Qubit leakage suppression by ultrafast composite pulses

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Abstract: The leakage suppression problem is considered for a three-level ladder-type quantum system, in which the first two levels are the qubit system and the third is the leakage state weakly coupled to the qubit system. We show that two (three) phase- and amplitude-controlled pulses are sufficient for arbitrary qubit controls from the ground (an arbitrary) initial state, with leakage suppressed up to the first order of perturbation without additional pulse-area cost. A proof-of-principle experiment was performed with shaped ultrafast optical pulses and cold rubidium atoms, and the result shows a good agreement with the theory.

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1. Introduction

Quantum two-level systems are the basic building blocks in quantum information science and engineering. However, many physical systems that are used to store and process quantum information are not perfect two-level systems. There are often leakage states weakly coupled to the two-level qubit systems, in atom and ion systems [1–3], superconducting qubits [4,5], and quantum dots [6]. Leakage transitions to unwanted energy levels are often a critical source of control errors in physical implementations of qubit logic operations. Pulse shaping and optimal control theories have been developed to deal with the leakages and to improve gate operations [7–12]. One example is developed through analytic waveform designing, known as derivative removal by adiabatic gate (DRAG) [4,13,14], which is in particular successful for superconducting qubits [5,15]. Another is the multiple-pulse approach known as Majorana decomposition [16,17], recently proposed and experimentally demonstrated [18].

In this paper, we consider short-pulse controls to remove the leakage. Short-pulse control schemes are useful for quantum systems with a limited coherence time. Quantum dots, for example, have a short dephasing time ($T_\text{2}$) ranging from 100 ps to ns [19,20], and pulses considerably shorter in time than the coherence time have broad spectrum often causing inevitable leakages. However, neither the DRAG nor Majorana decomposition methods are suitable for ultrafast-pulse based control schemes: the former requires complex waveforms, and the latter works for specific target states without individual coupling controls. In that regards, a leakage suppression scheme for ultra-short time-scale gate operations is worthy to consider.

Our approach is to use a programmed pulse sequence [21,22] to remove the leakage [23] through transition pathway engineering. As to be explained below with examples in a three-level system (of a qubit two-level system and a leakage state), it is found that one subsequent pulse can suppress the leakage caused after a single-pulse qubit preparation (from the ground initial state to an arbitrary final state) and that two subsequent pulses for an arbitrary qubit rotation (between arbitrary initial and final states).

2. Model description

We consider a three-level system ($|0\rangle$, $|1\rangle$, and $|2\rangle$) with energies $\hbar\omega_1$ and $\hbar\omega_2$, respectively) in the ladder-type configuration ($|0\rangle$-$|2\rangle$ is dipole-forbidden), in which the first two levels are the qubit states and the third is the leakage state. The interaction Hamiltonian $H$ (in unit of $\hbar \equiv 1$)
for electric-field \( E(t) = E_0(t) \cos(\omega_L t + \phi) \) is given, after the rotating wave approximation, by

\[
H = \sum_{m=0}^{2} \Delta_m \Pi_m + \sum_{m,n=0}^{2} \frac{\lambda_{mn}}{2} (\Omega_x \sigma_{mn}^{(x)} - \Omega_y \sigma_{mn}^{(y)}),
\]

(1)

where \( \Pi_m = |m\rangle \langle m| \) and \( \sigma_{mn}^{(k)} \) are the projection operator and Pauli matrices, respectively, for \( k = x, y, z \) and \( m, n = 0, 1, 2 \) (i.e., \( \sigma_{mn}^{(x)} = |m\rangle \langle n| + |n\rangle \langle m| \), \( \sigma_{mn}^{(y)} = -i|m\rangle \langle n| + i|n\rangle \langle m| \)). \( \Omega_x \) and \( \Omega_y \) are the real and imaginary parts of the Rabi oscillation frequency defined by \( \Omega = \mu_{01} E_0 \exp(i\phi) \) between \( |0\rangle \) and \( |1\rangle \), where \( \mu_{01} \) is the dipole moment. Scaled dipole moments, \( \lambda_{mn} = \mu_{mn} / \mu_{01} \), are given by \( \lambda_{mn} = 0 \) except \( \lambda_{01} = 1 \) and \( \lambda_{12} = \lambda \), and detunings are \( \Delta_1 = \omega_1 - \omega_L \) and \( \Delta_2 = \omega_2 - 2\omega_L \).

