantum logic gates can be realized by manipulating the spin states of the electrons confined to these quantum dots. Single and two qubit operations can be achieved by applying pulsed local electromagnetic fields and electrical gating of the tunneling barrier between neighboring quantum dots respectively [8]. Solid state spin based devices are expected to dominate the field of quantum computation by exploiting the developed field of semiconductor devices fabrication technology.

The aim of this paper is to realize quantum Hadamard gate by applying tailored control fields to the spin of a single electron confined to a semiconductor quantum dot. Quantum Hadamard gate is one of the most useful quantum logic gates. It maps a basis state to a superposition of basis states with equal weights. This property makes it useful in many quantum computing algorithms [9]. We have to consider physical restrictions in order to realize practical quantum logic gates. Undesired interaction of solid state qubits with environment leads to decoherence. Thus gate operation times should be much shorter than decoherence times [6]. Therefore, we need to perform transition of states in specified times. We would also like to keep the control fields small, in order not to disturb neighboring spins that, at the same time, are performing some other logic operations [10]. Optimal control theory provides a powerful set of tools and concepts to deal with quantum control problems. In the present work we apply optimal control theory to the problem of steering state of a spin qubit in a specified time while minimizing an energy-type cost functional. Due to complex nonlinear dynamics of the system it is inevitable to use numerical methods to solve this problem.

The paper is organized as follows. In Section II, we will briefly review a solid state spin qubit. Mathematical model of quantum Hadamard gate which describes the dynamics of the system will be derived in section III. Optimal control of the system is formulated within Pontryagin's principle in Section IV. In Section V, we present an iterative numerical procedure in the form of a gradient method to define optimal control fields. Concluding remarks are given in section VI.

II. SOLID STATE SPIN QUBITS

Qubit is the basic unit of representing data in quantum information science. Despite having two possible states like its classical analogue, either $|0\rangle$ or $|1\rangle$, a qubit can be in a superposition of basis states:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \tag{1}$$

where, α and β are complex numbers, restricted by the

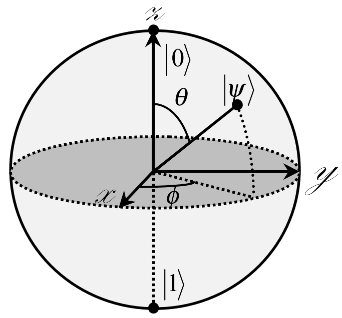

Figure 1. Bloch sphere representation of qubit states [1].

normalization condition:

$$|\alpha|^2 + |\beta|^2 = 1. \tag{2}$$

State of a qubit is a vector in a two dimensional vector space over complex numbers. States $|0\rangle$ and $|1\rangle$ are computational basis states and form an orthonormal basis for this vector space. Measuring the state of a qubit gives either the result$|0\rangle$, with probability $|\alpha|^2$, or the result $|1\rangle$, with probability $|\beta|^2$. Considering the normalization condition (2), the qubit state can be rewritten as:

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle. \tag{3}$$

Representing qubit state by a point on a sphere of unit radius, called *Bloch sphere*, would be useful. Specially in the case of spin qubits, where the point on the sphere denotes spin's direction. This scheme is shown in "Fig. 1."

The suggestion to use spin states of individual electrons confined to semiconductor quantum dots as qubits, *spin qubits*, was made for the first time by Daniel Loss and David P. DiVincenzo in their remarkable proposal [6]. These quantum dots are formed in a two dimensional electron gas by surface electrical gating. Electrostatic potentials confine electrons in small circles. Electron's spin-up and spin-down correspond to $|0\rangle$ and $|1\rangle$ basis states respectively. Single qubit operations can be achieved by applying pulsed local electromagnetic fields to electrons in single quantum dots. Two qubit operations can be accomplished by changing the height of the tunneling barrier between neighboring coupled quantum dots by a purely electrical gating [8].

