Quantum gates by inverse engineering of a Hamiltonian

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Abstract
Inverse engineering of a Hamiltonian (IEH) from an evolution operator is a useful technique for the protocol of quantum control with potential applications in quantum information processing. In this paper we introduce a particular protocol to perform IEH and we show how this scheme can be used to implement a set of quantum gates by using minimal quantum resources (such as entanglement, interactions between more than two qubits or auxiliary qubits). Remarkably, while previous protocols request three-qubit interactions and/or auxiliary qubits to implement such gates, our protocol requires just two-qubit interactions and no auxiliary qubits. By using this approach we can obtain a large class of Hamiltonians that allow us to implement single and two-qubit gates necessary for quantum computation. To conclude this article we analyze the performance of our scheme against systematic errors related to amplitude noise, where we show that the free parameters introduced in our scheme can be useful for enhancing the robustness of the protocol against such errors.

Keywords: quantum control, quantum computing, robustness against systematic errors

((Some figures may appear in colour only in the online journal)

1. Introduction

Currently, protocols of quantum control with time-dependent Hamiltonians like adiabatic passage [1], Lewis–Riesenfeld invariants [2, 3], transitionless quantum driving [4–6] and the current proposal of the inverse engineering of a Hamiltonian (IEH) from unitary evolution operators [7], have played an important role in quantum information processing (see [8] for a detailed review of many applications of the three first techniques). In addition, in the few last years, many experimental and theoretical studies have been performed in order to analyze the robustness of such protocols against decoherence effects [9–17].

Quantum control via time-dependent Hamiltonians is of great interest for many knowledge fields in physics, in particular for quantum computation (QC) and information (our focus in this paper). For example, these techniques are used to solve problems of satisfiability via adiabatic dynamics [18], engineering fast Hamiltonians for speeding up QC [19–21] and state preparation in quantum simulations of relativistic dynamics [22], for example. In addition, we can use such protocols to develop hybrid schemes of QC, where we obtain controllable time-dependent Hamiltonians to implement single and controlled quantum gates. For example, quantum gates of a circuit can be implemented via adiabatic Hamiltonians [23, 24], via counter-diabatic dynamics [19–21] and via shortcuts to adiabatic holonomic QC with transitionless quantum driving dynamics [25]. However, in order to implement universal QC, these schemes require auxiliary qubits, many body interactions, etc [19–21, 23, 24]. We say universal in the sense that, given an unknown input state, we should be able to implement any single- and two-qubit quantum gate on such a qubit.

In this paper, we introduce an alternative way of obtaining Hamiltonians for implementing quantum gates based on IEH from evolution operators. Different from methods previously developed for IEH and shortcuts to adiabaticity, ancilla qubits or highly degenerate Hamiltonians are not necessary for our scheme. In section 2, we discuss the general aspects of our approach and we show how to obtain a set of Hamiltonians which allows us to implement the quantum gates of a quantum circuit. In this sense, the scheme present here is an enhanced way of implementing quantum gates without auxiliary resources. In section 4, we illustrate the results obtained here by providing a set of Hamiltonians for implementing a restricted set of quantum gates necessary for QC [26, 27].
2. Inverse engineering of a Hamiltonian

Let us start by considering the Schrödinger equation (we set $\hbar = 1$ throughout the manuscript)

$$H(t)|\psi(t)\rangle = i\dot{\psi}(t).$$

(1)

For a unitary dynamics, there is an operator $U(t)$ that allows us to write $|\psi(t)\rangle = U(t)|\psi(0)\rangle$. From the equation above (valid for any $|\psi(0)\rangle$), the Hamiltonian reads as

$$H(t) = iU(t)U^\dagger(t),$$

(2)

the well-known equation to obtain the Hamiltonian associated with the evolution operator $U(t)$ [26, 28]. This equation is the starting point for protocols of inverse engineering in closed quantum systems [7, 29, 30], as well as transitionless quantum driving [4–6, 8]. In alternative approaches, the operator $U(t)$ has been considered as

$$U'(t) = |k(t)\rangle \langle k(0)| + \sum_{n,n'=k} \lambda_{nm}(t)|n(t)\rangle \langle n(0)|,$$

(3)

where $|n(t)\rangle$ is a complete orthonormal basis for the Hilbert space of the system, and $\lambda_{nm}(t)$ are free parameters. Therefore, any system driven by the Hamiltonian $H'(t) = iU'(t)U'^\dagger(t)$ is begun in the state $|k(0)\rangle$ and evolves to $|k(\tau)\rangle$ through path $|k(t)\rangle$, with $0 \leq t \leq \tau$. Since we can obtain the transitionless theory from a suitable choice of the parameters $\lambda_{nm}(t)$, we can consider the operator $U'(t)$ as the most general form of $U(t)$ [7].

On the other hand, our alternative approach of Hamiltonian engineering is obtained from a new definition of the operator $U(t)$ as

$$U(t) = e^{i\varphi_0(t)} \sum_n e^{i\varphi_n(t)} |n(t)\rangle \langle n(0)|,$$

(4)

where $|n(t)\rangle$ constitutes an orthonormal bases for the Hilbert space associated with the system and $\varphi_n(t)$ are real free parameters. It is easy to show that $U(t)$ satisfies the unitarity condition $U(t)U^\dagger(t) = 1$ for any set of parameters $\varphi_n(t)$. In addition, to obtain an operator that satisfies the initial condition $U(0) = 1$, we must impose initial conditions for the parameters $\varphi_n(t)$ given by $\varphi_0(t) = 2n\pi$ for $n \in \mathbb{Z}$.

