Designing robust gate implementations for quantum-information processing

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Quantum-information processing systems are often operated through time-dependent controls; choosing these controls in a way that makes the resulting operation insensitive to variations in unknown or uncontrollable system parameters is an important prerequisite for obtaining high-fidelity gate operations. In this article we present a numerical method for constructing such robust control sequences for a quite general class of quantum-information processing systems. As an application of the method we have designed a robust implementation of a phase-shift operation central to rare-earth-metal quantum computing, an ensemble quantum computing system proposed by Ohlsson *et al.* [Opt. Commun. **201**, 71 (2002)]. In this case the method has been used to obtain a high degree of insensitivity with respect to differences between ensemble members, but it is equally well suited for quantum computing with a single physical system.

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I. INTRODUCTION

Many potential quantum-information processing systems are controlled by means of a set of time-dependent parameters, such as quasistatic electromagnetic fields [1], radio frequency [2,3], or optical fields [4–7]. For most such systems, it is relatively simple to devise a set of controls that implement a given evolution in an ideal situation. Often, however, a more careful choice of controls can lead to an implementation that is less sensitive to variations in unknown or uncontrollable system parameters. Examples of such robust implementations include system specific solutions such as the hot gate for ion trap quantum computing, which is insensitive to vibrational excitations [8], as well as more general techniques such as composite pulses, a technique originating in NMR spectroscopy [9].

In this article we describe a numerical method for designing robust controls for systems that can be adequately described by the Schrödinger equation. We will allow the associated Hamiltonian to include non-Hermitian terms describing decay and the associated loss of coherence.

As an application of the method, we will consider the construction of a robust phase-shift operation for the rare-earth-metal quantum computing (REQC) system [4,10], which is based on rare-earth-metal ions embedded in a cryogenic crystal. In each ion, two metastable ground-state hyperfine levels, labeled $|0\rangle$ and $|1\rangle$, serve as a qubit register which is manipulated via optical transitions from both states to an inhomogeneously shifted excited state $|e\rangle$. The REQC system is an ensemble quantum computing system and macroscopic numbers of ions are manipulated in parallel, addressed by the value of the inhomogeneous shift of their $|e\rangle$ state. To obtain a sufficient number of ions within each frequency channel, it is necessary to operate on all ions within a finite range of inhomogeneous shifts, and the main difficulty in operating the REQC system is to achieve the same evolution for each of these ions independent of their particular inhomogeneous shift.

This article is divided into two sections: in Sec. I we describe the method we have used to design robust gate implementations; these results should be applicable to a variety of quantum-information processing systems. In Sec. II we present the results of applying the method to a specific problem relating to the REQC system and show that it is indeed possible to obtain very high degrees of robustness.

II. DESIGNING ROBUST GATE IMPLEMENTATIONS

We consider a collection of quantum system which evolve according to a set of time-dependent controls $\boldsymbol{\varepsilon}(t)$. In addition to $\boldsymbol{\varepsilon}$, the single system Hamiltonian $H(\boldsymbol{\xi};\boldsymbol{\varepsilon}(t))$ depends on a system specific set of uncontrollable or unknown parameters $\boldsymbol{\xi}$, such as field strength or quantum numbers corresponding to unused degrees of freedom. The evolution of each system is governed by the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\mathbf{U}(\boldsymbol{\xi};t)=H(\boldsymbol{\xi};\boldsymbol{\varepsilon}(t))\mathbf{U}(\boldsymbol{\xi};t),\quad \mathbf{U}(\boldsymbol{\xi};0)=\mathbf{1}, \tag{1}$$

where we will allow the Hamiltonian H to include non-Hermitian terms describing loss.

Our goal is to choose a set of controls that lead to an evolution $\mathbf{U}(\boldsymbol{\xi};T)$ which is as close as possible to a given desired evolution $\mathbf{U}_0(\boldsymbol{\xi})$ for all $\boldsymbol{\xi}$ values in a set X. To quantify this, we introduce an objective functional $J(\boldsymbol{\xi},\boldsymbol{\varepsilon})$ which describes the performance of a set of controls $\boldsymbol{\varepsilon}$ for a given value of $\boldsymbol{\xi}$. By convention we take a low value of J to indicate a good performance, and the problem of finding a robust set of controls thus corresponds to minimizing

$$J_X(\boldsymbol{\varepsilon})=\max_{\boldsymbol{\xi}\in X} J(\boldsymbol{\xi},\boldsymbol{\varepsilon}). \tag{2}$$

The conceptually simple approach we have taken to this problem is to replace X with a discrete subset $X'\subset X$, so that the minimization of $J_{X'}$ has the form of a so-called minimax problem, which can be solved efficiently provided that we are able to calculate $\partial J(\boldsymbol{\xi},\boldsymbol{\varepsilon})/\partial\boldsymbol{\varepsilon}$.