III. Mathematical Model

Assume a single electron confined to a quantum dot. As mentioned before, the spin-up and spin-down of the electron are denoted as $|0\rangle$ and $|1\rangle$, respectively. The underlying Hilbert space is

$$\mathcal{H} = \mathrm{span}\{|0\rangle, |1\rangle\}. \tag{4}$$

The wave function of the electron has two components:

$$|\psi(t)\rangle = \psi_1(t)|0\rangle + \psi_2(t)|1\rangle, \tag{5}$$

which satisfies the Schrödinger equation

$$\begin{cases} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, & t > 0 \\ |\psi(0)\rangle = |\psi_0\rangle \in \mathcal{H}, \end{cases}. \tag{6}$$

Hamiltonian of the system is given by [11]:

$$H(t) = \frac{\hbar}{2}\mathbf{\Omega}(t)\cdot\boldsymbol{\sigma}, \tag{7}$$

with $\mathbf{\Omega}(\mathrm{t})$ as the external control field which is defined by

$$\mathbf{\Omega}(t) = \mu_B g(t)\boldsymbol{B}(t), \tag{8}$$

where, μ_B and $g(t)$ are the Bohr magneton and the effective g-factor of the semiconductor material respectively, and $\boldsymbol{B}(t)$ is the applied magnetic field. The $\boldsymbol{\sigma}$ in (7) is the spin operator of the electron:

$$\boldsymbol{\sigma} = \sigma_x\boldsymbol{e}_x + \sigma_y\boldsymbol{e}_y + \sigma_z\boldsymbol{e}_z, \tag{9}$$

where, σ_x, σ_y and σ_z are usual Pauli matrices:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},\quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{10}$$

and $\boldsymbol{e}_x$, $\boldsymbol{e}_y$ and $\boldsymbol{e}_z$ are the unit vectors in directions of x, y and z. *Unitary rotation gate* is described beautifully in [12]: choosing the control field such that

$$\mathbf{\Omega}(t) = \Omega(t)\boldsymbol{e}(\phi),\quad t \in [0, T], \tag{11}$$

with $\Omega(t)$ satisfying

$$\int_0^T \Omega(t)dt = 2\theta,\quad \theta \in [0, 2\pi], \tag{12}$$

and

$$\boldsymbol{e}(\phi) = \cos\phi\,\boldsymbol{e}_x + \sin\phi\,\boldsymbol{e}_y, \tag{13}$$

as the direction of the applied field, the Hamiltonian of the system becomes

$$H(t) = \frac{\hbar}{2}\Omega(t)\boldsymbol{e}(\phi)\cdot\boldsymbol{\sigma}. \tag{14}$$

Note that to suppress the unwanted effect of the Lorentz force which produces an accumulated phase change [12], a constraining condition on the direction of the magnetic field has been imposed, i.e. $\mathbf{\Omega}(t)\cdot\boldsymbol{e}_z = 0$.

The time evolution operator of the quantum system which is equal to corresponding quantum gate will be

$$\begin{aligned} U(T) &= e^{-i\int_0^T H(t)dt/\hbar}, \\ &= e^{-i\int_0^T \Omega(t)\boldsymbol{e}(\phi)\cdot\boldsymbol{\sigma}dt}, \\ &= e^{-i[\int_0^T \Omega(t)dt/\hbar]\boldsymbol{e}(\phi)\cdot\boldsymbol{\sigma}}, \\ &= e^{-i\theta\boldsymbol{e}(\phi)\cdot\boldsymbol{\sigma}}, \end{aligned} \tag{15}$$

where

$$\boldsymbol{e}(\phi)\cdot\boldsymbol{\sigma} = \begin{bmatrix} 0 & \cos\phi - i\sin\phi \\ \cos\phi + i\sin\phi & 0 \end{bmatrix}. \tag{16}$$

Considering eigenvalues of (16), which are ± 1, time evolution of the system becomes:

$$U(T) = \frac{1}{2}e^{-i\theta}[\mathbf{1} + \boldsymbol{e}(\phi)\cdot\boldsymbol{\sigma}] + \frac{1}{2}e^{i\theta}[\mathbf{1} - \boldsymbol{e}(\phi)\cdot\boldsymbol{\sigma}]$$

$$= \begin{bmatrix} \cos\theta & -ie^{-i\phi}\sin\theta \\ -ie^{i\phi}\sin\theta & \cos\theta \end{bmatrix} = U_{\theta,\phi} \qquad (17)$$

which is the unitary rotation gate. Note that the boldface one, **1,** in (17) is the identity matrix.