Different from other protocols [1–7, 14, 16, 31], we can see that our definition of the operator $U(t)$ is an operator more general than some operators that drive the system from a known initial state $|n(0)\rangle$ to $|n(\tau)\rangle$. Therefore, this method is not dependent on the initial state $|n(0)\rangle$. As we shall see, this approach can be useful in some protocols of quantum information processing, e.g. to implement a set of quantum gates necessary for universal QC using minimal resources.

3. Quantum gates by IEH

3.1. Single-qubit gates

In this section, we will show how single quantum gates can be implemented, without additional resources, by using the scheme presented here. To this end, let us consider that a single-qubit gate can be viewed as a linear transformation on an arbitrary quantum state $|\psi_{\text{inp}}\rangle = a|0\rangle + b|1\rangle$, and so let us consider the transformation $|\psi(t)\rangle = U(t)|\psi_{\text{inp}}\rangle$, where the operator $U(t)$ is given by

$$U(t) = |n_+(t)\rangle \langle n_+(t)| + e^{i\varphi_0(t)} |n_-(t)\rangle \langle n_-(t)|,$$

(5)

where

$$|n_+(t)\rangle = \cos[\theta(t)/2]|0\rangle + e^{i\varphi(t)} \sin[\theta(t)/2]|1\rangle,$$

(6)

$$|n_-(t)\rangle = \cos[\theta(t)/2]|0\rangle - e^{i\varphi(t)} \sin[\theta(t)/2]|1\rangle,$$

(7)

with $\theta(t)$, $\varphi(t)$ and $\varphi_0(t)$ being real free parameters. It is easy to show that the conditions $U(t)U^\dagger(t) = 1$ and $U(0) = 1$ are satisfied if we choose $\varphi(t)$ such that $\varphi(0) = 2n\pi$, for $n$ integer. Parameters associated with the quantum gate to be implemented are encoded in the parameters $\theta(t)$, $\varphi(t)$ and $\varphi_0(t)$. To show that we can really implement single-qubit gates by using the operator $U(t)$, let us consider an arbitrary input state $|\psi_{\text{inp}}\rangle$ so that the evolved state $|\psi(t)\rangle$ is given by

$$|\psi(t)\rangle = U(t)|\psi_{\text{inp}}\rangle = \alpha(t)|0\rangle + \beta(t)|1\rangle,$$

(8)

where the coefficients $\alpha(t)$ and $\beta(t)$ are given, respectively by

$$\alpha(t) = \frac{a\sigma_0(t) - \sigma_z(t)\bar{\alpha}(t)}{2}, \quad \beta(t) = \frac{\sigma_x(t) + \sigma_z(t)\bar{\beta}(t)}{2},$$

(9)

with $\sigma_0(t) = (e^{-\varphi(t)/4} \pm 1)$, $\alpha(t) = a \cos \theta(t) + b e^{-i\varphi(t)} \sin \theta(t)$ and $\beta(t) = b \cos \theta(t) - a e^{-i\varphi(t)} \sin \theta(t)$. By using the initial condition $\varphi(0) = 2n\pi$ we can see that $\alpha(0) = a$ and $\beta(0) = b$, because $\sigma_0(0) = 2\delta_{1,2}$. Therefore, from equations (8)–(9), an arbitrary single-qubit rotation can be performed.

Notice that we have implemented an arbitrary rotation on an unknown input state $|\psi_{\text{inp}}\rangle$. Thus, arbitrary single-qubit universal operations can be performed by using this approach, where no additional quantum resource (such as entanglement or auxiliary qubits, for example) is required. In addition, as we shall see in the next section, this model allows us find both trivial and nontrivial Hamiltonians to implement the same gate.

3.2. Two-qubit quantum gates

To show that our protocol can be used to implement a universal set of quantum gates for QC, we must show how to implement two-qubit quantum gates. To this end, let us write the two-qubit input state generically as $|\psi_{\text{inp},2}\rangle = a|00\rangle + b|10\rangle + c|01\rangle + d|11\rangle$. In addition, we define the operator

$$U_2(t) = \sum_{k=1,2} [n_{k+}(t)|\langle n_{k+}(t)| + e^{i\varphi_0(t)} |n_{k-}(t)\rangle \langle n_{k-}(t)|,$$

(10)

where (with $\bar{k} = k - 1$)

$$|n_{k+}(t)\rangle = \cos[\theta_k(t)/2]|0\rangle + e^{i\varphi_k(t)} \sin[\theta_k(t)/2]|1\rangle,$$

(11)

$$|n_{k-}(t)\rangle = e^{i\varphi_k(t)} \cos[\theta_k(t)/2]|1\rangle - \sin[\theta_k(t)/2]|0\rangle,$$

(12)

with the initial conditions $\varphi_0(0) = \varphi_0(0) = 2n\pi$ (due to the requirement $U_2(0) = 1$). Now we have six free parameters, so we will use them in order to obtain an arbitrary two-qubit operation. It is easy to see that the operator $U_2(t)$ is a general
two-qubit operator. Therefore, we can adequately adjust our free parameters to obtain $U_2(t)$ as an entangled gate or a composition of two independent single-qubit gates (i.e. $U_2(t) = A_1(t) \otimes A_2(t)$). In order to analyze some results by using its most general form, we maintain our discussion without considering a particular case for $U_2(t)$, but particularizations for $U_2(t)$ will be taken into account in section 4.