A. Calculating $\partial J(\xi,\varepsilon)/\partial\varepsilon$

In this section we show how the control dependency of a quite general class of single system objective functionals may be calculated by methods from optimal control theory. To reduce notational complexity and avoid unnecessary restrictions, we will consider the following generalization of the single system Schrödinger equation (1),

$$\dot{\mathbf{U}}(t) = \mathbf{f}(\mathbf{U}(t),\boldsymbol{\varepsilon}(t)), \quad \mathbf{U}(0) = \mathbf{1}, \tag{3}$$

determining the evolution of a complex-valued, time-dependent matrix $\mathbf{U}(t)$ due to a set of real-valued, time-dependent controls $\boldsymbol{\varepsilon}(t)$. We consider single system objective functionals of the form,

$$J(\boldsymbol{\varepsilon}) = \phi\big(\mathbf{U}(T)\big) + \int_0^T l\big(\mathbf{U}(t),\boldsymbol{\varepsilon}(t)\big)dt. \tag{4}$$

Here $\phi(\mathbf{U}(T))$ is a real-valued function quantifying how close the final state $\mathbf{U}(T)$ is to our goal, and the real-valued function $l(\mathbf{U}(t),\boldsymbol{\varepsilon}(t))$, referred to as a penalty function, can be chosen to discourage the use of certain states or control values.

Our goal is to calculate $\partial J/\partial\boldsymbol{\varepsilon}$ subject to the constraint that $\boldsymbol{\varepsilon}$ and $\mathbf{U}$ obey Eq. (3). To achieve this, we introduce the modified objective functional:

$$J' = J - \int_0^T \mathrm{Tr}[\boldsymbol{\Lambda}^\dagger\{\dot{\mathbf{U}} - \mathbf{f}(\mathbf{U},\boldsymbol{\varepsilon})\} + \mathrm{H.c.}]dt, \tag{5}$$

where the complex time-dependent adjoint state matrix $\boldsymbol{\Lambda}$ is in effect a continuous set of Lagrange multipliers leaving J' identical to J, provided that $\mathbf{U}$ and $\boldsymbol{\varepsilon}$ obey Eq. (3). Introducing

$$h(\boldsymbol{\varepsilon},\mathbf{U},\Lambda) = l(\mathbf{U},\boldsymbol{\varepsilon}) + \mathrm{Tr}[\boldsymbol{\Lambda}^\dagger\mathbf{f}(\mathbf{U},\boldsymbol{\varepsilon}) + \mathrm{H.c.}], \tag{6}$$

we can express the first-order change in J' due to a variation $\delta\boldsymbol{\varepsilon}$ in $\boldsymbol{\varepsilon}$ and resulting variation $\delta\mathbf{U}$ in $\mathbf{U}$ as

$$dJ' = \int_0^T \frac{\partial h}{\partial\boldsymbol{\varepsilon}}\delta\boldsymbol{\varepsilon}dt + 2\,\mathrm{Re}\,\mathrm{Tr}\left(\left\{\frac{\partial\phi}{\partial\mathbf{U}^\dagger} - \boldsymbol{\Lambda}\right\}^\dagger\delta\mathbf{U}\right)\Bigg|_T + \int_0^T 2\,\mathrm{Re}\,\mathrm{Tr}\left(\left\{\frac{\partial h}{\partial\mathbf{U}^\dagger} + \dot{\boldsymbol{\Lambda}}\right\}^\dagger\delta\mathbf{U}\right)dt, \tag{7}$$

where $\mathbf{U}$ and $\mathbf{U}^\dagger$ should be considered as independent with respect to the partial derivative. We now require the adjoint state $\boldsymbol{\Lambda}$ to obey the adjoint equations

$$\dot{\boldsymbol{\Lambda}}^\dagger = -\frac{\partial h}{\partial\mathbf{U}}, \quad \boldsymbol{\Lambda}^\dagger(T) = \frac{\partial\phi}{\partial\mathbf{U}}\Bigg|_T, \tag{8}$$

in which case Eq. (7) reduces to [11]

$$dJ' = \int_0^T \frac{\partial h}{\partial\boldsymbol{\varepsilon}}\delta\boldsymbol{\varepsilon}(t)dt. \tag{9}$$