Quantum Hadamard gate is a one input one output gate that causes a rotation followed by a reflection of the Bloch sphere representation of the qubit state. An example of Hadamard operation is presented in "Fig. 3." First the point representing the qubit state on the Bloch sphere is rotated by $\pi/2$ around the y axis. Then the resulting state will be reflected by the xy plane. Matrix operator of the Hadamard gate is given by

$$U_H = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}. \qquad (18)$$

It is obvious that the Hadamard gate cannot be implemented using (17) directly. But we can decompose (18) into two canonical matrices which are feasible on (17). By choosing appropriate control fields, Hadamard gate can be realized in two steps. As shown in "Fig. 2," control fields are chosen such that the first control field, in direction of y, satisfies

$$\int_0^{T_m} \Omega_1(t)dt = \pi/4, \qquad (19)$$

and second control field, in direction of x, satisfies

$$\int_{T_m}^{T} \Omega_2(t)dt = \pi/2. \qquad (20)$$

The corresponding matrix operators become

$$U_{\frac{\pi}{4},\frac{\pi}{2}} = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \;\&\; U_{\frac{\pi}{2},0} = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}, \qquad (21)$$

and the resulting matrix is the Hadamard gate with an unwanted phase factor:

$$U_{\frac{\pi}{2},0}U_{\frac{\pi}{4},\frac{\pi}{2}} = e^{-i\frac{\pi}{2}} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}. \qquad (22)$$

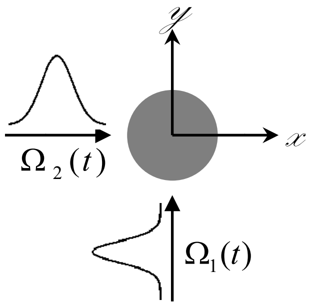

Figure 2. Directions of control fields applied to an electron spin confined to a quantum dot (grey circle).

IV. QUANTUM OPTIMAL CONTROL PROBLEM

Let time t be in the interval $[0, T]$, for T fixed. Dynamics of the system is described by the controlled Schrödinger equation:

$$\begin{cases} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(\Omega(t))|\psi(t)\rangle \\ |\psi(0)\rangle = |\psi_0\rangle \in \mathcal{H} \end{cases}, \qquad (23)$$

where, both the wave function $|\psi(t)\rangle$ and the Hamiltonian $H(\Omega(t))$ are complex quantities. In order to express the problem in terms of real quantities only, we write [13]:

$$|\psi(t)\rangle = |\psi_{\Re e}(t)\rangle + i|\psi_{\Im m}(t)\rangle, \qquad (24)$$

and

$$H(\Omega(t)) = H_{\Re e}(\Omega(t)) + iH_{\Im m}(\Omega(t)). \qquad (25)$$

By placing (24) and (25) into (23) we obtain

$$\begin{cases} \hbar\frac{\partial}{\partial t}|\psi_{\Re e}\rangle = H_{\Im m}(\Omega)|\psi_{\Re e}\rangle + H_{\Re e}(\Omega)|\psi_{\Im m}\rangle \\ \hbar\frac{\partial}{\partial t}|\psi_{\Im m}\rangle = H_{\Im m}(\Omega)|\psi_{\Im m}\rangle - H_{\Re e}(\Omega)|\psi_{\Re e}\rangle \end{cases}. \qquad (26)$$

By defining $\phi = [\langle\psi_{\Re e}|, \langle\psi_{\Im m}|]^T$ and

$$\widetilde{\mathrm{H}} = \frac{1}{\hbar}\begin{bmatrix} H_{\Im m} & H_{\Re e} \\ -H_{\Re e} & H_{\Im m} \end{bmatrix}, \qquad (27)$$

dynamics of the system can be written as a system of nonautonomous linear ordinary differential equations [14]:

$$\dot{\phi}(t) = \widetilde{\mathrm{H}}(\Omega(t))\phi(t), \qquad (28)$$

where $\phi \in \mathbb{R}^4$, and $\widetilde{\mathrm{H}}$ is a real valued 4×4 matrix.