From equations (10)–(12) we can write the evolved state as
\begin{equation}
[\psi_{\text{imp}, 2}] = U_2(t)[\psi_{\text{imp}, 2}] = \alpha(t)[00] + \beta(t)[10] + \gamma(t)[01] + \delta(t)[11],
\end{equation}
with the following coefficients
\begin{align}
\alpha(t) &= \frac{a\sigma_{+}(t) - \sigma_{-}(t)\hat{\alpha}(t)}{2}, \\
\beta(t) &= \frac{b\sigma_{+}(t) + \sigma_{-}(t)\hat{\beta}(t)}{2}, \\
\gamma(t) &= \frac{c\sigma_{+}(t) - \sigma_{-}(t)\hat{\gamma}(t)}{2}, \\
\delta(t) &= \frac{d\sigma_{+}(t) + \sigma_{-}(t)\hat{\delta}(t)}{2}.
\end{align}

Again we have defined $\sigma_{\pm}(t) = (e^{i\varphi(t)} \pm 1)$, $\hat{\alpha}(t) = a\cos \theta(t) + be^{i\varphi(t)} \sin \theta(t)$, $\hat{\beta}(t) = b\cos \theta(t) + ae^{i\varphi(t)} \sin \theta(t)$, $\hat{\gamma}(t) = c\cos \theta(t) + de^{i\varphi(t)} \sin \theta(t)$, and $\hat{\delta}(t) = d\cos \theta(t) - ce^{-i\varphi(t)} \sin \theta(t)$. Thus, an arbitrary two-qubit gate can be implemented with this scheme.

In this discussion, we have not labeled the target and control qubit; however, this choice can be made through the definition of the free parameters. The operator $U_2(t)$ encompasses a large class of two-qubit gates, i.e. $U_2(t)$ can be an entangling quantum gate (as CNOT or some controlled single-qubit unitary rotations) or non-entangling gates (such as the SWAP gate).

4. Quantum gates for (approximately) universal QC

In order to show how we can implement a set of universal quantum gates by using the results developed here, in this section we consider some choices for the free parameters previously discussed. As an application of this method, we discuss Hamiltonians able to implement a set of quantum gates necessary for implementing universal QC with arbitrary precision, namely, the set \{H, S, T, CZ\}, where $H$ represents the Hadamard gate, $S$ and $T$ are $\pi/4$ and $\pi/8$ gates, respectively, and $CZ$ is the controlled-phase gate [26, 32].

4.1. Single-qubit gates

The Hamiltonian for implementing single quantum gates that can be obtained from equation (2) is not trivial and written as (in order to obtain simple Hamiltonians, throughout the manuscript we consider that the system evolves up to a global phase)
\begin{equation}
H(t) = \frac{1}{2} \hat{\omega}(t) \cdot \hat{\sigma},
\end{equation}
where $\hat{\sigma}$ is a ‘vector’ with its components given by the Pauli matrices $\sigma_x$, $\sigma_y$ and $\sigma_z$, and $\hat{\omega}(t)$ is a vector where its components are given by
\begin{align}
\omega_x(t) &= (\cos \varphi - 1) \phi \cos \phi \cos \theta \sin \theta \\
&\quad + (\theta \cos \theta \sin \varphi + \phi \sin \theta) \cos \phi \\
&\quad + [\hat{\phi} \sin \theta \sin \varphi + (\cos \varphi - 1)\hat{\theta}] \sin \phi, \\
\omega_y(t) &= (\cos \varphi - 1) \phi \sin \phi \sin \theta \cos \theta \\
&\quad + \sin \phi (\theta \cos \theta \sin \varphi + \phi \sin \theta) \\
&\quad + [\hat{\phi} \sin \theta \sin \varphi - (\cos \varphi - 1)\hat{\theta}] \cos \phi, \\
\omega_z(t) &= -\hat{\theta} \sin \theta \sin \varphi - (\cos \varphi - 1) \phi \sin^2 \theta + \phi \cos \theta.
\end{align}

Therefore, now we are able to particularize the Hamiltonian of equation (16) in order to obtain a restricted set of Hamiltonians associated with quantum gates used to implement universal QC (approximately) [26, 32].

**Hamiltonian for phase shift gates.** For phase shift gates, given any entry $|\psi_{\text{imp}}\rangle = a|0\rangle + b|1\rangle$ we have the corresponding output $|\psi_{\text{out}}\rangle = a|0\rangle + e^{i\varphi}b|1\rangle$, for an arbitrary value $0 < \xi < 2\pi$. Thus, from equation (9), we see that such a gate is implemented if we choose $\varphi(\tau) = \xi$ and $\theta(\tau) = 2\pi n$, with $n \in \mathbb{Z}$ and $\tau$ being the total evolution time. Since we have boundary conditions for the parameter $\varphi(\tau)$, namely $\varphi(0) = 0$ and $\varphi(\tau) = \xi$, so $\varphi(t)$ cannot assume an arbitrary form. On the other hand, we see that no consideration has been given to the parameter $\phi(t)$, so that we can consider it arbitrary. For simplicity we will consider that $\phi(t) = 0$. Therefore, the components of $\hat{\omega}(t)$ associated with the Hamiltonian $H_{\text{ph}}(t) = (1/2)\hat{\omega}(t) \cdot \hat{\sigma}$ become
\begin{align}
\omega_x^{\text{ph}}(t) &= \cos(\theta^{\text{ph}}) \sin(\phi^{\text{ph}}) \phi^{\text{ph}} + \sin(\theta^{\text{ph}}) \phi^{\text{ph}}, \\
\omega_y^{\text{ph}}(t) &= -[\cos(\phi^{\text{ph}}) - 1] \theta^{\text{ph}}, \\
\omega_z^{\text{ph}}(t) &= \cos(\theta^{\text{ph}}) \phi^{\text{ph}} - \sin(\theta^{\text{ph}}) \sin(\phi^{\text{ph}}) \hat{\theta},
\end{align}
where we have labeled the parameters by using ‘ph’ in order to specify that these parameters depend on the gate to be implemented.