Equation (9) is the main result of this section, as it allows us to calculate explicitly the change in J due to a change $\delta\boldsymbol{\varepsilon}(t)$ in the controls. To accomplish this we proceed as follows: from the dynamical equation (3) and the initial controls we determine $\mathbf{U}(t)$ for all t. Based on $\mathbf{U}(T)$ we can calculate the adjoint state boundary condition which we back propagate according to Eq. (8) to obtain $\Lambda(t)$ for all t. Knowing both $\mathbf{U}(t)$ and $\boldsymbol{\Lambda}(t)$ for all t we can compute dJ for any $\delta\boldsymbol{\varepsilon}$ according to Eq. (9). In an actual application $\boldsymbol{\varepsilon}(t)$ will be parametrized in some way, e.g., $\boldsymbol{\varepsilon}(t)=\Sigma_k\, c_k f_k(t)$, and we will be interested in the dependence of J on the parameters, which according to Eq. (9) would be $\partial J/\partial c_k = \int_0^T \partial h(\boldsymbol{\varepsilon},\mathbf{U},\boldsymbol{\Lambda})/\partial\boldsymbol{\varepsilon} f_k(t)dt$ for this simple parametrization.

We now return to the case of a quantum system governed by the Schrödinger equation (1). If we assume the penalty function l to be independent of $\mathbf{U}$, the adjoint equations in this case are

$$i\hbar\frac{\partial}{\partial t}\boldsymbol{\Lambda}(\boldsymbol{\xi};t) = H^\dagger(\boldsymbol{\xi};\boldsymbol{\varepsilon}(t))\boldsymbol{\Lambda}(\boldsymbol{\xi};t), \tag{10a}$$

$$\boldsymbol{\Lambda}(\boldsymbol{\xi};T) = \frac{\partial\phi(\boldsymbol{\xi},\mathbf{U})}{\partial\mathbf{U}^\dagger}\Bigg|_T, \tag{10b}$$

and dJ is given by Eq. (9) with

$$\frac{\partial h}{\partial\boldsymbol{\varepsilon}} = \frac{\partial l}{\partial\boldsymbol{\varepsilon}} + \frac{2}{\hbar}\mathrm{Im}\,\mathrm{Tr}\left(\boldsymbol{\Lambda}^\dagger\frac{\partial H}{\partial\boldsymbol{\varepsilon}}\mathbf{U}\right). \tag{11}$$

The role of the adjoint state and the adjoint equations is often described as back propagating the errors in achieving the desired final state. If H is Hermitian, the boundary value for $\boldsymbol{\Lambda}$ can be optimized for numerical computation as shown in Appendix B.

B. Fidelity of quantum evolution

We will now discuss the choice of the function ϕ, quantifying how well an obtained evolution $\mathbf{U}$ approximates $\mathbf{U}_0$. As we are concerned with quantum-information processing we will assume that all operations start out with an unknown state in the qubit subspace $\mathcal{H}_Q$ of the full system Hilbert space $\mathcal{H}$, and that this subspace is invariant under the ideal evolution $\mathbf{U}_0$. The function ϕ should not depend on the evolution of states outside $\mathcal{H}_Q$, nor on collective phases on the states originating in $\mathcal{H}_Q$. A cautious choice of ϕ fulfilling these conditions could be based on the gate fidelity [12]:

$$\mathcal{F}(\mathbf{U}_0,\mathbf{U}) = \min_{|\psi\rangle\in\mathcal{H}_Q} |\langle\psi|\mathbf{U}_0^\dagger\mathbf{U}|\psi\rangle|, \tag{12}$$

which measures the least possible overlap between the obtained output state $\mathbf{U}|\psi\rangle$ and the ideal output $\mathbf{U}_0|\psi\rangle$ for initial states in $\mathcal{H}_Q$. This fidelity measure has the desirable quality that both population transfer from $\mathcal{H}_Q$ to $\mathcal{H}_Q^\perp$ and population transfer completely out of $\mathcal{H}$, as described by a nonunitary evolution, is counted as loss of fidelity.