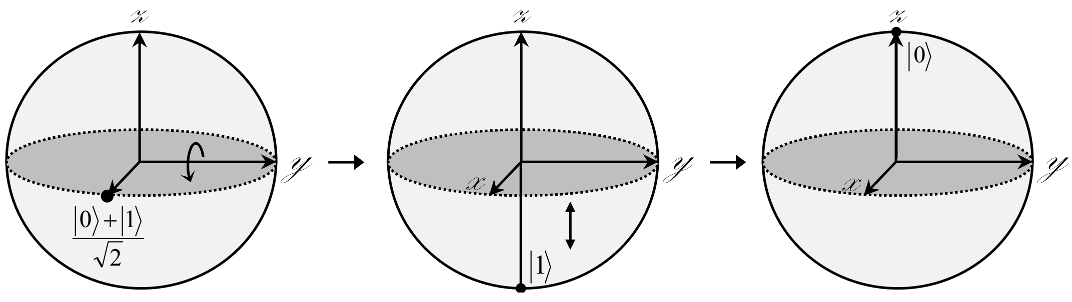

Figure 3. Bloch sphere representation of Hadamard gate operation [1]. First the initial state $(|0\rangle + |1\rangle)/\sqrt{2}$ is rotated around the y axis by $\pi/2$. The resulting state $|1\rangle$ will be reflected by the xy plane in second step, giving the final state $|0\rangle$.

The optimal control problem is to design a control field which steers our system from an initial state ϕ_0 to a desired final state ϕ_T at specified final time T. Note that ϕ_0 and ϕ_T correspond to $|\psi_0\rangle$ and $|\psi_T\rangle = U_{\mathrm{H}}|\psi_0\rangle$ states respectively. This problem can be formulated in terms of a cost functional that also takes into account practical constraints, such as energy of the control fields:

$$J(\Omega) = \frac{1}{2}\|\phi(T) - \phi_T\|^2 + \frac{1}{2}\int_0^T \alpha(t)\Omega^2(t)dt, \quad (29)$$

where, the first term represents measure of distance of the final state from the desired one, and the second integral term penalizes the field fluency. $\alpha(t)$ is a weight function which forces the control field to approach zero near the end points of the time interval $[0, T]$ in accordance with reality where magnetic fields are of finite duration. For this purpose we use the shape function [15], [16]:

$$\alpha(t) = \alpha_0 + W_0 e^{-t/\tau} + W_T e^{-(T-t)/\tau}, \quad (30)$$

where the positive constants α_0, W_0 and W_T are the penalty parameters and τ is a rise time.

First order optimality conditions in the form of Pontryagin's minimum principle offer an optimal solution of this problem. These conditions are formulated using a Hamiltonian which in our problem has the following form:

$$\mathcal{H}\big(\phi(t), \Omega(t), \lambda(t)\big) = \tfrac{1}{2}\alpha(t)\Omega^2(t) + \lambda^T(t)\big[\widetilde{\mathrm{H}}\big(\Omega(t)\big)\phi(t)\big], \quad (31)$$

where $p(t)$ is called the co-state vector. Pontryagin's minimum principle states that necessary conditions to simultaneously minimize $J\big(\Omega(t)\big)$ and satisfy (28) are as follows [17]:

$$\frac{d}{dt}\phi(t) = \frac{\partial\mathcal{H}(\phi(t), \Omega(t), t)}{\partial\lambda}, \quad t \in [0, T], \quad (32)$$

$$\frac{d}{dt}\lambda(t) = -\frac{\partial\mathcal{H}(\phi(t), \Omega(t), t)}{\partial\phi}, \quad t \in [0, T], \quad (33)$$

$$0 = \frac{\partial\mathcal{H}(\phi(t), \Omega(t), t)}{\partial\Omega}, \quad t \in [0, T]. \quad (34)$$

The set of state and co-state equations, (32) and (33), together with the algebraic equation (34) form a boundary value problem which is extremely difficult to solve analytically because of the apparent nonlinearity in the system of differential equations.