For some experimental architecture, the operation $\sigma_x$ is not easily implementable, for example in systems composed of Bose–Einstein condensates in optical lattices [33], and experimental architecture of superconducting circuits [34–37]. Thus, such an experimental difficulty is not a problem if we set $\theta^{\text{ph}}(t) = \theta_0 = \text{cte}$.

Therefore, by taking into account those considerations related to parameters $\phi^{\text{ph}}(t)$, $\theta^{\text{ph}}(t)$ and $\varphi(t)$, let us put $\theta^{\text{ph}}(t) = \phi^{\text{ph}}(t) = 0$, so that the Hamiltonian for phase shift gates is given by
\begin{equation}
H_{\text{ph}}(t) = \frac{\hat{\omega}^{\text{ph}}(t)}{2} \sigma_z,
\end{equation}
The Hamiltonian above can be implemented in nuclear magnetic resonance (NMR) experimental setups, where a magnetic \( \vec{B} \) field is used to driving nuclear spins of atoms and molecules. In general, such a field is taken to be constant [38], thus we can set \( \varphi(t) = \xi \frac{t}{\tau} \), where \( \xi \) is the shift phase to be implemented and \( \tau \) is the total evolution time. Therefore, we obtain the time-independent Hamiltonian

\[
H_{\text{ph}}(t) = \frac{\xi}{2\tau} \sigma_z,
\]

(24)

where \( 1/\tau \) can be identified as the Larmor frequency \( \omega_0 \propto \gamma_B B_z \) of a nuclear spin, where the magnetic field is \( \vec{B} = B_z \hat{\mathbf{z}} \) and \( \gamma_B \) is the gyromagnetic ratio of the nucleus. Thus, we can set the total evolution time from the intensity of the magnetic field \( \vec{B} \). In particular, if we put \( \xi = \xi_0 = \pi/2 \), \( \xi = \xi_0 = \pi/4 \) and \( \xi = \xi_0 = \pi \), we obtain the Hamiltonian that implements the \( S, T \) and \( Z \) gates [26], respectively.

It is worth mentioning that this choice is not unique and there are many other possibilities if we set \( \theta_{\text{ph}}(t) \neq 0 \). However, if we pick \( \theta_{\text{ph}}(t) = 0 \), the corresponding Hamiltonian will be not as simple as the Hamiltonian obtained above. In conclusion, we have shown that our approach allows us to find both trivial and nontrivial Hamiltonians to perform the same task. Moreover, we can obtain time-independent Hamiltonians feasible in the lab.

**Hamiltonian for the Hadamard gate.** The Hadamard gate is an exclusive gate of quantum computers due to its particular task of generating quantum superpositions with elements of the computational basis. More specifically, given a quantum state \( |\psi_{\text{inp,2}}\rangle = a|0\rangle + b|1\rangle \), we obtain its corresponding output \( |\psi_{\text{out,2}}\rangle = (a + b)/\sqrt{2} |0\rangle + (a - b)/\sqrt{2} |1\rangle \). To implement such an operation we set \( \theta(\tau) = \pi/4 \), \( \phi(\tau) = 0 \) and \( \varphi(\tau) = \pi \). In this case, there are no free parameters, but due to the boundary condition on \( \phi(t) \), we can consider \( \phi = 0 \) in order to simplify the Hamiltonian

\[
H_{\text{Had}}(t) = \frac{\omega_{\text{Had}}(t) \cdot \sigma}{2},
\]

that implements a Hadamard gate.

Under this condition, from equations (17)–(19), we can see that \( \omega_{\text{Had}} = \omega_{\text{ph}} \), but with different boundary conditions for parameters \( \theta \) and \( \varphi \). Thus, we have the set \( \{ \omega_{\text{Had}}(t), \omega_{\text{ph}}(t), \omega_{\text{ph}}(t), \omega_{\text{ph}}(t) \} \) given by equations (20)–(22), where the functions \( \omega_{\text{ph}}(t) \) and \( \varphi_{\text{ph}}(t) \) must now satisfy \( \theta(\tau) = \pi/4 \) and \( \phi(\tau) = 0 \), respectively. In particular, if we set \( \theta(\tau) = \pi/4 \), we find

\[
H_{\text{Had}}(t) = \frac{\varphi(t)}{2\sqrt{2}}(\sigma_x + \sigma_z),
\]

(25)

where \( \varphi(t) \) is an arbitrary function that satisfies the conditions \( \phi(\tau) = 0 \) and \( \varphi(\tau) = \pi \). For example, we can pick \( \varphi(t) = \pi t/\tau \). To describe how we can implement this Hamiltonian, let us consider an NMR experimental setup, where we have a time-dependent magnetic field \( \vec{B}(t) = B_t \hat{\mathbf{t}} + B_m(t) \), where \( B_m(t) \) is a transverse (rotating) field, called a radio-frequency field, given by \( B_m(t) = |J_0| \cos(\omega t) \hat{\mathbf{z}} + |J_0| \sin(\omega t) \hat{\mathbf{k}} \), where \( \omega \) is the frequency of such a field. It is possible to show that the Hamiltonian equation (25) can be implemented/simulated using the magnetic field \( \vec{B}(t) \) once we set the frequency \( \omega \) of the radio-frequency field \( B_t \) near to the resonance, i.e. if we put \( \omega \approx \omega_0 \). In fact, in the rotating frame, the Hamiltonian of the system can be written as a Landau–Zener Hamiltonian. The demonstration of such a result can be found in [26, p 326].