Quantum information is carried by the first two states, \( |0\rangle \) and \( |1\rangle \), (e.g., initial state \( |\psi_i\rangle = a_0 |0\rangle + b_1 |1\rangle \)), so it is convenient to divide the Hamiltonian into two parts [12], namely the qubit-system Hamiltonian \( H_q \) and the leakage Hamiltonian \( H_l \):

\[
H_q = \sum_{m=0}^{2} \Delta_m \Pi_m + \frac{\lambda_{01}}{2} (\Omega_x \sigma_{01}^{(x)} - \Omega_y \sigma_{01}^{(y)}),
\]

(2a)

\[
H_l = \frac{\lambda_{12}}{2} (\Omega_x \sigma_{12}^{(x)} - \Omega_y \sigma_{12}^{(y)}).
\]

(2b)

Then, the unitary matrix for the total system dynamics can also be conveniently divided into two parts, i.e., \( U \equiv U(q)U(l) \), where \( U(q) \) is the qubit dynamics and \( U(l) \) is the leakage dynamics, respectively governed by the following equations:

\[
i \frac{dU(q)}{dt} = H_q U(q),
\]

(3a)

\[
i \frac{dU(l)}{dt} = U(q)^\dagger H_l U(q) U(l) = H'_l U(l).
\]

(3b)

Here, Eq. (3a) represents the qubit-system evolution that is uncoupled from the leakage state, and Eq. (3b) is the additional dynamics due to leakage-state coupling defined on the qubit evolution basis \( (U(q)) \). The resulting effective leakage Hamiltonian is given by

\[
H'_l = \frac{\lambda}{2} (\Omega_x U_{10}^{(q)} e^{i\Delta_2 t} \sigma_{02}^+ + \Omega_y U_{10}^{(q)} e^{-i\Delta_2 t} \sigma_{02}^+) + \frac{\lambda}{2} (\Omega_x U_{11}^{(q)} e^{i\Delta_2 t} \sigma_{21}^+ + \Omega_y U_{11}^{(q)} e^{-i\Delta_2 t} \sigma_{12}^+),
\]

(4)

where \( U_{mn}^{(q)} \) are the effective couplings defined by Eq. (3a) and \( \sigma_{mn}^{(x)} = (\sigma_{mn}^{(x)} + i\sigma_{mn}^{(y)}) / 2 \). As a result, the leakage dynamics \( (U(l)) \) is obtained as a function of the electric field \( (\lambda \Omega) \) and the qubit-system dynamics \( (U(q)) \).

The leakage is therefore obtained through eliminating the first-order perturbation terms of the Dyson series, when \( \lambda \) is small (weakly-coupled leakage). The leakage-state coefficient after the interaction, defined by \( c_l \equiv \langle 2 | U(l = \infty) | \psi \rangle \), is given by

\[
c_l = -\frac{i\lambda}{2} \int_{-\infty}^{\infty} \Omega^* \left( a_1 U_{10}^{(q)} + b_1 U_{11}^{(q)} \right) e^{i\Delta_2 t} dt.
\]

(5)

3. Leakage suppression with two pulses: qubit preparation

Now we consider the leakage suppression \( (c_l = 0) \) for the case in which the system evolves from the ground initial state, \( |\psi_i\rangle = |0\rangle \) \( (a_i = 1, b_i = 0) \), to an arbitrary final state. As a simplest
possible approach, we use two time-delayed short pulses to achieve \( c_l = 0 \), where the second pulse makes the leakage, \( c_l \), made by the first pulse, return exactly to zero in the complex plane.