From the point of view of optimal control, a significant drawback of the gate fidelity $\mathcal{F}$ is that it is computationally complicated [13]. A computationally accessible fidelity measure which share many appealing features with $\mathcal{F}$ is the trace fidelity [14],

$$\mathcal{T}(\mathbf{U}_0,\mathbf{U}) = \frac{1}{n}\left|\mathrm{Tr}_{\mathcal{H}_Q}(\mathbf{U}_0^\dagger \mathbf{U})\right|, \tag{13}$$

where $n=\dim(\mathcal{H}_Q)$. As shown in Appendix A, $\mathcal{T}$ is related to $\mathcal{F}$ by the strict bound

$$1-\mathcal{F} \leqslant n(1-\mathcal{T}), \tag{14}$$

indicating that we can safely replace $\mathcal{F}$ by $\mathcal{T}$ for numerical computations on a few qubits at high fidelity.

For numerical calculations it is beneficial to use $\mathcal{T}^2$ rather than $\mathcal{T}$ [15]; in the calculations presented in the following section we have used $\phi(\boldsymbol{\xi},\mathbf{U}(\boldsymbol{\xi};T))=1-\mathcal{T}^2(\mathbf{U}_0(\boldsymbol{\xi}),\mathbf{U}(\boldsymbol{\xi};T))$, which according to Eq. (10b) yields an adjoint state boundary condition of

$$\mathbf{\Lambda}(\boldsymbol{\xi};T) = -\frac{1}{n^2}\mathbf{U}_0(\boldsymbol{\xi})\mathrm{Tr}_{\mathcal{H}_Q}(\mathbf{U}_0(\boldsymbol{\xi})^\dagger \mathbf{U}(\boldsymbol{\xi};T)). \tag{15}$$

C. Minimization algorithms

One approach to minimizing the single system objective functional $J(\boldsymbol{\xi},\boldsymbol{\varepsilon})$ is to directly solve the extremum condition $\partial J/\partial \boldsymbol{\varepsilon}=0$ for $\boldsymbol{\varepsilon}$. This task is significantly simplified if a penalty function proportional to $\boldsymbol{\varepsilon}^2$ is introduced, $h=\lambda\boldsymbol{\varepsilon}^2+h_0$, so that the extremum condition according to Eq. (9) reads,

$$\boldsymbol{\varepsilon}(t) = -\frac{1}{2\lambda}\frac{\partial h_0}{\partial \boldsymbol{\varepsilon}}, \tag{16}$$

which may be used as an iterative formula for calculating $\boldsymbol{\varepsilon}$. Variations over this iterative approach give rise to the Krotov [16] and Zhu-Rabitz [17,18] algorithms which have been shown to have excellent convergence properties, and have been successfully applied to optimal control of unitary transformations for one set of parameters by Palao *et al.* [14,15]. A unifying view of these direct methods can be found in Ref. [19].

In the present setting we are interested in optimizing the performance for a number of parameter sets simultaneously, corresponding to minimizing $J_{X'}$ as introduced in the start of this section. For the direct approach to be applied to this problem it appears that it would be necessary to replace $J_{X'}(\boldsymbol{\varepsilon})$ with some smooth function of the various $J(\boldsymbol{\xi},\boldsymbol{\varepsilon})$.

As an alternative to this approach, we have chosen to use an indirect minimization algorithm: rather than trying to solve the extremum condition directly, we have used the gradient information obtained through Eq. (9) as input for a general minimax algorithm based on a constrained quasi-Newton sequential quadratic programming procedure [20–22]. The primary advantage of this approach is that we have total freedom to choose the parametrization of the controls and can place arbitrary bounds on these. This allows us to more accurately model the fact that the experimental limitations most often only distinguish between possible and impossible controls: no possible controls are significantly harder than others. An explicit field strength limit also serves to introduce an absolute scale on which to introduce decay strengths, etc.