### 4.2. Controlled phase shift gate

A phase-controlled phase shift gate is a two-qubit gate that introduces a phase \( e^{i\phi} \) controlled by one qubit, where for any input state given by \( a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle \) the output state is \( a|00\rangle + b|01\rangle + c|10\rangle + e^{i\delta}|11\rangle \). In particular, for \( \xi = \pi \) we get the CZ gate (controlled-phase gate, also known as CPHASE or CSign). In general, the CZ is a gate that naturally can be implemented in linear optical quantum computing [39] and constitutes a required gate for universal quantum computing [26]. In addition, we can use a CZ gate and single-qubit gates to implement a CNOT gate in different experimental architecture [26, 41]. Here we will consider the simplest Hamiltonian for implementing such a gate.

Without loss of generality, let us consider a bipartite system initially in the state

\[
|\psi_{\text{inp,2}}\rangle = a|0\rangle|0\rangle + b|0\rangle|1\rangle + c|1\rangle|0\rangle + d|1\rangle|1\rangle,
\]

(26)

where subscripts ‘c’ and ‘t’ are the control and target qubits, respectively. Thus, under this encoding, the state of the system at the end of the evolution can be written as

\[
|\psi_{\text{out,2}}\rangle = a|0\rangle|0\rangle + b|0\rangle|1\rangle + \gamma|\tau\rangle|1\rangle|0\rangle + \delta|\tau\rangle|1\rangle|1\rangle,
\]

(27)

where \( \gamma(t) \) and \( \delta(t) \) are given by equation (15), respectively. Now, we can discuss the parameters \( \varphi_1(t), \theta_2(t) \) and \( \phi_2(t) \) necessary to obtaining such a gate. Firstly, because the coefficients \( a \) and \( b \) were not changed, from equation (14) we conclude that such an evolution can be achieved if we set the parameter \( \varphi_1(t) = 0 \), where no condition regarding \( \theta_2(t) \) and \( \phi_2(t) \) is necessary, thus \( \theta_2(t) \) and \( \phi_2(t) \) become additional free parameters that can be used to simplify the Hamiltonian. Secondly, in order to obtain a correct CZ operation, we need to choose our functions so that \( \gamma(\tau) = c \) and \( \delta(\tau) = e^{i\delta}d \). From equation (15), this result can be achieved if we choose \( \theta_2(\tau) = 0 \) and \( \varphi_2(\tau) = \xi \). Therefore, we have two free parameters that can be used to obtain feasible Hamiltonians, namely, \( \phi_2(t) \) and \( \theta_2(t) \).

In particular, we can obtain a familiar Hamiltonian if we pick \( \phi_2(t) = \theta_2(t) = 0 \), where the corresponding Hamiltonian is written as

\[
H(t) = \frac{\varphi_2(t)}{4}[\sigma_x \otimes \sigma_z + \sigma_z \otimes \sigma_z - \sigma_z \otimes \sigma_z],
\]

(28)

for an arbitrary function \( \varphi(t) \) satisfying the boundary conditions \( \varphi_2(0) = 0 \) and \( \varphi_2(\tau) = \xi \). Remarkably, we can see that the Hamiltonian above requires an interaction ZZ between the physical qubits of the system. Such an interaction is a common interaction between nuclear spins present in NMR experimental setups [42, 43], therefore the Hamiltonian in equation (28) can be implemented for such physical systems.
5. Robustness against systematic errors

Now, we will explore the free parameters in order to show how such parameters can be useful in our model for providing robustness against systematic errors. To this end, we will study the stability of our protocol against deviations of physical parameters of the Hamiltonian. Basically, here we will follow the general formalism for such errors in two-level systems, as detailed in [44], where the authors have studied protocols where we can find parameters in order to cancel systematic errors. Unlike [44], our protocol allows us to find parameters in order to minimize such systematic errors. In particular, we will consider systematic errors associated with Rabi frequency that can be simply described by the Hamiltonian $H_{ae}(t) = \omega(t)\sigma_x/2$, where $\omega(t)$ is the x-component of the ideal Hamiltonian $H(t)$ given by equation (16). In general, such systematic errors are related to deviations in the amplitude of the field from an ideal value. These errors are very common in Hamiltonians driven by laser fields [45, 46] and nuclear magnetic resonance [47–50], for example. Therefore, the dynamics is given by

$$|\dot{\psi}(t)| = [H(t) + \varepsilon H_{ae}(t)]|\psi(t)|,$$

where $\varepsilon$ is a small real parameter that sets the perturbation strength. In this case, from perturbation theory, the evolved state of the system is given by [51, 52]

$$|\psi(t)| = |\psi(0)| + \varepsilon \int_0^t U(t')H_{ae}(t)|\psi(0)|dt' + \left(\frac{\varepsilon}{\hbar}\right)^2 \int_0^t \int_0^{t'} U(t')H_{ae}(t)U(t'')H_{ae}(t)|\psi(0)|dt''dt' + \mathcal{O}(\varepsilon^3),$$

(30)

where $|\psi(0)|$ is the ideal evolved state (unperturbed) and $U(t)$ is the ideal propagator. For the scheme developed in this paper $U(t) = U_1(t)$, where $U_1(t)$ is given by equation (5), and $|\psi(0)| = U_1(t)|\psi_{inp}|$ is given by equation (8). It is important to mention that in our notation we have $|\psi(0)| = U_1(t)|\psi_{inp}| = |\psi_{oa0}|$. Therefore, the probability of obtaining $|\psi_{oa0}|$ can be computed from equation (up to second order) [44, 51–55]

$$P(\tau) = |\langle\psi_{oa0}|\psi(\tau)\rangle|^2$$

$$= 1 - \varepsilon^2 \left[\int_0^\tau \langle\psi_{oa0}(t)|H_{ae}(t)|\psi(0)\rangle dt\right]^2,$$

(31)

where $|\psi_{oa0}(t)|$ is also a solution of the unperturbed Schrödinger equation (29) ($\varepsilon = 0$) and it satisfies $|\psi_{oa0}(0)| = 0$ [44].

