High-fidelity quantum state preparation using neighboring optimal control

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Abstract We present an approach to single-shot high-fidelity preparation of an \(n\)-qubit state based on neighboring optimal control theory. This represents a new application of the neighboring optimal control formalism which was originally developed to produce single-shot high-fidelity quantum gates. To illustrate the approach, and to provide a proof-of-principle, we use it to prepare the two qubit Bell state \(|\beta_{01}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)\) with an error probability \(\varepsilon \sim 10^{-6} (10^{-5})\) for ideal (non-ideal) control. Using standard methods in the literature, these high-fidelity Bell states can be leveraged to fault-tolerantly prepare the logical state \(|\beta_{01}\rangle\). 

Keywords Quantum state preparation, quantum optimal control theory, neighboring optimal control, Bell states

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1 Introduction

In optimal control theory the problem is to determine a control field profile \(F_*(t)\) that optimizes system performance relative to a set of design criteria. A cost function is introduced that quantifies the degree to which a particular assignment of the control and system variables satisfies these criteria, with optimal assignment being one of minimum cost \([1]\). In the quantum version of this problem the optimal control \(F_*(t)\)
drives an optimal unitary transformation $U$, that yields a high-fidelity approximation to a target unitary $U_{tgt}$. The target $U_{tgt}$ might represent a desired quantum gate, or it might be used to prepare a quantum state $|\psi_{tgt}\rangle = U_{tgt} |\psi_{in}\rangle$, given an easily prepared initial state $|\psi_{in}\rangle$. Note that a perturbation of the quantum dynamics can cause the optimal control $F_*(t)$ to become nonoptimal. If the perturbation is small, however, the optimal control problem can be linearized about the unperturbed optimal control, and a family of perturbed optimal controls found from a single feedback control law. In the classical literature this perturbed problem is referred to as neighboring optimal control (NOC) \cite{1}.

In this paper we present a general approach to single-shot high-fidelity quantum state preparation based on NOC theory. This represents a new application of the neighboring optimal control formalism which was originally developed to produce single-shot high-fidelity quantum gates. In Section 2 we formulate the NOC problem and determine the Euler-Lagrange equations whose solution determines the optimal control $F_*(t)$ and the resulting optimal quantum state $|\psi_\ast\rangle$. In Section 3\cite{4} we illustrate the general approach by using it to prepare a high-fidelity approximation to the two qubit Bell state $|\beta_{01}\rangle = (1/\sqrt{2}) [|01\rangle + |10\rangle]$ with error probability $\varepsilon \sim 10^{-6} (10^{-5})$, assuming ideal (non-ideal) control. The high-fidelity of the final state provides proof-of-principle for the performance gains possible using NOC, even in the presence of imperfect control. Note that standard methods in the literature \cite{2} can leverage these high-fidelity Bell states to fault-tolerantly prepare the logical state $|\beta_{01}\rangle$. We close in Section 5 with a discussion of our results. Finally, in Appendix A we briefly review the essential features of a type of non-adiabatic rapid passage used in Sections 3 and 4 and specify the Hamiltonian used to drive the two-qubit dynamics.

2 High-fidelity state preparation using NOC

In this Section we present an approach to $n$-qubit state preparation based on NOC. The task is to find a control field $F(t)$ that produces a quantum state $|\psi_f\rangle$ which is a high-fidelity approximation to a target state $|\psi_{tgt}\rangle$. In Section 2.1 we transform the state preparation problem to that of implementing a high-fidelity approximation $U_f$ to a desired unitary gate $U_{tgt}$. Sections 2.2 and 2.3 summarize earlier work \cite{3} that used NOC theory to produce such a high-fidelity approximation. These Sections formulate the optimization problem whose solution yields the optimal control field $F_*(t)$ and unitary gate $U_\ast$; derive the equations governing the optimization; and describe a procedure for obtaining a solution.

2.1 Reformulating the control problem

Consider an $n$-qubit system whose Hamiltonian is a functional of a control field $F(t)$: $\mathcal{H}(t) = \mathcal{H}[F(t)]$. Throughout this paper we assume: (i) the control $F(t)$ acts for times $-T/2 \leq t \leq T/2$; and (ii) the control duration $T$ is much shorter than the longitudinal ($T_1$) and
transverse ($T_2$) relaxation times so that a qubit is weakly decohering and a state vector description is appropriate. See Section 5 for further discussion of assumption (ii).

Suppose the initial $n$-qubit state is the “all-zeros” computational basis state (CBS) $|\psi(-T/2)\rangle = |0\cdots0\rangle$. The control field $F(t)$ drives a unitary transformation $U(t)$ that produces the final state

$$|\psi_f\rangle = U_f|0\cdots0\rangle,$$

where $U_f \equiv U(T/2)$. Let $\{ |\beta_i\rangle : i = 1,\ldots,M = 2^n \}$ be an orthonormal basis for the $n$-qubit Hilbert space that has $|\beta_1\rangle = |\psi_{tgt}\rangle$. Defining the target gate $U_{tgt}$ as the unitary matrix whose columns are the basis vectors $\{|\beta_i\rangle\}$,

$$U_{tgt} = \begin{bmatrix} |\beta_1\rangle & \cdots & |\beta_i\rangle & \cdots & |\beta_M\rangle \end{bmatrix},$$

we see that, by construction,

$$|\psi_{tgt}\rangle = U_{tgt}|0\cdots0\rangle.$$ (3)

These definitions reformulate the problem of preparing a high-fidelity approximation $|\psi_f\rangle$ to the target state $|\psi_{tgt}\rangle$ to that of implementing a high-fidelity approximation $U_f$ to the target gate $U_{tgt}$ (Eq. (2)). A solution to this problem was found in Ref. [3] using NOC. In the remainder of this Section we summarize that solution and refer the reader to Ref. [3] for a detailed presentation.