We define two pulses \( E_1(t) \) and \( E_2(t) \), that are temporally sequential and non-overlapping, as

\[
E_1(t) + E_2(t) = E_0 e^{-\frac{t^2}{\tau^2}} \cos(\omega_L t) + \gamma E_0 e^{-\frac{(t-t_d)^2}{\tau^2}} \cos[\omega_L (t-t_d) + \phi]
\]

with respective Rabi frequencies \( \Omega_1 \) and \( \Omega_2 \), where \( \gamma \) and \( t_d \) are the amplitude ratio and the time delay between the pulses, respectively. We set the carrier-envelope phase \( \phi = 0 \) without loss of generality. If we define \( A(t) = \int_{-\infty}^{t} \mu_0(1 + \gamma) E_0 \exp(-t'^2/\tau^2) dt' \), the time-dependent pulse areas for the two pulses are given by \( A(t)/(1 + \gamma) \) and \( \gamma A(t-t_d)/(1 + \gamma) \), respectively. The targeted final state is given by \( \ket{\psi_f} = \cos \Theta/2(0) - i \sin \Theta/2(1) \) with the total pulse area \( \Theta = A(\infty) \). Then \( U_{10}^{(q)} \) in Eq. (5) becomes

\[
U_{10}^{(q)}(t) = -i \cos \frac{A(t)}{2(1 + \gamma)} \sin \frac{\gamma A(t-t_d)}{2(1 + \gamma)} - i \sin \frac{A(t)}{2(1 + \gamma)} \cos \frac{\gamma A(t-t_d)}{2(1 + \gamma)}
\]

Then, the condition of leakage suppression \( (c_l = 0) \), for the ground initial state \( (a_i = 1, b_i = 0) \), is obtained through substitution of Eq. (7) in Eq. (5) as

\[
\int_{-\infty}^{\infty} \frac{\Omega_1(t)}{2} \sin \frac{A(t)}{2(1 + \gamma)} e^{i\Delta t'} dt + \int_{-\infty}^{\infty} \frac{\Omega_2(t-t_d)}{2} \cos \frac{A(\infty)}{2(1 + \gamma)} \sin \frac{\gamma A(t-t_d)}{2(1 + \gamma)} e^{i\Delta t'} dt \\
+ \int_{-\infty}^{\infty} \frac{\Omega_1(t-t_d)}{2} \sin \frac{A(\infty)}{2(1 + \gamma)} \cos \frac{\gamma A(t-t_d)}{2(1 + \gamma)} e^{i\Delta t'} dt = 0.
\]

Figure 1(a) shows the result of the time-dependent Schrödinger equation (TDSE) calculation for various laser bandwidths \( (\Delta \omega_{\text{FWHM}}, \text{electric-field bandwidth}) \). For a wide range of laser bandwidth, leakage suppression below 1% is achieved, which is especially successful at the short pulse limit \( (\Delta \omega_{\text{FWHM}} \to \infty) \).

Furthermore, there exists an asymptotic solution at the limit of the large bandwidth compared to the two-photon detuning \( \Delta_2 \). Under this short-pulse approximation (SPA), the phase factor \( \Delta_2 t \) in Eq. (8) remains constant during the interaction. So, if we set the three terms in Eq. (8) to be
all in phase, with a time-delay phase \(\phi_d \equiv \Delta_2\tau_d = \pi\) defined between the pulse peaks, a simple algebraic solution can obtained as

\[
y = \left(1 - \frac{2}{\Theta} \cos^{-1} \left(\frac{1 + \cos \frac{\Theta}{2}}{2}\right)\right)^{-1} \left(\frac{2}{\Theta} \cos^{-1} \left(\frac{1 + \cos \frac{\Theta}{2}}{2}\right)\right)^{-1}.
\]

(9)

This solution is valid for the full coverage of \(\Theta \in [0, \pi]\), as shown in Fig. 1(b).