Through this analyses, we can define a sensitivity systematic error $q_s(\tau)$ given by [44]

$$q_s(\tau) = \int_0^\tau \langle\psi_{oa0}(t)|H_{ae}(t)|\psi(0)\rangle dt,$$

(32)

that quantifies how robust (sensitive) the protocol is against systematic errors. Therefore, a robust protocol requests a tiny value for $q_s(\tau)$. Therefore, our aim is to minimize the function $q_s(\tau)$ in order to maximize the fidelity $P(\tau)$ of the protocol.

To compute $q_s(\tau)$ associated with our protocol, we need to find $|\psi_0(\tau)|$ and $|\psi_{0}^\dagger(\tau)|$. It is easy to see that the evolved state $|\psi_0(\tau)|$ can be obtained from equation (8) with the complex functions $\alpha(t)$ and $\beta(t)$ defined in equation (9), while the state $|\psi_{0}^\dagger(\tau)|$ can be written as $|\psi_{0}^\dagger(\tau)| = \alpha(t)|0\rangle + \beta(t)|1\rangle$, so that the condition $|\psi_{0}^\dagger(\tau)||\psi_0(\tau)| = 0$ imposes that $\alpha(t)\alpha^*(t) + \beta(t)\beta^*(t) = 0$. In addition, once functions $\alpha(t)$ and $\beta(t)$ depend on the input state $|\psi_{inp}|$, it is possible to show (because the propagator $U_1(t)$ is unitary) that functions $\alpha(t)$ and $\beta(t)$ are associated with another input state $|\psi_{inp}^\dagger|$, so that $|\psi_{inp}^\dagger| = \alpha(0)|0\rangle + \beta(0)|1\rangle$, where $a$ and $b$ are real and complex numbers, respectively. Consequently, if we change $a \to b^*$ and $b \to -a$ in equation (9), we can obtain $\alpha(t)$ and $\beta(t)$, respectively. In conclusion, in this case, we get

$$q_s(\tau) = \frac{1}{4} \int_0^\tau \omega(t)[\beta(t)\alpha^*(t) + \alpha(t)\beta^*(t)]dt.$$

(33)

Thus, now we can consider some particular case where we can study (analytically or not) the function $q_s(\tau)$.

**Case one.** For simplicity, let us consider an arbitrary single-qubit gate applied to the particular input state $|\psi_{inp}| = |0\rangle$. Furthermore, we consider a gate where we have the parameters $\phi = 2n\pi$, for $n \in \mathbb{Z}$, and $\theta(t) = \theta_0$ (for example, the gates discussed in section 4.1). In this case, we get

$$q_s(\tau) = \frac{\sin^2\theta_0}{4} \int_0^\tau \varphi(t) \left[\cos(2\theta_0)\sin^2\varphi(t) - \cos^2\varphi(t) + i\cos\theta_0\sin\varphi(t)\right] dt.$$  

(34)

Firstly, it is worth highlighting that, different from others protocols of inverse engineering where the parameter $q_s$ was studied [44, 53–55], in this particular case we have the parameter $q_s$ independent of the total evolution time $\tau$. In fact, let us define the normalized time $s = \tau/\tau$; so that $s \in [0; 1]$. Therefore, with the definition we can rewrite the above equation as

$$q_s = \frac{\sin^2\theta_0}{4} \int_0^1 \varphi(s) \left[\cos(2\theta_0)\sin^2\varphi(s) - \cos^2\varphi(s) + i\cos\theta_0\sin\varphi(s)\right] ds,$$

(35)

therefore we have $q_s$ independent of the total evolution time $\tau$. In addition, in this particular case we can analytically solve the above equation for any function $\varphi(t)$ as

$$q_s = \frac{\sin^2\theta_0}{4} \left[\cos^2\theta_0[\cos\varphi(t) - 1]^2 + [\cos^2\theta_0\sin\varphi(t) + \varphi(t)\sin^2\theta_0]\right],$$

(36)

where we have used the boundary condition $\varphi(0) = 0$. Remarkably, we can see that $q_s$ depends on the boundary conditions for parameter $\varphi(t)$. However, it is important to mention that such a result is due to our consideration of the Hamiltonian $H_{ae}(t)$; for others Hamiltonian we can obtain a different result.
In order to show that we can optimize the protocol against the systematic error considered here, let us consider the gates discussed in this paper. Since we have considered the initial state as a computational basis state, let us discuss the gates discussed in this paper. Since we have considered against the systematic error considered here, let us consider the role of the free parameters introduced here, let us keep the parameter that satisfies the boundary condition \( \theta(\tau) = \theta_0 \). Here we will consider: (i) a constant function \( \theta_{\text{lin}}(t) = \theta_0 \), (ii) the linear interpolation \( \theta_{\text{lin}}(t) = \theta_0 t / \tau \), (iii) quadratic interpolation \( \theta_{\text{quad}}(t) = \theta_0 t^2 / \tau^2 \), (iv) a trigonometric interpolation \( \theta_{\text{tri}}(t) = \theta_0 \sin^2(\pi t / 2\tau) \) and (v) a nontrivial interpolation given by an arc of a cycloid, i.e. we consider

\[
\theta_{\text{cyc}}(t) = r \arccos\left(1 - \frac{1}{r^2} \frac{t}{\tau} \right) - \frac{L}{\tau} \left[2r - \frac{t}{\tau}\right],
\]

where \( r \) is the ratio of the cycloid. However, we will use the parameter \( r \) in order to satisfy the boundary condition \( \theta_{\text{cyc}}(\tau) = \pi / 4 \). In particular, we use \( r \approx 0.69294 \), so that \( \theta_{\text{cyc}}(\tau) \approx \pi / 4 \). In figure 1(b) (inset), we plot each function \( \theta(t) \) considered here.