III. APPLICATION TO RARE-EARTH-METAL QUANTUM COMPUTING

The motivation for the work presented in this article has been the design of robust gate implementations for the REQC system mentioned in the Introduction. As an example, we will consider the construction of a robust implementation of the single qubit phase shift operation described by the evolution

$$\mathbf{U}_{\mathrm{PS}} = |1\rangle\langle 1| - |0\rangle\langle 0| \tag{17}$$

of $\mathcal{H}_Q$. We will model the REQC system by the single-ion Hamiltonian

$$H = -\delta|e\rangle\langle e| + \frac{\gamma}{2}\sum_{i=0,1}(\Omega_i(t)|e\rangle\langle i| + \mathrm{H.c.}), \tag{18}$$

where Ω_1 and Ω_2 are the time-dependent complex Rabi frequencies of the fields addressing the $|0\rangle$-$|e\rangle$ and $|1\rangle$-$|e\rangle$ transitions, respectively, and $\hbar$ has been set to 1. H does not include any effects of decay or decoherence, so that if we were not concerned with robustness, we could simply implement $\mathbf{U}_{\mathrm{PS}}$ by a single 2π pulse on the $|0\rangle$-$|e\rangle$ transition, causing a phase shift of -1 on the $|e\rangle$ and $|0\rangle$ states of an ideal ion with $\delta=0$ and $\gamma=1$. Our primary concern will be to find an implementation of $\mathbf{U}_{\mathrm{PS}}$ which is robust with respect to variations in the inhomogeneous shift δ of the $|e\rangle$ state in order to allow the use of finite width channels. Since it is experimentally difficult to obtain a homogeneous field strength over the crystal, we would also prefer the implementation to be insensitive to variations in the relative field strength γ.

In addition to requiring the implementation of $\mathbf{U}_{\mathrm{PS}}$ to be robust with respect to variations in δ and γ, we will add the requirement that ions outside the channel should not be affected, as this allows us to use the obtained implementation of $\mathbf{U}_{\mathrm{PS}}$ as a part of a controlled phase-shift operation [4,7]: If the $|e\rangle$ states of the qubit ion and a controlling ion are coupled sufficiently strongly by static dipole interaction, an excitation of the controlling ion will effectively shift the qubit ion out of the channel, thus conditioning the evolution of the qubit on the state of the controlling ion.

Even though the simplest implementation of $\mathbf{U}_{\mathrm{PS}}$ for an ideal ion with $\delta=0$ and $\gamma=1$ would address only the $|0\rangle$-$|e\rangle$ transition, a robust implementation must also involve the $|1\rangle$-$|e\rangle$ transition, since the coupling of $|0\rangle$ to $|e\rangle$ will result in a δ-dependent phase on $|0\rangle$ which can only be compensated by introducing the same phase on the $|1\rangle$ state, e.g., through phase compensating rotations [13]. A highly successful example of this approach is the sech-pulse sequence suggested by Roos and Mølmer [23], which as illustrated by Fig. 1(a) yields a very robust implementation, achieving high fidelities over a wide range of parameter values.

In the notation introduced in Sec. I, the system parameters are $\boldsymbol{\xi}=(\gamma,\delta)$, the controls are $\boldsymbol{\varepsilon}=(\Omega_0,\Omega_1)$, and the qubit subspace is $\mathcal{H}_Q=\{|0\rangle,|1\rangle\}$. The objective functional is chosen to be $J(\boldsymbol{\xi},\boldsymbol{\varepsilon})=1-\mathcal{T}^2(\mathbf{U}_0(\boldsymbol{\xi}),\mathbf{U}(\boldsymbol{\xi};T))$, with