In comparison, leakage suppression in other systems, such as V-type and Λ-type three-level systems, can be also considered. It is simple to show that Λ-type systems provide the exactly same leakage suppression condition as Eq. (9). In V-type systems, for example, with \(\lambda_1 = 0\) but \(\lambda_2 = \lambda\) in Eq. (1), the condition is obtained in a slightly different form as

\[
y(V) = \left(1 - \frac{2}{\Theta} \sin^{-1} \left(\frac{\sin \frac{\Theta}{2}}{2}\right)\right)^{-1} \left(\frac{2}{\Theta} \sin^{-1} \left(\frac{\sin \frac{\Theta}{2}}{2}\right)\right)^{-1}.
\]

(10)

4. **Experimental verification of leakage-free qubit preparation**

Experimental verification of the scheme in Sec. 3 for arbitrary qubit preparation, was performed with ultrashort laser interactions with cold rubidium atoms. The setup is described in our previous works [24–27]. In brief, \(^{87}\)Rb cold atoms were prepared in a magneto optical trap (MOT), and the size of the atomic cloud was kept below about 80% of laser field diameter, to ensure uniform laser-atom interaction [25]. Ultrafast laser pulses were produced from a Ti:sapphire mode-locked laser amplifier operating at 1 kHz repetition, and the sequence of two pulses was programmed with an acousto-optic programmable dispersive filter (AOPDF) [28, 29].

We used 5S\(_{1/2}\), 5P\(_{3/2}\), and 5D states (\(|0\rangle\), \(|1\rangle\), and \(|2\rangle\), respectively). The resonance wavelengths are \(\lambda = 780\) nm for 5S-5P and 776 nm for 5P\(_{3/2}\)-5D, where the 5D fine-structures are treated as one through Morris–Shore transformation [30]. The short pulses were produced with the center wavelength of \(\lambda_{center} = 780\) nm and with the bandwidth of \(\Delta\lambda_{FWHM} = 4.5 \times 10^{13}\) rad/s (corresponding to \(\tau = 75\) fs), where the bandwidth was limited by the other one-photon transition to 5P\(_{1/2}\). The time delay between pulses was about 714 fs, corresponding to \(2\Delta\tau_d = 3.1\pi\), and the relative phase shift was kept less than \(\pi/10\). The pulse area was fine-controlled with a half-wave plate placed between a pair of cross polarizers. The leakage state (5D) population was probed through ionizing the 5D state atoms, where the ion signal was collected with a micro-channel plate (MCP) detector. Three-photon ionization signals (directly from 5S, blue) and full (\(\Theta = 2\pi\), red) Rabi cycles, in Fig. 2(c), as a function of \(\gamma\). Overall measurement error is estimated to about 10% after 30 repeated measurements, mainly caused by laser power fluctuation (shot-to-shot noise, about 10%), MOT density fluctuation (less than 10%, standard error), and relative amplitude shift due to pulse-shaper imperfection.

5. **Leakage suppression with three pulses: arbitrary initial state**

The previous sections, Secs. 3 and 4, dealt with qubit rotations from the ground initial state \((a_i = 1, b_i = 0)\). We now consider general initial states. In this case, the leakage defined in
Fig. 2. (a) Experimental result for the leakage state (5D) population measured as a function of total pulse area $\Theta$ and relative amplitude $\gamma$. The white dashed line represents the leakage suppression condition under the short-pulse approximation from Eq. (9). (b) Corresponding numerical calculation. (c) Comparison between the experiment (diamonds) and theory (solid lines) for $\Theta = \pi$ and 2$\pi$, extracted along the white dotted lines in Fig. 2(a) and 2(b).