2.2 Quantum dynamics of NOC

Ref. [3] showed how NOC could be used to improve the performance of a good quantum gate. The starting point is a nominal control $F_0(t)$ which enacts a unitary $U_0(t)$ such that $U_{0,f} = U_0(T/2)$ is a good approximation to the target $U_{tgt}$. Then $U_{0,f}$ is close to the inverse of $U_{tgt}$ so that

$$U_{0,f}^\dagger U_{tgt} = I - i\delta \beta + O(\Delta^2).$$ (4)

NOC was then used to determine a control modification $\Delta F(t)$ which yields a new control $F(t) = F_0(t) + \Delta F(t)$ which drives a unitary $U(t)$ that provides a better approximation $U_f = U(T/2)$ to $U_{tgt}$. Since $F_0(t)$ is a good control, $\Delta F(t)$ is expected to be small. To begin, we write $U(t)$ as

$$U(t) = U_0(t)\delta U(t),$$ (5)

where

$$\delta U(t) = I - i\delta A(t) + O(\Delta^2).$$ (6)

Substituting Eqs. (5) and (6) into the Schrodinger equation ($\hbar = 1$)

$$i \frac{d}{dt} U(t) = \mathcal{H}[F(t)]U(t),$$

(7)
gives the equation of motion for $\delta A(t)$,

$$\frac{d}{dt} \delta A(t) = \sum_{j=1}^{3} \overline{G}_j(t) \Delta F_j(t) + \mathcal{O}(\Delta^2),$$  \tag{8}$$

with

$$\overline{G}_j(t) = U_0^\dagger(t) \mathcal{G}_j(t) U_0(t)$$  \tag{9}$$

and

$$\mathcal{G}_j(t) = \frac{\delta H}{\delta F_j} |_{F_0(t)}.$$  \tag{10}$$

It proves convenient to vectorize all matrices by concatenating their columns. For example, let $\Delta x(t)$ be the vectorization of $\delta A(t)$:

$$\Delta x(t) = \begin{pmatrix} \delta A \cdot 1(t) \\ \vdots \\ \delta A \cdot M(t) \end{pmatrix}.$$  

Similarly, we write $\delta \beta$ and $\overline{G}_j(t)$ as the vectors $\Delta \beta$ and $G_j(t)$. Lastly, we define the $2^n \times 3$ matrix $G(t)$ as

$$G(t) = \begin{pmatrix} G_1(t) & G_2(t) & G_3(t) \end{pmatrix}.$$  

With these definitions, and introducing $\Delta y(t) = \Delta x(t) - \Delta \beta$, Eq. (8) becomes

$$\frac{d}{dt} \Delta y(t) = G(t) \Delta F(t),$$  \tag{11}$$

with initial condition

$$\Delta y(-T/2) = -\Delta \beta,$$  \tag{12}$$

which is a consequence of $\delta A(-T/2) = 0$.

2.3 Optimal control problem

To determine the optimal control modification $\Delta F(t)$ and the associated improved unitary gate $U_f$, we introduce a cost function $J$ whose variation yields the equations governing the optimization:

$$J = \Delta y^\dagger(T/2) \Delta y(T/2)$$

$$+ \int_{-T/2}^{T/2} dt \left[ \Delta y^\dagger(t) Q(t) \Delta y(t) + \frac{1}{2} \Delta F^T(t) R(t) \Delta F(t) \right]$$

$$+ \int_{-T/2}^{T/2} dt \left[ \Delta \lambda^\dagger(t) \left\{ G(t) \Delta F(t) - \frac{d}{dt} \Delta y(t) \right\} + \text{h.c.} \right].$$  \tag{13}$$
The cost function: (i) penalizes controls which yield $U_f \neq U_{tgt}$ and large $\Delta F(t)$ and $\Delta y(t)$; and (ii) introduces a Lagrange multiplier $\Delta \lambda(t)$ that insures the optimization does not violate the Schrodinger dynamics. The matrices $Q(t)$ and $R(t)$ are required to be positive-definite and Hermitian, though are otherwise at our disposal. Requiring that $J$ be stationary under variation of $\Delta y(t)$, $\Delta y(T/2)$, $\Delta F(t)$, and $\Delta \lambda(t)$ gives the optimization equations of motion (EOM):

$$\frac{d}{dt} \Delta \lambda(t) + Q(t) \Delta y(t) = 0 \quad ; \quad \Delta \lambda(T/2) = \Delta y(T/2) \quad (14b)$$

$$\frac{d}{dt} \Delta y(t) - G(t) \Delta F(t) = 0 \quad ; \quad \Delta y(-T/2) = -\Delta \beta. \quad (14c)$$

To simplify the solution of Eqs. (14) we introduce the Ricatti matrix $S(t)$ via

$$\Delta \lambda(t) = S(t) \Delta y(t). \quad (15)$$

Differentiating Eq. (15) and using Eqs. (14) yields the differential equation for $S(t)$:

$$\frac{dS}{dt} = -Q + SGR^{-1}G^\dagger S. \quad (16)$$

Its initial condition follows from Eq. (15) evaluated at $t = T/2$ and Eq. (14b):

$$S(T/2) = I. \quad (17)$$

Inserting Eq. (15) into Eq. (14a) gives the feedback control law

$$\Delta F(t) = -C(t)\Delta y(t), \quad (18)$$

where

$$C(t) = R^{-1}(t)G^\dagger(t)S(t) \quad (19)$$

is the control gain matrix.

Eqs. (14a), (14c), and (16–19) form an equivalent set of EOM which are easier to solve. The first step is to solve Eqs. (16) and (17) for $S(t)$. Since these Eqs. are independent of $\Delta y(t)$ and $\Delta F(t)$, they can be solved immediately. Knowing $S(t)$, Eq. (19) allows the gain matrix $C(t)$ to be determined. Substituting Eq. (18) into Eq. (14c) gives

$$\frac{d}{dt} \Delta y = -GC\Delta y. \quad (20)$$

This can be integrated for $\Delta y(t)$ subject to the initial condition $\Delta y(-T/2) = -\Delta \beta$.