General procedure to solve the problem is as follows: choose an initial guess for the control field $\Omega(t)$ and solve state equations for $\phi(t)$ by integration forward in time. Using obtained $\phi(t)$ integrate co-state equations backward in time. Use (34) to update the control field and run this loop until the desired cost function value is achieved. The numerical method to solve this problem is described in details in the following section.

V. Numerical Algorithm

Numerically, there exist two main classes of methods to solve optimal control problems, *direct* and *indirect* [18]. An indirect method forms the Hamiltonian of the system and solves the necessary conditions of optimality in the form of a boundary value problem. Here we will use a gradient method which by an iterative algorithm improves estimates of the control field histories, $\Omega(t)$, so as to come closer to satisfy optimality and boundary conditions [19].

A first order gradient algorithm for solving our problem is presented below [20]:

1. Choose an initial guess for the control field $\Omega^{(0)}(t)$ in the time interval $[0, T]$.
2. Using the control field history $\Omega^{(i)}$, integrate the state equations (32) from 0 to T with initial conditions ϕ_0.
3. Calculate $\lambda^{(i)}(T)$ by substituting $\phi^{(i)}(T)$ from step 2 into $\lambda^{(i)}(T) = \phi^{(i)}(T) - \phi_T$. Using this value of $\lambda^{(i)}(T)$ as the initial condition and $\phi^{(i)}(t)$ obtained in the previous step, integrate co-state equations (33) from T to 0.
4. If $\partial\mathcal{H}^{(i)}/\partial\Omega^{(i)} < \gamma$, where γ is a preselected small positive constant, terminate the procedure. Otherwise set $\Omega^{(i+1)} = \Omega^{(i)} - \beta\,\partial\mathcal{H}^{(i)}/\partial\Omega^{(i)}$ and go to step 2. Here, β is the step size.

Various numerical methods can be used to integrate the Schrödinger equation and the associated co-state system. Here, we used explicit Runge-Kutta-Fehlberg method of order 4(5) to carry out the numerical integrations [21].

Optimum control fields and corresponding evolution of spin state are shown in “Fig. 4.” Note that the mapping shown in “Fig. 4,” which is the transformation of two superposition states into a final basis state, is not the basic application of Hadamard gate. Hadamard gate is mainly used for transforming a basis state into the superposition of basis states. Two superposition states are chosen as the input in order to illustrate the two stage operation of the Hadamard gate. The second stage would have been eliminated in our simulation if we had chosen a basis state as the input. The value of the performance measure as a function of the number of iterations is shown in “Fig. 5.”

VI. Concluding Remarks

We addressed the realization of the quantum Hadamard gate based on the spin of a single electron confined to a semiconductor quantum dot. Hadamard gate cannot be implemented using in plane control fields directly, thus we decomposed the Hadamard operator into two canonical forms which are feasible by applying in plane fields. By deriving the Hamiltonians of the system we accessed to the dynamics of the quantum system. The problem of finding tailored control fields which drive the quantum system in a specified time, while minimizing the energy of the control fields, is formulated within optimal control theory and Pontryagin's minimum principle. Using a gradient based iterative numerical procedure we solved this optimal control problem.

In this paper we studied the ideal case of an isolated solid state spin qubit subject to the external control fields. While in practice, there exist several types of interactions with environment which lead to decoherence. Major sources of decoherence in solid state spin qubits are addressed in [22]. The effect of these undesired interactions on dynamics of the quantum system can be considered by adding uncontrolled Hamiltonians to the Schrödinger equation. Optimal control theory can be used to design control fields in order to realize robust quantum gates even in the presence of an environment [23].