Eq. (5) must be zero irrespective of both $a_i$ and $b_i$. In order to make the complex coefficients of $a_i$ and $b_i$ simultaneously zero, we need at least three pulses. With three pulses defined by

$$a E_0 \exp(-t^2/\tau^2), \quad \beta E_0 \exp(-(t-t_{d1})^2/\tau^2), \quad \text{and} \quad (1-\alpha-\beta) E_0 \exp(-(t-t_{d2})^2/\tau^2),$$

respectively, the leakage suppression condition ($c_i = 0$) is obtained under the short pulse approximation as

$$
(1 - e^{i\phi_{d1}}) \cos \frac{\alpha\Theta}{2} + (e^{i\phi_{d1}} - e^{i\phi_{d2}}) \cos \frac{(\alpha + \beta)\Theta}{2} + e^{i\phi_{d2}} \cos \Theta = 0, \quad (11a)
$$

$$
(1 - e^{i\phi_{d1}}) \sin \frac{\alpha\Theta}{2} + (e^{i\phi_{d1}} - e^{i\phi_{d2}}) \sin \frac{(\alpha + \beta)\Theta}{2} + e^{i\phi_{d2}} \sin \Theta = 0, \quad (11b)
$$

where $\alpha\Theta$ and $\beta\Theta$ are the pulse-areas, and $\phi_{d1, d2}$ are the phase delay due to the pulse intervals. When $\phi_{d1} = \pi$ and $\phi_{d2} = 0$, for example, a simple solution is obtained as

$$2 \cos \frac{\alpha\Theta}{2} - 2 \cos \frac{(\alpha + \beta)\Theta}{2} + \cos \Theta = 1, \quad (12a)$$

$$2 \sin \frac{\alpha\Theta}{2} - 2 \sin \frac{(\alpha + \beta)\Theta}{2} + \sin \Theta = 0. \quad (12b)$$

Figure 3 shows the leakage population $P_l = |c_i|^2$ after an $X(\pi)$ rotation, plotted as a function of $\alpha$ and $\beta$. The results are shown for three distinct initial states: Fig. 3(a) the ground state $|\psi_i\rangle = |0\rangle$, Fig. 3(b) a superposition state $|\psi_i\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, and Fig. 3(c) the excited state $|\psi_i\rangle = |1\rangle$. The optimal solutions (shown with star marks in the figures) are the same, suggesting that Eq. (12) results in the same ($\alpha, \beta$) values for all initial states ($a_i, b_i$), as expected. Note that experimental verification of this three-pulse leakage-suppression scheme is not provided, due to experimental limitation in our current setup.

6. Discussion: leakage population vs. fidelity error

As a discussion, we consider the contribution of the leakage population ($|c_i|^2$) to the fidelity error ($\delta F$) of qubit operation. When a final state is given by $|\psi(\eta)\rangle$, after an imperfect control, near the target $|\psi(\eta = 0)\rangle$ (the perfectly controlled final state), the fidelity can be defined as

$$F = |\langle \psi(0) | \psi(\eta) \rangle|,$$

where $\eta$ parameterizes small imperfection $[26, 31, 32]$. Using the Taylor expansion, $|\psi(\eta)\rangle$ is given by

$$|\psi(\eta)\rangle = |\psi(0)\rangle + \partial_\eta |\psi\rangle |\eta = 0\rangle + \frac{1}{2} \partial^2_\eta |\psi\rangle |\eta = 0\rangle \eta^2 + \cdots.$$  

(14)
Therefore, we get leakage population. Note that the perturbation estimation for the fidelity error contributed to by and \(H\). However, because \(\lambda = 0.34\) (scaled dipole moment for atomic rubidium) and \(\Delta\omega_{F\text{WHM}} = 15\Delta_0\) (near the SPA condition).