In figure 1(a) we show the fidelity \( P(\tau) \) for each \( \theta(t) \) discussed above, where we vary parameter \( \varepsilon \). We choose to vary the parameter \( \varepsilon \) within the interval \([-0.1; 0.1]\). Under this consideration, we take into account a systematic error so that an experimental implementation is performed with some \( \omega_{\text{exc}}(t) \in [\omega_{\text{exc}}(t) - 0.1 \omega_{\text{exc}}(t); \omega_{\text{exc}}(t) + 0.1 \omega_{\text{exc}}(t)] \). This assumption is reasonable, since the error due to imperfect calibration of the RF pulse for some experimental implementations in NMR is about 1% – 10% [47–50]. Figure 1(a) shows that the parameter \( \theta(t) \) develops an interesting role for obtaining a robust protocol against systematic errors. Thus, as we have said, the free parameters introduced in our approach may be useful for providing robust Hamiltonians against the systematic errors considered here.

As an ‘experimental guide’ for understanding how the physical parameters \( \omega_{\text{exc}}(t) \) and \( \omega_{\text{c}}(t) \) work, figure 1(b) shows the behavior of the Rabi (respectively Larmor) frequency \( \omega_{\text{exc}}(t) \) (respectively \( \omega_{\text{c}}(t) \)) (always in multiples of the total evolution time \( \tau \)) for each \( \theta(t) \) considered above. Therefore, if the total evolution time is of the order of milliseconds (microseconds), the intensity of \( \omega_{\text{exc}}(t) \) and \( \omega_{\text{c}}(t) \) is of the order of MHz (GHz). From figures 1(a) and (b), we can see that we can obtain a robust protocol with simple functions \( \omega_{\text{exc}}(t) \) and \( \omega_{\text{c}}(t) \); however, we can obtain an enhanced scheme with more complicated functions \( \omega_{\text{exc}}(t) \) and \( \omega_{\text{c}}(t) \). In addition, obtaining the better function \( \theta(t) \) that minimizes the sensitivity function given by equation (37) can be difficult.

In addition, it is important to highlight that our approach can be limited by the experimental setup used for implementing it. For instance, if we wish to implement a Hadamard gate, the protocol does not work with Hamiltonians driven by laser fields where we have the boundary conditions \( \theta(0) = \theta(\tau) = 0 \) [7, 56]. Moreover, the protocol does not work for any boundary condition where we need \( \theta(t) \approx \pi / 4 \). However, as we have discussed, we can implement such a
protocol by using another physical system. For example, quantum dots [57], trapped ions [58], nuclear magnetic resonance [26] and any experimental setup where the Landau–Zener Hamiltonian can be implemented with the boundary $\theta(\tau) = \pi/4$.

6. Conclusion

In summary, in this paper we have introduced a new scheme to perform universal QC via IEH from an evolution operator. We discuss the general aspects of our approach and show how we obtain a set of Hamiltonians that allow us to implement a universal set of quantum gates. Our method is an economic scheme that can be viewed as an alternative to other methods present in the literature. In fact, while many protocols require auxiliary qubits to perform universal QC, our approach does not need the help of auxiliary elements to implement single and controlled arbitrary quantum gates. In particular, we have discussed a restricted set of quantum gates that can be used for QC. Furthermore, by using this approach, we can obtain a large class of Hamiltonians to implement single and two-qubit gates where we use only two-qubit interactions.

In conclusion, we have studied the robustness of our approach against systematic errors due to imprecise calibration of experimental apparatus. In particular, we have considered errors related to Rabi frequency (for example, when there are deviations in the amplitude of the RF field in NMR). We show that the free parameters introduced in this paper can be useful for compensating such systematic errors from a suitable choice of such parameters. In general, the discussion considered here may not be efficient for other kinds of errors; however, we can obtain the ideal free parameters for each case independently, with the intent of providing an enhanced dynamics against such errors.