Note that $\Delta \beta$ is determined by Eq. (4) (for an example, see Section 1). With $\Delta y(t)$ in hand, the control modification $\Delta F(t)$ follows from the feedback control law (Eq. (18)). The new control is then $F(t) = F_0(t) + \Delta F(t)$, and the new gate $U_f = U(T/2)$ is found by plugging $F(t)$ into the Hamiltonian $\mathcal{H}[F(t)]$ and integrating the Schrodinger equation (Eq. (7)) for $U(t)$. The improved state is then

$$|\psi_f\rangle = U_f|0\cdots0\rangle. \quad (21)$$
with fidelity

$$\mathcal{F} = |\langle \psi_f | \psi_{tgt} \rangle|$$

and error probability

$$\epsilon = 1 - \mathcal{F}^2. $$

From an experimental point of view, the essential result is the new control $F(t)$ which drives the state $|0 \cdots 0\rangle$ to a high-fidelity approximation to $|\psi_{tgt}\rangle$. We illustrate this approach in the following Section.

3 Bell state preparation—ideal control

Here we show how the approach to quantum state preparation described in Section 2 can be used to prepare a high-fidelity approximation to the Bell state

$$|\beta_{01}\rangle = (1/\sqrt{2})[|01\rangle + |10\rangle].$$

As that discussion was general, no specific form was assumed for the Hamiltonian $\mathcal{H}[F(t)]$. In Sections 3 and 4 we assume the two-qubit Hamiltonian $\mathcal{H}_2$ couples each qubit to the control field $F(t)$ through the Zeeman interaction, and couples the qubits through an anisotropic Heisenberg interaction. In the lab frame ($h = 1$):

$$\mathcal{H}_2[F(t)] = -\sum_{i=1}^3 \frac{\gamma_i}{2} \sigma_i \cdot F(t) - \frac{\pi}{2} \left[ J_z \sigma_z^2 + J_{xy} (\sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2) \right].$$

(24)

Since $F(t) = F_0(t) + \Delta F(t)$, we have

$$\mathcal{H}_2[F(t)] = \mathcal{H}_2[F_0(t)] + \sum_{j=1}^3 g_j(t) \Delta F_j(t),$$

(25)

where

$$\mathcal{H}_2[F_0(t)] = -\sum_{i=1}^3 \frac{\gamma_i}{2} \sigma_i \cdot F_0(t) - \frac{\pi}{2} \left[ J_z \sigma_z^2 + J_{xy} (\sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2) \right],$$

(26)

and

$$g_j(t) = -\frac{1}{2} \sum_{i=1}^3 \gamma \sigma_i^j.$$ 

(27)

Thus $\mathcal{H}_2[F_0(t)]$ is the nominal Hamiltonian that drives the good starting gate $U_0(t)$ introduced in Section 2.2 and the dynamical contribution of the control modification $\Delta F(t)$ is contained in the second term on the RHS of Eq. (25).
3.1 Nominal dynamics

As noted earlier, the nominal control $F_0(t)$ enacts a unitary transformation $U_0(t)$ which maps the initial state $|\psi_0(-T/2)\rangle = |00\rangle$ to the final state $|\psi_0(T/2)\rangle = |\psi_{0,f}\rangle$:

$$|\psi_{0,f}\rangle = U_{0,f}|00\rangle,$$

where $|\psi_{0,f}\rangle$ is a good approximation to the Bell state $|\beta_{01}\rangle$. In this subsection we use a form of non-adiabatic rapid passage known as twisted rapid passage (TRP) [4][5] to provide the nominal control $F_0(t)$. The reader will find a summary of TRP essentials in Appendix A. We stress that NOC theory is not restricted to this particular type of starting control; any other control can be used so long as it produces a sufficiently good approximation to $|\beta_{01}\rangle$. See Section 5 for further discussion of this point.

In the lab frame the TRP control is

$$F_0(t) = B_0\hat{\mathbf{x}} + B_{rf} \cos \phi_{rf}(t) \hat{\mathbf{x}} - B_{rf} \sin \phi_{rf}(t) \hat{\mathbf{y}}. \quad (28)$$

The transformation to the detector frame [5][6] is carried out by the unitary

$$U_{det}(t) = \exp \left[ i \frac{\tau}{\lambda} \phi_{det}(t) \left( \sigma_z^1 + \sigma_z^2 \right) \right].$$

Appendix A (see also Ref. [4]) shows that $\phi_{rf}(t) = \phi_{det}(t) - \phi_{trp}(t)$, where $\phi_{trp}(t)$ is the instantaneous rate at which the control field $F_0(t)$ rotates about the $z$-axis in the detector frame (see Eq. (31) below). We restrict ourselves to quartic twist $\phi_{trp}(t) = (1/2)Bt^4 \equiv \phi_4(t)$ in this paper. The nominal Hamiltonian in the detector frame is then

$$\hat{H}^0_{det}(t) = U_{det}^\dagger(t)\hat{H}_0^0(t)U_{det}(t) - iU_{det}^\dagger(t) \frac{d}{dt} U_{det}(t). \quad (29)$$

It proves useful for the numerical simulations to recast the Schrödinger dynamics into dimensionless form. This is done in Appendix A (see also Ref. [3]) with the result

$$\hat{H}^0_{det}(\tau) = \hat{H}^0_{1}(\tau) + \hat{H}^0_{int}(\tau), \quad (30)$$

where the one-qubit term is

$$\hat{H}^0_{1}(\tau) = \left[ -\frac{d_1 + d_2}{2} + \frac{\tau}{\lambda} \right] \sigma_z^1 - \frac{d_3}{\lambda} \left[ \cos \phi_4(\tau) \sigma_z^1 + \sin \phi_4(\tau) \sigma_x^1 \right] + \left[ -\frac{d_2}{2} + \frac{\tau}{\lambda} \right] \sigma_z^2 - \frac{1}{\lambda} \left[ \cos \phi_4(\tau) \sigma_z^2 + \sin \phi_4(\tau) \sigma_y^2 \right]. \quad (31)$$

and the interaction term is

$$\hat{H}^0_{int}(\tau) = -\frac{\pi}{2} \left[ d_c \sigma_z^1 \sigma_z^2 + d_{xy} \left( \sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2 \right) \right]. \quad (32)$$