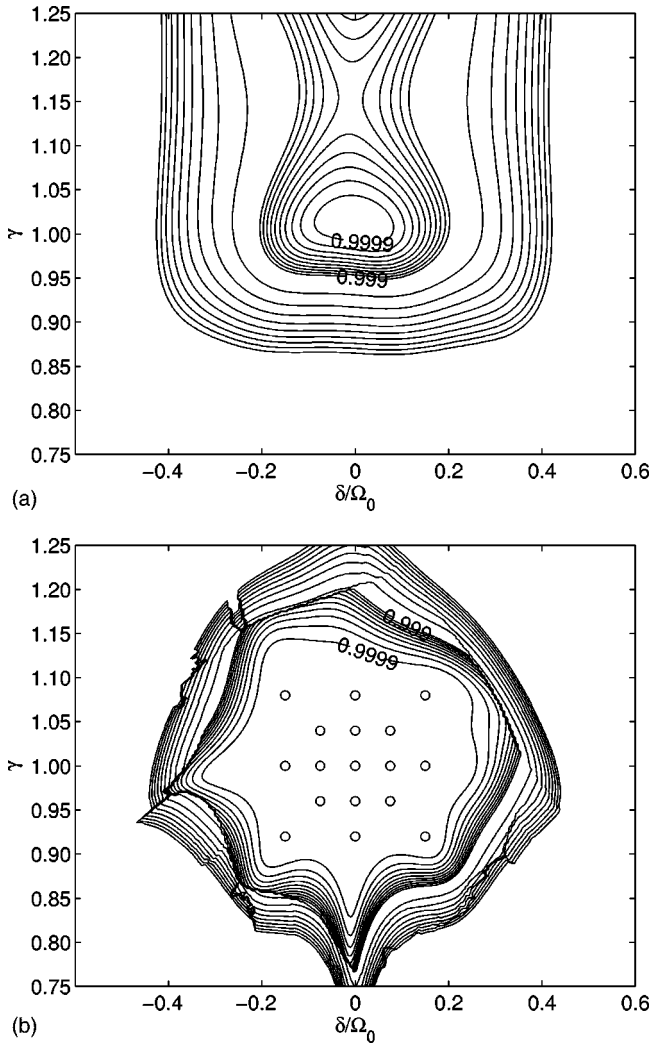

FIG. 1. The gate fidelity of two implementations of $\mathbf{U}_{\mathrm{PS}}$ plotted as a function of relative field strength γ and inhomogeneous shift δ relative to the maximal Rabi frequency Ω_0. The gate is implemented by (a) a series of sech pulses as suggested by Roos and Mølmer [23], and (b) by an optimized pulse obtained by minimizing $J_{X'}(\boldsymbol{\varepsilon})$, corresponding to simultaneously minimizing $J(\boldsymbol{\xi},\boldsymbol{\varepsilon})$ for $\boldsymbol{\xi}$ in a set X' of parameter values indicated by circles in the plot. The duration of both pulses is $24\pi/\Omega_0$.

$$\mathbf{U}_0(\boldsymbol{\xi}) = \begin{cases} \mathbf{U}_{\mathrm{PS}} & \text{for } |\delta| < \Omega_0, \\ \mathbf{1} & \text{for } |\delta| > \Omega_0, \end{cases} \tag{19}$$

where Ω_0 is the maximal resonant Rabi frequency at $\gamma=1$. No penalty function is used; instead we limit the field by strict bounds on $|\Omega_i(t)|$ as this is the relevant limiting parameter in the REQC system. Inspired by the success of the sech-based solution and the hatlike Fourier spectrum of the sech pulse, $\Omega_i(t)$ is parametrized in terms of a truncated Fourier basis. Based on trial and error we have arrived at 49 $\boldsymbol{\xi}$ values to constitute X', some within the neighborhood of $\delta=0$, $\gamma=1$, and some at large detunings where the ions should not be disturbed. The result of the optimization with this choice of X' is shown in Fig. 1(b), where the circles indicate the members of X'. It is evident from the plot that the optimization has achieved a high fidelity over an even larger range of parameters than the sech-pulse sequence illustrated in Fig. 1(a).

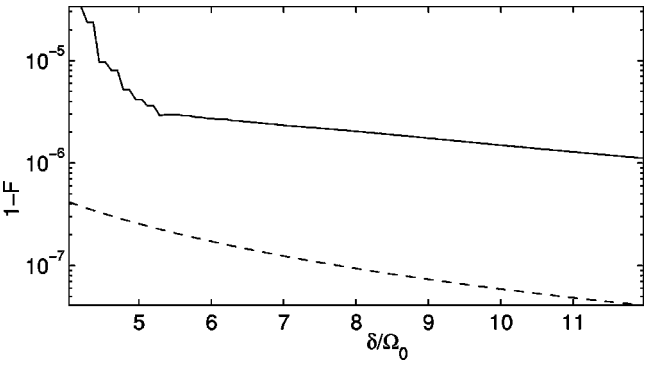

FIG. 2. The effect of the sech-pulse sequence (dashed line) and the optimized (solid line) implementation of $\mathbf{U}_{\mathrm{PS}}$ on far-detuned ions, as described by $1-\mathcal{F}$ where $\mathcal{F}$ is calculated with respect to the identity, since these ions should ideally not be disturbed. Both implementations achieve gate fidelities very close to unity, with the sech-pulse sequence achieving the best results. The curve for the optimized pulse is a running maximum as the actual value of $1-\mathcal{F}$ oscillates with a period of $2\pi/T$.