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References

[1] Gaubatz U, Rudecki P, Schiemann S and Bergmann K 1990 J. Chem. Phys. 92 5363–76
[2] Lewis H R 1967 Phys. Rev. Lett. 18 510–2
[3] Lewis H R Jr and Riesenfeld W 1969 J. Math. Phys. 10 1458
[4] Demirplak M and Rice S A 2003 J. Phys. Chem. A 107 9937
[5] Demirplak M and Rice S A 2005 J. Phys. Chem. B 109 6838
[6] Berry M 2009 J. Phys. A: Math. Theor. 42 365303
[7] Kang Y H, Chen Y H, Wu Q C, Huang B H, Xia Y and Song J 2016 Sci. Rep. 6 30151
[8] Torrontegui E, Ibañez S, Martínez-Garaot S, Modugno M, Del Campo A, Guir-y-Odellin D, Raschhaupt A, Chen X and Muga J G 2013 Adv. At. Mol. Opt. Phys. 62 117
[9] Childs A M, Farhi E and Preskill J 2001 Phys. Rev. A 65 012322
[10] Amin M H S, Averin D V and Nesteroff J A 2009 Phys. Rev. A 79 022107
[11] Du Y, Liang Z, Li Y, Yue X, Lv Q, Huang W, Chen X, Yan H and Zhu S 2016 Nat. Commun. 7 12479
[12] Beau M, Jaramillo J and del Campo A 2016 Entropy 18 168
[13] Santos A C and Sarandy M S 2017 J. Phys. A: Math. Theor. (https://doi.org/10.1088/1751-8121/aa9f61)
[14] Chen Y H, Xia Y, Wu Q C, Huang B H and Song J 2016 Phys. Rev. A 93 052109
[15] Chen Y H, Xia Y, Chen Q Q and Song J 2014 Phys. Rev. A 89 033856
[16] Chen Y H, Xia Y, Chen Q Q and Song J 2015 Phys. Rev. A 91 012325
[17] Lu M, Xia Y, Shen L T, Song J and An N B 2014 Phys. Rev. A 89 012326
[18] Farhi E, Goldstone J, Gutmann S, Lapan J, Lundgren A and Preda D 2001 Science 292 472–5
[19] Santos A C and Sarandy M S 2015 Sci. Rep. 5 15775
[20] Santos A C, Silva R D and Sarandy M S 2016 Phys. Rev. A 93 012311
[21] Coullamy I B, Santos A C, Hen I and Sarandy M S 2016 Frontiers in ICT 3 19
[22] Song X-K, Deng F-G, Lamata L and Muga J G 2017 Phys. Rev. A 95 022332
[23] Bacon D and Flammia S T 2009 Phys. Rev. Lett. 103 120504
[24] Hen I 2015 Phys. Rev. A 91 022309
[25] Song X-K, Zhang H, Ai Q, Qiu J and Deng F-G 2016 New J. Phys. 18 023001
[26] Nielsen M A and Chuang I L 2011 Quantum Computation and Quantum Information: 10th Anniversary Edition 10th edn (New York: Cambridge University Press)
[27] Hen I 2014 Frontiers Phys. 2 44
[28] Messiah A 1962 Quantum Mechanics (Amsterdam: North-Holland)
[29] Herrera M, Sarandy M S, Duzzioni E I and Serra R M 2014 Phys. Rev. A 89 022323
[30] Jing J, Wu L A, Sarandy M S and Muga J G 2013 Phys. Rev. A 88 053422
[31] Chen Y H, Wu Q C, Huang B H, Song J and Xia Y 2016 Sci. Rep. 6 38484
[32] Barenco A, Bennett C H, Cleve R, DiVincenzo D P, Margolus N, Shor P, Sleator T, Smolin J A and Weinfurter H 1995 Phys. Rev. A 52 3457–67
[33] Bason M G, Viteau M, Malossi N, Huillery P, Arimondo E, Ciampini D, Fazio R, Giovannetti V, Manneb R and Moroch O 2012 Nat. Phys. 8 147
[34] Johnson M G et al 2011 Nature 473 194
[35] Harris R et al 2010 Phys. Rev. B 82 024511
[36] Orlando T P, Moej E J, Tian L, van der Wal C H, Levitov L S, Lloyd S and Mazo J J 1999 Phys. Rev. B 60 15398
[37] You J and Nori F 2005 Phys. Today 58 42
[38] Oliveira I, Sarthour R J, Bonagamba T, Azvedo E and Freitas J C 2011 NMR Quantum Information Processing (Oxford: Elsevier)
[39] Kok P, Munro W J, Nemoto K, Ralph T C, Dowling J P and Milburn G J 2007 Rev. Mod. Phys. 79 135–74
[40] Chatterjee D and Roy A 2015 Prog. Theor. Exp. Phys. 2015 093A02
[41] Filidou V, Simmons S, Karlen S, Giustino F, Anderson H and Morton J 2012 Nat. Physics 8 596–600
[42] Vandersypen L M K and Chuang I L 2005 *Rev. Mod. Phys.* **76** 1037–69

[43] Le Bellac M 2006 *A Short Introduction to Quantum Information and Quantum Computation* (New York: Cambridge University Press)

[44] Ruschhaupt A, Chen X, Alonso D and Muga J 2012 *New J. Phys.* **14** 093040

[45] Ivanov S S and Vitanov N V 2015 *Phys. Rev. A* **92** 022333

[46] Low G H, Yoder T J and Chuang I L 2014 *Phys. Rev. A* **89** 022341

[47] Mitra A, Tulsi A and Kumar A 2009 arXiv:0912.4071

[48] Raitz C, Souza A M, Auccaise R, Sarthour R S and Oliveira I S 2015 *Quantum Inf. Process.* **14** 37–46

[49] Bernardes N K, Peterson J P, Sarthour R S, Souza A M, Monken C, Roditi I, Oliveira I S and Santos M F 2016 *Sci. Rep.* **6** 33945

[50] Silva I A *et al* 2016 *Phys. Rev. Lett.* **117** 160402

[51] Sakurai J J 1993 *Modern Quantum Mechanics*. 2nd edn (Reading, MA: Addison-Wesley)

[52] Zettili N 2009 *Quantum Mechanics: Concepts and Applications* 2nd edn (Chichester: Wiley)

[53] Lu X J, Chen X, Ruschhaupt A, Alonso D, Guérin S and Muga J G 2013 *Phys. Rev. A* **88** 033406

[54] Tseng S Y, Wen R D, Chiu Y F and Chen X 2014 *Opt. Express* **22** 18849–59

[55] Kiely A and Ruschhaupt A 2014 *J. Phys. B: At. Mol. Opt. Phys.* **47** 115501

[56] Chen Z, Chen Y, Xia Y, Song J and Huang B 2016 *Sci. Rep.* **6** 22202

[57] Shinkai G, Hayashi T, Ota T and Fujisawa T 2009 *Phys. Rev. Lett.* **103** 056802

[58] Cui J M *et al* 2016 *Sci. Rep.* **6** 33381