The parameters $d_1, d_2, d_3, d_c, d_{xy}$ are dimensionless versions of the qubit couplings to the TRP control as well as to each other and are defined below Eq. (51). The remaining parameters $\tau$ (dimensionless time), $\lambda$ (dimensionless TRP inversion rate),
Simulated annealing (SA) was used to find values for the parameters \( \eta_4, \lambda, d_1, d_2, d_3, d_z, d_{xy} \) that minimize the error probability for preparing a high-fidelity approximation to the Bell state \(|\beta_{01}\rangle\). MATLAB was used to implement SA with an initial (dimensionless) temperature \( T_0 = 100 \) and an exponential annealing schedule with a reduction factor of 0.95. The starting parameter values were \( \eta_4 = 10^{-4}, \lambda = d_1 = d_2 = d_3 = d_z = d_{xy} = 1 \). The parameter values found are listed below and produced a state preparation error probability \( \bar{e}_0 = 6.68 \times 10^{-4} \).

| Parameter | Value       |
|-----------|-------------|
| \( \eta_4 \) | \( 4.526 \times 10^{-4} \) |
| \( \lambda \) | 9.579       |
| \( d_1 \) | 1.386       |
| \( d_2 \) | 9.622       |
| \( d_3 \) | 8.905       |
| \( d_z \) | 0.918       |
| \( d_{xy} \) | 4.331       |

\( \eta_4 \) (dimensionless twist strength), and \( \tau_0 \) (dimensionless TRP inversion time) are defined above Eq. (51) and they determine the actual TRP control profile \( F_0(t) \) applied to the qubits.

For the TRP dynamics to produce a good approximation to \(|\beta_{01}\rangle\) we must search for suitable values for the parameters appearing in \( \mathcal{H}_{det}^0(\tau) \). We used simulated annealing to find a parameter assignment that minimized the state preparation error probability

\[
\bar{e}_0 = 1 - |\langle \psi_{0,f} | \beta_{01} \rangle|^2. \tag{33}
\]

As in the two-qubit simulations done in Ref. [3], we set \( \tau_0 = 120 \) in this paper. Table 1 lists the minimizing control parameter values found. Numerical integration of the two-qubit Schrödinger equation using the TRP control Hamiltonian \( \mathcal{H}_{det}^0(\tau) \) gave the final state \(|\psi_{0,f}\rangle\) in the detector frame which was then transformed back to the lab frame. The state obtained (in the computational basis) is

\[
|\psi_{0,f}\rangle = \begin{pmatrix}
-0.0070 - 0.0066i \\
-0.2503 - 0.6870i \\
-0.2006 - 0.667i \\
0.0080 + 0.0164i
\end{pmatrix} = -e^{1.28i} \sqrt{1 - \bar{e}_0} |\beta_{01}\rangle + O(\sqrt{\bar{e}_0}), \tag{34}
\]

with (state preparation) error probability

\[
\bar{e}_0 = 6.68 \times 10^{-4} \tag{35}
\]

and associated fidelity

\[
\mathcal{F}_0 = \sqrt{1 - \bar{e}_0} = 0.9997. \tag{36}
\]

The TRP nominal control thus provides an excellent starting point for the NOC approach to preparing \(|\beta_{01}\rangle\).

### 3.2 NOC dynamics

The TRP driven dynamics with parameter values as in Table 1 map the initial state \(|00\rangle\) to \( U_{0,f}|00\rangle = |\psi_{0,f}\rangle \) (see Eq. (34)):

\[
U_{0,f}|00\rangle = -e^{1.28i} \sqrt{1 - \bar{e}_0} |\beta_{01}\rangle + O(\sqrt{\bar{e}_0}). \tag{37}
\]
The same TRP control drives the remaining CBS \( |ij\rangle \) to

\[
U_{0,f}|01\rangle = \begin{pmatrix}
-0.7054 - 0.1678i \\
0.0036 + 0.0139i \\
-0.0130 - 0.0143i \\
-0.6694 - 0.1595i
\end{pmatrix} = -e^{0.24i} \sqrt{1 - \epsilon_{ij}^{(1)}}|\beta_{00}\rangle + \mathcal{O}(\sqrt{\epsilon_{ij}^{(1)}}) \tag{38a}
\]

\[
U_{0,f}|10\rangle = \begin{pmatrix}
-0.6686 - 0.1591i \\
0.0188 + 0.0311i \\
0.0051 - 0.0182i \\
0.7053 + 0.1683i
\end{pmatrix} = -e^{0.24i} \sqrt{1 - \epsilon_{ij}^{(1)}}|\beta_{10}\rangle + \mathcal{O}(\sqrt{\epsilon_{ij}^{(1)}}) \tag{38b}
\]

\[
U_{0,f}|11\rangle = \begin{pmatrix}
0.0374 - 0.0172i \\
0.1214 + 0.6853i \\
0.1267 - 0.7055i \\
-0.0115 + 0.0006i
\end{pmatrix} = e^{1.39i} \sqrt{1 - \epsilon_{ij}^{(1)}}|\beta_{11}\rangle + \mathcal{O}(\sqrt{\epsilon_{ij}^{(1)}}) \tag{38c}
\]

where \( \epsilon_{ij}^{(1)} \sim \epsilon_0 \). For the reader’s convenience we list all two-qubit Bell states in Table 2. We see that TRP provides excellent approximations for all four Bell states. Based on Eqs. (37) and (38) we use the following target unitary for the NOC state preparation procedure

\[
U_{fg} = \begin{pmatrix}
-e^{1.28i}|\beta_{01}\rangle & -e^{0.24i}|\beta_{00}\rangle & -e^{0.24i}|\beta_{10}\rangle & e^{1.39i}|\beta_{11}\rangle
\end{pmatrix} \tag{39}
\]