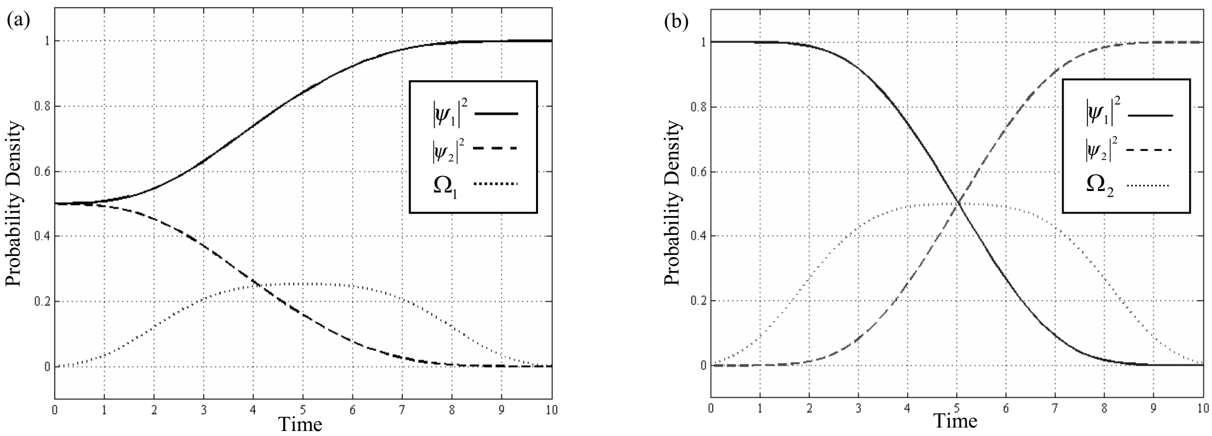

Figure 4. Time evolution of the spin states during quantum Hadamard gate operation. (a) Initial state $(|0\rangle + |1\rangle)/\sqrt{2}$ turns into state $|0\rangle$ by applying first optimal control field. (b) Resulting spin states will be flipped by applying second optimal control field, giving the final state $|1\rangle$. Note that $|\psi_1|^2$ is the probability density of the basis state $|0\rangle$, and $|\psi_2|^2$ is the probability density of the basis state $|1\rangle$.

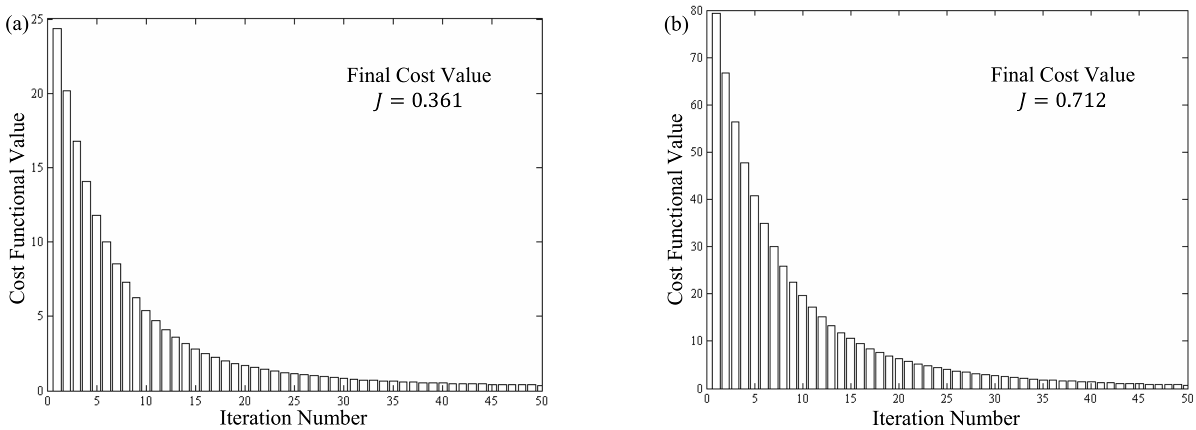

Figure 5. The value of the cost functional as a function of the number of iterations. First fifty iterations for (a) the first and (b) the second control fields. An extremely small value is chosen for the termination constant γ, in order not to terminate the iterative procedure before fifty iterations.

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