Using the relations \(\langle \partial_\eta \psi | \psi \rangle + \langle \psi | \partial_\eta \psi \rangle = 0\) and \(\text{Re}(\langle \partial_\eta^2 \psi | \psi \rangle) = -\text{Re}(\langle \partial_\eta \psi | \partial_\eta \psi \rangle)\) (both from \(\partial_\eta \langle \psi | \psi \rangle = 0\), we get

\[
\mathcal{F} = \sqrt{\langle \psi(\eta) | \psi(0) \rangle \langle \psi(0) | \psi(\eta) \rangle} \approx \sqrt{1 + \langle \partial_\eta \psi | \partial_\eta \psi \rangle} \eta^2 - \text{Re}(\langle \partial_\eta \psi | \partial_\eta \psi \rangle) \eta^2.
\]

In our case, \(\eta = \lambda\) (the small coupling to the leakage state) and the state evolves according to Eq. (3b), which leads to \(|\psi(\lambda)\rangle \approx |\psi(0)\rangle - i \int H'_t dt |\psi(0)\rangle\), where \(|\psi(0)\rangle = |\psi_i\rangle\) is the initial state (in the qubit space). Therefore, we get

\[
\partial_\lambda \langle \psi_i | \psi_i \rangle \bigg|_{\lambda=0} \approx -i \int_{-\infty}^{\infty} H'_t dt |\psi_i\rangle.
\]

However, because \(H'_t\) is the coupling from the qubit space to the leakage state, we get \(\langle \psi_q | \int_{-\infty}^{\infty} H'_t dt |\psi_i\rangle = 0\) for any state \(|\psi_q\rangle\) in the qubit space \(|0\rangle, |1\rangle\), which leads to \(\langle \partial_\lambda \psi | \psi \rangle = 0\) and \(\langle \partial_\lambda \psi | \partial_\lambda \psi \rangle = \langle \partial_\lambda \psi | \partial_\lambda \psi \rangle\) in Eq. (15). As a result, the fidelity can be obtained as

\[
\mathcal{F} \approx 1 - \frac{1}{2} \left( |\langle \psi_i | \int_{-\infty}^{\infty} H'_t dt |\psi_i\rangle - \int_{-\infty}^{\infty} H'_t dt |\psi_i\rangle |^2 \right) \approx 1 - \frac{1}{2} |c|^2.
\]

so the perturbation estimation indicates that the fidelity error is linearly contributed to by the leakage population. Note that the perturbation estimation for the fidelity error contributed to by the leakage process is less than 1% up to \(\Theta \approx 1.0\pi\) in our current experimental condition.

Fig. 3. (a–c) The leakage population map \(P_\eta(\alpha, \beta)\) for \(X(\pi)\)-rotations initiated from three characteristic states: (a) the ground state \((\alpha_i = 1, \beta_i = 0)\), (b) the superposition state \((\alpha_i = 1/\sqrt{2}, \beta_i = 1/\sqrt{2})\), and (c) the excited state \((\alpha_i = 0, \beta_i = 1)\). TDSE calculations for the regions of small leakages are respectively plotted, where white stars indicate the Eq. (12) solution points \((\alpha = 0.27, \beta = 0.46\) in each figure) for \(X(\pi)\)-rotation. (d) The solutions of Eq. (12) for \((\alpha, \beta)\). TDSE calculations are performed with \(\lambda = 0.34\) (scaled dipole moment for atomic rubidium) and \(\Delta\omega_{F\text{WHM}} = 15\Delta_0\) (near the SPA condition).
7. Conclusion

We have proposed a pulsed leakage suppression scheme and performed a proof-of-principle experimental verification. In a ladder-type three-level system, the leakage to the third level from the two-level qubit system is successfully suppressed for qubit $X$ rotations from the ground initial qubit state. We used coherent destructive interference to suppress the overall leakage, where the leakage caused by the first pulse was controlled with a subsequent pulse. Likewise, the qubit $X$ rotation from an arbitrary initial state requires two additional pulses for leakage suppression. Experimental verification was performed with femtosecond laser and atomic rubidium, for the qubit rotations of ground-state atoms using two pulses with controlled relative amplitude and time-delay, and the result shows good qualitative agreement with the prediction. Since pulse sequences is in general simpler to produce than other pulse shapes, our leakage suppression method may be useful in experiments with limited pulse shaping capability.

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