As discussed in Section 2.3 to obtain the control modification \( \Delta \mathbf{F}(t) \) we first integrate the Ricatti equation (Eqs. (16) and (17)). To that end, we chose \( R(\tau) = rG^T(\tau)G(\tau) \), \( Q(\tau) = \mathcal{G}(\tau)G(\tau)^T G^T(\tau)/r \), and \( r = 70 \). The solution to the Ricatti equation is then \( S(\tau) = \mathcal{I}_{16x16}, \) the 16 \times 16 identity matrix. Eq. (19) then gives the feedback control matrix \( C(\tau) \) which allows Eq. (20) to be integrated subject to the initial condition \( \Delta y(-T/2) = -\Delta \beta \). The constant vector \( \Delta \beta \) is found by concatenating the columns of \( \delta \beta \) (see Eq. (16)). With \( \Delta y(\tau) \) in hand, Eq. (18) determines the control modification \( \Delta \mathbf{F}(\tau) \). The improved control \( \mathbf{F}(\tau) = \mathbf{F}_0(\tau) + \Delta \mathbf{F}(\tau) \) is then plugged into the Schrodinger equation using Eq. (25) for \( \mathcal{H}_2[\mathbf{F}(\tau)] \). With initial state \( |00\rangle \), the resulting final state is

\[
|\psi_{f,\text{NOC}}\rangle = \begin{pmatrix}
-0.0043 - 0.0043i \\
-0.2044 - 0.6849i \\
-0.2006 - 0.6701i \\
0.0059 + 0.0118i
\end{pmatrix} \tag{40}
\]
which has error probability

\[ \varepsilon_{\text{NOC}} = 1 - |\langle \psi_a^{\text{NOC}} | \beta_{01} \rangle|^2 = 2.58 \times 10^{-6} \]  

and fidelity

\[ \mathcal{F}_{\text{NOC}} = 0.999999. \]  

We see that NOC has significantly improved the approximation to \(|\beta_{01}\rangle\), reducing the error probability by two orders-of-magnitude and adding three 9’s to the fidelity.

We can estimate the bandwidth needed for \(\Delta F(t)\) from Figure 1 which shows

\[ \Delta F_x(\omega) \]  

the Fourier transform \(\Delta F_x(\omega)\) of \(\Delta F_x(\tau)\); the \(y\)- and \(z\)-components behave comparably. We see that \(\Delta F_x(\omega)\) is reduced to 1-2% of its peak value for \(|\omega| \gtrsim 60\), giving a dimensionless bandwidth \(\Delta \omega \sim 60\). Choosing a control operation time \(T = 5\mu s\) which corresponds to a dimensionless inversion time \(\tau_0 = 120\), gives a dimensionful bandwidth \(\Delta \omega = (120/5\mu s) \Delta \omega = 1.44\) GHz. This is well within the range of commercially available arbitrary waveform generators (AWG). From the known values of the control operation time \(T\) and the dimensionless parameters in Table 1 it is straightforward to determine the values of dimensionful Hamiltonian parameters (see formulas in Appendix A). With these values the improved control \(F(t)\) is fully specified.

4 Performance impact of non-ideal control

In this Section we examine the robustness of NOC state preparation to two types of imperfections in the AWG that generates the control field: (i) finite-precision control parameters; and (ii) timing jitter. Although our interest here is in the effects of these control errors on NOC performance gains, we do not mean to imply that these are the only types of errors that can afflict a qubit.
Table 3 Sensitivity of the state preparation error probability $\varepsilon$ to small variation of $\eta_4$ away from its optimum value (marked with an asterisk). The other Hamiltonian parameters remain at their optimum (Table 1) values.

| $\eta_4$          | $\varepsilon$   |
|-------------------|-----------------|
| $4.525 \times 10^{-4}$ | $1.90 \times 10^{-5}$ |
| $4.526 \times 10^{-4}$ | $2.58 \times 10^{-6}$ |
| $4.527 \times 10^{-4}$ | $1.35 \times 10^{-5}$ |

Table 4 Sensitivity of the state preparation error probability $\varepsilon$ to small variation of $\lambda$ away from its optimum value (marked with an asterisk). The other Hamiltonian parameters remain at their optimum (Table 1) values.

| $\lambda$ | $\varepsilon$   |
|-----------|-----------------|
| 9.578     | $7.89 \times 10^{-6}$ |
| $^*9.579$ | $2.58 \times 10^{-6}$ |
| 9.580     | $3.35 \times 10^{-5}$ |

Table 5 Sensitivity of the state preparation error probability $\varepsilon$ to small variation of $d_1$ away from its optimum value (marked with an asterisk). The other Hamiltonian parameters remain at their optimum (Table 1) values.

| $d_1$ | $\varepsilon$   |
|-------|-----------------|
| 1.385 | $2.37 \times 10^{-5}$ |
| $^*1.386$ | $2.58 \times 10^{-6}$ |
| 1.387 | $1.99 \times 10^{-5}$ |

4.1 Finite-precision

The NOC formalism requires a nominal control $F_0(t)$ that can produce a good approximation $U_{0,f}$ to a target unitary $U_{10}$. The NOC modification $\Delta F(t)$ is then optimum relative to $F_0(t)$. Altering the nominal control field $F_0(t) \rightarrow F'_0(t)$ may cause $\Delta F(t)$ to become sub-optimal relative to $F'_0(t)$. Because the hardware (viz. AWG) used to produce $F_0(t)$ has limited precision it is important to examine the degree of precision the control parameters must have to achieve the NOC performance gains.