With respect to not disturbing the detuned ions, both the optimized pulse and the sech pulses obtain fidelities within 10^{-5} of unity for $|\delta|>5\Omega_0$. As illustrated by Fig. 2, which only shows fidelities at $\gamma=1$ as $\mathbf{U}(\boldsymbol{\xi};T)$ is nearly independent of γ at $|\delta|\gg\Omega_0$, the sech-pulse sequence performs better than the optimized pulse in this regime.

IV. CONCLUSIONS AND OUTLOOK

We have shown that it is possible to construct highly robust gate implementations for quantum-information processing by a quite general method. In particular, the method has been used to greatly enhance the performance of a gate implementation for a model REQC system by extending the range of inhomogeneous shifts and relative field strengths over which an acceptable performance is achieved.

The model REQC system used in this article ignores many performance degrading factors, the two most important being decoherence and implementation noise. Decoherence could in the present case be adequately modeled by a non-Hermitian Hamiltonian, for which we expect the method described in this paper to be able to find a robust implementation as in the decoherence-free case. It is not clear, however, how the method could be extended to address the problem of robustness with respect to implementation imperfections.

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APPENDIX A: THE TRACE FIDELITY

In this section we prove the relation (14) between the gate fidelity $\mathcal{F}$ and the trace fidelity $\mathcal{T}$. Referring to the definition (12), we note that $\mathcal{F}(\mathbf{U}_0,\mathbf{U})$ is completely determined by the restriction $\mathbf{O}$ of the operator $\mathbf{U}_0^\dagger\mathbf{U}$ to $\mathcal{H}_Q$. Since $\mathbf{U}$ describes the evolution of a quantum system, it is possible to extend it to a unitary operation on a Hilbert space containing $\mathcal{H}$, and $\mathbf{O}$ is consequently the restriction of a unitary operator to $\mathcal{H}_Q$. In the ideal case $\mathbf{O}$ will be equal to the identity on $\mathcal{H}_Q$, perhaps with the exception of a complex phase.

$\mathcal{F}$ is defined as the minimum of the overlap $\langle\psi|\mathbf{O}|\psi\rangle$ for $|\psi\rangle\in\mathcal{H}_Q$. Since the unit sphere of $\mathbb{C}^n$ is compact, this minimum will be attained for some $|\psi_0\rangle$: $\mathcal{F}=|\langle\psi_0|\mathbf{O}|\psi_0\rangle|$. We now extend $\{|\psi_0\rangle\}$ to an orthonormal basis $\{|\psi_k\rangle\}_{k=0,\ldots,n-1}$ of $\mathcal{H}_Q$ by the Gram-Schmidt process. Evaluating the trace fidelity in this basis we find by the triangle inequality:

$$\mathcal{T}\leqslant\frac{1}{n}\sum_{k=0}^{n-1}|\langle\psi_k|\mathbf{O}|\psi_k\rangle| \tag{A1a}$$

$$\leqslant\frac{1}{n}[\mathcal{F}+(n-1)], \tag{A1b}$$

where we have used that $|\langle\psi|\mathbf{O}|\psi\rangle|\leqslant 1$ for all $|\psi\rangle$ since $\mathbf{O}$ is the restriction of a unitary operator. By rewriting Eq. (A1b) we obtain the desired relation (14).

We note that the established bound is strict in the sense that for any $0\leqslant\mathcal{F}_0\leqslant 1$, the operator

$$\mathbf{O}_{\mathcal{F}}=\mathbf{1}-(1-\mathcal{F}_0)|\psi\rangle\langle\psi| \tag{A2}$$

will fulfill Eq. (14) with equality for any $|\psi\rangle$.

APPENDIX B: OPTIMIZED ADJOINT STATE BOUNDARY CONDITION

In this section we will show that in the case of a Hermitian Hamiltonian and a penalty function that does not depend on the state $\mathbf{U}$, it is possible to modify the adjoint state boundary condition (10b) to reduce the required accuracy of the adjoint state propagation. To reduce notational complexity, we will not explicitly include the $\boldsymbol{\xi}$ dependency in this appendix.