We have seen that the parameter values appearing in Table 1 produce an approximate Bell state $|\psi^{NOC}\rangle$ (Eq. (40)) with error probability $\varepsilon_{NOC} = 2.58 \times 10^{-6}$. To examine the robustness of this result to finite-precision Hamiltonian parameters we shifted one parameter away from its optimum value in its fourth significant digit, while keeping the remaining parameters fixed. This alters the nominal control $F_0(t) \rightarrow F'_0(t)$. To study the effect on performance we numerically simulated the Schrödinger dynamics driven by $i\mathcal{H}_2[F'(t)]$ using $F'(t) = F'_0(t) + \Delta F(t)$ with $\Delta F(t)$ the NOC modification relative to $F_0(t)$. Tables 3,9 show the state preparation error probability $\varepsilon$ found as we varied each Hamiltonian parameter. For example, Table 3 shows that as $\eta_4$ is varied away from its optimum value by $(+1/-1)$ in its fourth significant digit the error probability shifts from $2.58 \times 10^{-6}$ at optimum to $(1.35/1.90) \times 10^{-5}$. Examination of the Tables shows that performance is most sen-
Table 6 Sensitivity of the state preparation error probability $\varepsilon$ to small variation of $d_2$ away from its optimum value (marked with an asterisk). The other Hamiltonian parameters remain at their optimum (Table 1) values.

| $d_2$  | $\varepsilon$ |
|--------|---------------|
| 9.621  | $5.31 \times 10^{-3}$ |
| *9.622 | $2.58 \times 10^{-6}$ |
| 9.623  | $2.70 \times 10^{-3}$ |

Table 7 Sensitivity of the state preparation error probability $\varepsilon$ to small variation of $d_3$ away from its optimum value (marked with an asterisk). The other Hamiltonian parameters remain at their optimum (Table 1) values.

| $d_3$  | $\varepsilon$ |
|--------|---------------|
| 8.904  | $4.68 \times 10^{-6}$ |
| *8.905 | $2.58 \times 10^{-6}$ |
| 8.906  | $8.05 \times 10^{-6}$ |

Table 8 Sensitivity of the state preparation error probability $\varepsilon$ to small variation of $d_z$ away from its optimum value (marked with an asterisk). The other Hamiltonian parameters remain at their optimum (Table 1) values.

| $d_z$  | $\varepsilon$ |
|--------|---------------|
| 0.917  | $1.67 \times 10^{-6}$ |
| *0.918 | $2.58 \times 10^{-6}$ |
| 0.919  | $8.70 \times 10^{-6}$ |

Table 9 Sensitivity of the state preparation error probability $\varepsilon$ to small variation of $d_{xy}$ away from its optimum value (marked with an asterisk). The other Hamiltonian parameters remain at their optimum (Table 1) values.

| $d_{xy}$ | $\varepsilon$ |
|----------|---------------|
| 4.330    | $5.59 \times 10^{-3}$ |
| *4.331  | $2.58 \times 10^{-6}$ |
| 4.332    | $1.33 \times 10^{-4}$ |

Note however that if the control parameters can be controlled to 1 part in 10,000 or better, then the NOC performance gains are achievable. This corresponds to parameters with 14-bit precision (viz. 1 part in $2^{14} = 16,384$). On the other hand, 13-bit precision (1 part in $2^{13} = 8192$) will cause uncertainty in the fourth significant digit and should result in non-optimal NOC performance.

4.2 Timing jitter

Timing jitter arises from timing errors in the clock used in an AWG. Ideally the clock outputs a sequence of “ticks” with constant time separation $T_{\text{clock}}$ derived from an oscillation with phase $\phi(t) = 2\pi f_{\text{clock}} t$, where $f_{\text{clock}} = 1/T_{\text{clock}}$. In a real clock,
however, the time $T$ between ticks is a stochastic process $T = T_{\text{tick}} + \delta t$, where the stochastic timing error $\delta t$ has vanishing time average $\overline{\delta t} = 0$ and standard deviation $\sigma_t = \sqrt{\overline{\delta t}^2}$ that quantifies the spread of tick intervals about $T_{\text{tick}}$. The timing error $\delta t$ causes a phase error $\delta \phi = (2\pi f_{\text{clock}})\delta t$ which has $\overline{\delta \phi} = 0$ and standard deviation $\sigma_\phi = \sqrt{\overline{\delta \phi}^2}$. It is straightforward to show \[3\] that $\sigma_\phi = (2\pi f_{\text{clock}})\sigma_t$.

Timing jitter causes phase noise in the TRP nominal control $F_0(t)$. Specifically, the TRP quartic twist profile $\phi_4(t) = (\eta_4/2\lambda)\tau^4$ picks up phase noise $\delta \phi(\tau)$ due to the timing error $\delta \tau$ (we switch over to dimensionless time): $\phi_4(\tau) \rightarrow \phi_4(\tau) + \delta \phi(\tau)$. This causes the TRP control to twist incorrectly and yields a noisy nominal control $F_0(\tau) \rightarrow F'_0(\tau)$. As the phase noise cannot be known in advance, it is not possible to determine a control modification that is optimal for $F'_0(\tau)$. All one can do is calculate the control modification $\Delta F(\tau)$ which is optimal for the jitter-free control $F_0(\tau)$ and add it to the noisy nominal control $F'_0(\tau)$. Since $\Delta F(\tau)$ is not optimal for $F'_0(\tau)$, timing jitter is expected to reduce NOC performance.

To quantitatively study the effects of timing jitter on NOC performance we modelled the phase noise $\delta \phi(\tau)$ as shot noise and used the model to generate numerical realizations of the phase noise $\delta \phi(\tau)$. The details of the model and the protocol used to generate a noise realization are described in Ref. \[3\] (see also Ref. \[11\]). For each noise realization we determined the state $|\psi(\tau)\rangle$ by numerically integrating the Schrodinger dynamics driven the noisy control $F'(\tau) = F'_0(\tau) + \Delta F(\tau)$ and used it to determine the error probability $\varepsilon$ for the state produced. We generated 10 phase noise realizations $\delta \phi_i(\tau)$ and determined 10 error probabilities $\varepsilon_i$. From these we determined the average error probability $\overline{\varepsilon}$ and standard deviation $\sigma_\varepsilon$. These were used to estimate the noise-averaged performance of NOC state preparation with TRP providing the nominal control. For timing jitter $\sigma_t = 5.03 \text{ ps}$ and clock frequency $f_{\text{clock}} = 1 \text{ GHz}$ (typical of a commercially available AWG), the simulations found $\overline{\varepsilon} \pm \sigma_\varepsilon = (1.64 \pm 0.16) \times 10^{-5}$. We see that timing jitter does impact NOC performance, though the resulting error probability remains quite small at jitter levels typical of present-day AWGs. In closing, note that for nominal controls whose good performance is not due to controllable quantum interference effects, timing jitter may have less impact on NOC performance than for the TRP nominal control considered here.

5 Discussion

We have presented a procedure for single-shot high-fidelity quantum state preparation based on NOC theory. We illustrated the procedure by using it to prepare a high-fidelity approximation to the Bell state $|\beta_0\rangle$. The resulting state had error probability $\varepsilon_{\text{NOC}} \sim 10^{-6}$ ($10^{-5}$) for ideal (non-ideal) control. The excellent fidelity of the final state provides proof-of-principle of the performance gains possible using NOC, even in the presence of control imperfections.

We have assumed throughout this paper that the qubit longitudinal ($T_1$) and transverse ($T_2$) relaxation times are long compared to the state preparation time $T_{sp}$. This assumption is essential for any discussion of fault-tolerant quantum computing and
error correction as it ensures that the qubit state does not decohere away before the error-syndrome extraction circuit can be applied, and likely errors identified. When \( T_{sp} \ll T_1, T_2 \), control imperfections may be anticipated to be the primary source of errors during the time for state preparation, and the qubit environment a secondary source. On the other hand, when \( T_1, T_2 \approx T_{sp} \), the qubits are of sufficiently poor quality that errors from the qubit environment can be expected to be (at least) as bad as the types of errors we have examined in this paper. Our NOC procedure for improving state preparation does not remove the need for high-quality qubits as the objects of these controls.

In this paper we used TRP to provide a good starting control to be improved by NOC. Other controls could be used as well. It would be very interesting to use GRAPE [12] to provide the input control for the NOC formalism and to examine what kind of performance gains are possible. We plan to carry out such a study in future work.

The high-fidelity NOC preparation of \( |β_{01}⟩ \) can be straightforwardly incorporated into Knill’s procedure for fault-tolerant logical Bell state preparation [2]. This requires working with two codeblocks of a [4,2,2] quantum error detecting code. In Ref. [2] each physical Bell state is prepared using a Hadamard and a CNOT gate. With NOC, each physical Bell state is prepared in a single-shot as described in Section 3 reducing the depth of state preparation by a factor of two. As many Bell states are needed in a large-scale quantum computation, the cumulative effect of this reduction could be significant.

As noted in Section 2, the NOC state preparation procedure can be used to prepare \( n \)-qubit states. It would be interesting to examine the effectiveness of this procedure for single-shot high-fidelity preparation of logical states in small to moderate size quantum error correcting codes. Efforts along this direction are currently underway.

Finally, we have included as supplementary material the MATLAB source files used to obtain the numerical results presented in this paper.

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Conflicts of Interest The authors declare that they have no conflict of interest.

A TRP Essentials and the Dimensionless Hamiltonian \( \mathcal{H}_{det}^0 (τ) \)

(i) TRP Essentials: To introduce twisted rapid passage (TRP) [13] we consider a single-qubit interacting with an external field \( \mathbf{F}(t) \) via the Zeeman interaction \( H(t) = -\mathbf{σ} \cdot \mathbf{F}(t) \), where the \( \mathbf{σ}_i \) are the Pauli matrices \( (i = x, y, z) \). TRP is a generalization of adiabatic rapid passage (ARP). In ARP the control field \( \mathbf{F}(t) \) is slowly inverted over a time \( T \) with \( \mathbf{F}(t) = a\mathbf{z} + b\mathbf{x} \). In TRP, however, the control field is allowed to twist in the \( x-y \) plane with time-varying azimuthal angle \( φ(t) \), while simultaneously undergoing inversion along the \( z \)-axis:

\[
\mathbf{F}_0(t) = a\mathbf{z} + b \cos φ(t)\mathbf{x} + b \sin φ(t)\mathbf{y}.
\]

Here \( t \in [-T/2, T/2] \) and we consider TRP with nonadiabatic inversion. As shown in Ref. [3], the qubit undergoes resonance when

\[
αt - \frac{b}{2} \frac{d}{dt} φ(t) = 0. \tag{43}
\]

For polynomial twist, the twist profile \( φ(t) \) takes the form

\[
φ_n(t) = \frac{2}{n} Re^n.
\]
In this case Eq. (43) has \( n - 1 \) roots, though only real-valued roots correspond to resonance. Ref. [7] showed that for \( n \geq 3 \), the qubit undergoes resonance \textit{multiple} times during a single TRP sweep: (i) for all \( n \geq 3 \) when \( B > 0 \); and (ii) for odd \( n \geq 3 \) when \( B < 0 \). In this paper we restrict ourselves to \( B > 0 \) and quartic twist \( (n = 4) \). During quartic twist the qubit passes through resonance at time \( t = 0, \pm \sqrt{\pi/4B} \). It is thus possible to alter the time separating the resonances by varying the TRP sweep parameters \( B \) and \( a \).

Ref. [3] showed these multiple resonances have a strong influence on the qubit transition probability, allowing transitions to be strongly enhanced or suppressed through small variation of the sweep parameters. Ref. [4] observed these quantum interference effects in the transition probability using NMR and found excellent agreement between theory and experiment. Subsequently, TRP controls were used to produce a high-fidelity universal set of quantum gates \([7,8,9,10]\) which were further improved using NOC \([3]\). 