Under the assumptions stated above, we find according to Eqs. (9) and (11) that dJ has the form

$$dJ=\int_0^T\left[\frac{\partial l}{\partial\boldsymbol{\varepsilon}}+2\ \mathrm{Im}\left(\sum_k\boldsymbol{\lambda}_k^\dagger\frac{\partial H}{\partial\boldsymbol{\varepsilon}}\mathbf{u}_k\right)\right]\delta\boldsymbol{\varepsilon}(t)dt, \tag{B1}$$

where $\mathbf{u}_k$ and $\boldsymbol{\lambda}_k$ denote the kth columns of $\mathbf{U}$ and $\boldsymbol{\Lambda}$, respectively. Since H and thus $\partial H/\partial\boldsymbol{\varepsilon}$ are assumed to be Hermitian, dJ as given by Eq. (B1) is not affected by replacing $\boldsymbol{\lambda}_k$ with $\tilde{\boldsymbol{\lambda}}_k(t)=\boldsymbol{\lambda}_k(t)+\alpha_k\mathbf{u}_k(t)$ for any real constants α_k. Since we assume l to be independent of $\mathbf{U}$ and H to be Hermitian, we see from Eq. (10a) that $\boldsymbol{\Lambda}$ and $\mathbf{U}$ evolve according to the same linear equation. As the same is thus true for $\boldsymbol{\lambda}_k$ and $\mathbf{u}_k$, replacing $\boldsymbol{\lambda}_k$ with $\tilde{\boldsymbol{\lambda}}_k$ is seen to correspond to replacing the boundary conditions for the adjoint state columns to read

$$\tilde{\boldsymbol{\lambda}}_k(T)=\boldsymbol{\lambda}_k(T)+\alpha_k\mathbf{u}_k(T), \tag{B2}$$

where $\boldsymbol{\lambda}_k(T)$ are the columns of the unmodified adjoint state boundary value $\boldsymbol{\Lambda}(T)$ as given by Eq. (10b).

One use of the freedom in the choice of the constants α_k is to minimize the norm of the adjoint state $|\tilde{\boldsymbol{\lambda}}_k|$, in order to relax the requirements of the relative precision of the adjoint state propagation. This minimum is easily calculated from Eq. (B2), but we prefer to illustrate the physical background of the result by calculating it in a different way: To do so we introduce $\tilde{\phi}$ as $\tilde{\phi}(\mathbf{U})=\phi(\hat{\mathbf{U}})$, where $\hat{\mathbf{U}}$ denotes $\mathbf{U}$ with all columns normalized to unit length. Since H is assumed to be Hermitian, all these columns $\mathbf{u}_k$ will have unit length at all times, so $\tilde{\phi}(\mathbf{U})=\phi(\mathbf{U})$. The derivatives of $\tilde{\phi}$ and ϕ with respect to $\mathbf{u}_k$ will, however, not be equal. As a result, the adjoint state boundary condition, as given by Eq. (10b), corresponding to $\tilde{\phi}$ is found to be

$$\tilde{\boldsymbol{\lambda}}_k(T)=\boldsymbol{\lambda}_k(T)-\mathrm{Re}\{\mathbf{u}_k^\dagger(T)\boldsymbol{\lambda}_k(T)\}\mathbf{u}_k(T). \tag{B3}$$

Comparing this expression to Eq. (B2), it is tempting to let $\alpha_k=\mathrm{Re}[\mathbf{u}_k^\dagger(T)\boldsymbol{\lambda}_k(T)]$, which is indeed found to be the value that minimizes $|\tilde{\boldsymbol{\lambda}}_k|$ subject to Eq. (B2).

In conclusion, we have shown that in the case of a Hermitian Hamiltonian and a state-independent penalty function, we are free to replace the adjoint state $\boldsymbol{\Lambda}$ with a modified adjoint state $\tilde{\boldsymbol{\Lambda}}$, which evolves according to Eq. (8), but with boundary conditions given by Eq. (B3). $\tilde{\boldsymbol{\Lambda}}$ will carry the same error information as $\boldsymbol{\Lambda}$, but the required relative numerical precision when propagating the adjoint state will be reduced, since the norm of the columns of $\tilde{\boldsymbol{\Lambda}}$ will be smaller than those of $\boldsymbol{\Lambda}$.

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