\( \text{(ii) Dimensionless Hamiltonian:} \) The two-qubit Hamiltonian \( \mathcal{H}_0(t) \) describes qubits coupled to an external control field \( F(t) \) via the Zeeman interaction and to each other via an anisotropic Heisenberg interaction. In the lab frame the control field \( F_0(t) \) is

\[
F_0(t) = B_0 \hat{a} + B_f \cos \phi_f(t) \hat{a} - B_f \sin \phi_f(t) \hat{a},
\]

and \( \mathcal{H}_0(t) \) is \( \hbar = 1 \)

\[
\mathcal{H}_0(t) = - \sum_{i=1}^{2} \frac{\gamma_i}{2} \sigma_i \cdot F_0(t) + \frac{\pi}{2} \left[ J_x \sigma_x^1 \sigma_x^2 + J_y \left( \sigma_y^1 \sigma_y^2 + \sigma_y^1 \sigma_y^2 \right) \right].
\]

Introducing \( \omega_0 = \gamma B_0 \) and \( \omega_{ij} = \gamma B_f \) \( (i = 1, 2) \) gives

\[
\mathcal{H}_0(t) = - \frac{\omega_0}{2} \sigma_z^1 - \frac{\omega_{ij}}{2} \left[ \cos \phi_f \sigma_y^1 \sigma_y^2 \right] - \frac{\omega_0}{2} \sigma_z^2 - \frac{\omega_{ij}}{2} \left[ \cos \phi_f \sigma_y^2 - \sin \phi_f \sigma_y^2 \right] - \frac{\pi}{2} \left[ J_x \sigma_x^1 \sigma_x^2 + J_y \left( \sigma_y^1 \sigma_y^2 + \sigma_y^1 \sigma_y^2 \right) \right].
\]

We switch to the detector frame \([56]\) by applying the unitary

\[
U_{det}(t) = \exp \left[ \frac{i}{\hbar} \phi_{det}(t) \left( \sigma_z^1 + \sigma_z^2 \right) \right].
\]

The detector frame Hamiltonian is

\[
\mathcal{H}_{det}^0(t) = U_{det}^\dagger(t) \mathcal{H}_0(t) U_{det}(t) - iU_{det}^\dagger(t) \frac{d}{dt} U_{det}(t).
\]

Inserting Eqs. (45) and (46) into (47) gives

\[
\mathcal{H}_{det}^0 = - \frac{\omega_0 + \Delta_{det}}{2} \sigma_z^1 - \frac{\omega_{ij}}{2} \left[ \cos \left( \phi_{det} - \phi_f \right) \sigma_y^1 + \sin \left( \phi_{det} - \phi_f \right) \sigma_y^2 \right] - \frac{\omega_0 - \Delta_{det}}{2} \sigma_z^2 - \frac{\omega_{ij}}{2} \left[ \cos \left( \phi_{det} - \phi_f \right) \sigma_y^2 + \sin \left( \phi_{det} - \phi_f \right) \sigma_y^1 \right] - \frac{\pi}{2} \left[ J_x \sigma_x^1 \sigma_x^2 + J_y \left( \sigma_y^1 \sigma_y^2 + \sigma_y^1 \sigma_y^2 \right) \right].
\]

To produce a TRP sweep in the detector frame it is necessary to sweep \( \phi_{det} \) and \( \phi_f \) through a Larmor resonance frequency \([3]\). Without loss of generality we chose to sweep through the Larmor Frequency \( \omega_2 \) and introduce a detuning \( \Delta \):

\[
\phi_{det}(t) = \omega_2 \frac{t}{\hbar} + \Delta \quad \phi_f(t) = \phi_{det}(t) - \phi_{trp}(t).
\]
Here $a$ is the TRP inversion rate and for quartic twist $\phi_{TRP}(t) = \phi_0(t) = (1/2)Bt^4$. Introducing $\delta \omega = \omega - \omega_c$, Eq. (46) becomes

\[
\mathcal{H}_{\text{det}}(t) = \left[ -\frac{(\delta \omega + \Delta)}{2} + \frac{a t}{\hbar} \right] \sigma_1^a \left[ \cos \phi_0(t) \sigma_1^a + \sin \phi_0(t) \sigma_2^a \right] \\
- \left[ -\frac{\Delta}{2} + \frac{a t}{\hbar} \right] \sigma_2^a \left[ \cos \phi_0(t) \sigma_2^a + \sin \phi_0(t) \sigma_1^a \right] \\
- \frac{\pi}{2} \left[ J_x \sigma_1^a \sigma_2^a + J_y \left( \sigma_1^a \sigma_1^a + \sigma_2^a \sigma_2^a \right) \right].
\]

It proves convenient for the numerical simulations to transform $\mathcal{H}_{\text{det}}(t)$ to dimensionless form. To that end we introduce $b_1 = h\omega_0/2$, $b_2 = h\omega_0$, $b_3 = h\omega_0$, the dimensionless time $\tau = (a/b_2)t$, and the dimensionless inversion time $\tau_0 = (b_2/a)T$. The dimensionless quartic twist profile is $\phi_0(\tau) = (\eta_4/2\lambda)\tau^4$, where $\eta_4 = h\lambda b_2^2/a^2$. Multiplying both sides of Eq. (50) by $b_2/a$ gives the dimensionless Hamiltonian

\[
\mathcal{H}_{\text{det}}^0 = \left[ \frac{(d_1 + d_2)}{2} + \frac{\tau}{\lambda} \right] \sigma_1^a \left[ \cos \phi_0(\tau) \sigma_1^a + \sin \phi_0(\tau) \sigma_2^a \right] \\
- \left[ \frac{d_2}{2} + \frac{\tau}{\lambda} \right] \sigma_2^a \left[ \cos \phi_0(\tau) \sigma_2^a + \sin \phi_0(\tau) \sigma_1^a \right] \\
- \frac{\pi}{2} \left[ d_1 \sigma_1^a \sigma_2^a + d_4 \left( \sigma_1^a \sigma_1^a + \sigma_2^a \sigma_2^a \right) \right],
\]

where: $(i) \; d_1 = (b_2/a)\delta \omega$; $d_2 = (b_2/a)\lambda$; $d_3 = (b_2/a)\Delta$; $d_4 = (b_2/a)J_x$; and $d_5 = (b_2/a)J_y$. This is the dimensionless Hamiltonian that appears in Eqs. (30)–(32). We see that $\mathcal{H}_{\text{det}}^0(\tau)$ depends on the TRP sweep parameters $(\lambda, \eta_4)$ as well as the coupling parameters $(d_1, d_2, d_3, d_4)$. The latter set of parameters are dimensionless ratios of, respectively, the Lambor frequency difference $\delta \omega$, the detuning $\Delta$, the Zeeman coupling ration $b_1/b_2$, and the Heisenberg couplings $J_x$ and $J_y$.

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