Simple Circuits for Exact Elimination of Leakage in a Qubit Embedded in a Three-level System

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Leakage errors damage a qubit by coupling it to other levels. Over the years, several theoretical approaches to dealing with such errors have been developed based on perturbation arguments. Here we propose a different strategy: we use a sequence of finite rotation gates to exactly eliminate leakage errors. The strategy is illustrated by the recently proposed charge quadrupole qubit in a triple quantum dot, where there are two logical states to support the qubit and one leakage state. We find an \( su(2) \) subalgebra in the three-level system, and by using the subalgebra we show that ideal Pauli \( x \) and \( z \) rotations, which are universal for single-qubit gates, can be generated by two or three propagators of experimentally-available Hamiltonians. The proposed strategy does not require additional pulses, is independent of error magnitude, and potentially reduces experimental overheads. In addition, the magnitude of detuning fluctuation can be estimated based on the exact solution.

The physical realization of quantum computer poses an unprecedented challenge to our capabilities of controlling the dynamics of quantum systems. While there have been many attempts to overcome this challenge, the perfect controllability of semiconducting quantum dots makes them promising candidates for universal quantum computation [1–6]. A universal quantum computer is the ultimate information processor in modern quantum technology, which uses quantum bits (qubits) and quantum circuits to perform computations. A qubit consists of an idealized pair of orthonormal quantum states. However, this idealization neglects other states which are typically present and can mix with those supporting the qubit. Such mixing is termed as leakage. Leakage may be the result of the application of gate operations, or induced by system-bath interactions [7–13]. Several strategies for combating the leakage errors have been developed for different systems, in particular the semiconducting qubit setup which is the main subject of this work, including analytic pulse shaping [10, 14] and optimal quantum control [15, 16]. Ref. [17] also presents a general leakage-elimination method for removing such errors by using simple decoupling and recoupling pulse sequences of the leakage elimination operator (LEO). Nonperturbative LEO was recently introduced for nonideal composite pulses, with emphasis on application of three-level nitrogen-vacancy centers [18]. It is shown that, for a three-level system, the effectiveness of LEOs does not depend on the details of the composite pulses but on the integral of the pulse sequence in the time domain. Recent studies show a significant advantage of a three-level system embedded in a triple quantum dot, which is associated with a decoherence-free subspace of a charge quadrupole qubit [19]. The leakage errors are caused by noise and could be reduced by smoothly-varying short control pulses which are experimentally feasible. The system is modelled by two logical states and a leakage state coupled to one of them. Using perturbation technique and the quasistatic noise approximation, the leakage errors of single qubit operations can be suppressed by simple pulse sequences up to the sixth order in noise amplitude. While it is simple and efficient, the approach needs additional well-controlled pulses, and is only valid for small-amplitude noise. These requirements may not be well satisfied during gate operations, especially when the strength and time-dependence of noise are not negligible in comparison with other control parameters.

Here we present an exact solution to leakage elimination for a three-level system where the leakage state is coupled to one of the logical states, by using a simple sequence or circuit of experimentally-available finite rotations (gates). The coupling strength between the logical state and the leakage state is assumed to be static during the operation time, which is experimentally feasible for semiconducting quantum dots [19–21]. This assumption may not be necessary as the later numerical simulation shows that our exact circuit performs perfectly, even in the presence of time-dependent noise. Moreover, we explain the parameter settings in our approach including estimation of noise strength based on the exact circuit.

The model.—We start with a model Hamiltonian represented in the basis spanned by two logical states and one leakage state [19].

\[ H = H_x + H_z + H_{\text{leak}}, \]

where

\[ H_x = \sum_{i} |i\rangle \langle i | x |i\rangle \langle i |, \]

\[ H_z = \sum_{i} |i\rangle \langle i | z |i\rangle \langle i |, \]

\[ H_{\text{leak}} = \sum_{i,j} |i\rangle \langle j | \text{leak} |i\rangle \langle j |, \]

with
where we use the same notations as in Ref. [19]. Here \( \epsilon_d \) and \( g \) are independent control parameters for rotations with respect to the \( z \) and \( x \) directions. \( H_{\text{leak}} \) stands for a coupling between the leakage state and one of the logical states, and \( \zeta \) is the scaled leakage state energy in the absence of coupling [22–24]. A charge quadrupole (CQ) qubit is formed in three adjacent semiconductor quantum dots sharing a single electron and is embedded in the localized charge basis \( \{ |100\rangle, |010\rangle, |001\rangle \} \), where the basis states denote the electron being in the first, second or the third dot, respectively. The system Hamiltonian reads

\[
H_{\text{CQ}} = \left( \begin{array}{cccc}
\epsilon_d & t_A & 0 \\
t_A & \epsilon_q & t_B \\
0 & t_B & -\epsilon_d
\end{array} \right) + \frac{U_1 + U_3}{2},
\]

where \( U_{1,2,3} \) are the on-site potentials for the three dots.

\[
|C\rangle = |010\rangle, \quad |E\rangle = \frac{|100\rangle + |001\rangle}{\sqrt{2}}, \quad |L\rangle = \frac{|100\rangle - |001\rangle}{\sqrt{2}},
\]

and a schematic diagram is presented in Fig. (1). The Hamiltonian in the new basis is transformed into

\[
\tilde{H}_{\text{CQ}} = \left( \begin{array}{ccc}
\frac{\epsilon_d}{2} & \frac{t_A + t_B}{\sqrt{2}} & \frac{t_A - t_B}{\sqrt{2}} \\
\frac{t_A + t_B}{\sqrt{2}} & \epsilon_q & \epsilon_d \\
\frac{t_A - t_B}{\sqrt{2}} & \epsilon_d & -\frac{\epsilon_d}{2}
\end{array} \right),
\]

where a term proportional to the identity has been dropped. \( \tilde{H}_{\text{CQ}} \) is reduced to Eq. (1) under the conditions of \( \zeta = 1, \xi = \epsilon_d, \) and \( g = (t_A + t_B)/\sqrt{2} \). In case that \( t_A = t_B \) and \( \epsilon_d = 0 \) are satisfied, \( \tilde{H}_{\text{CQ}} \) supports a decoherence-free subspace against uniform electric field fluctuations [20].

In the triple quantum dot system, \( \epsilon_d \) corresponds to an average dipolar detuning control parameter. Although \( \epsilon_d \) is set to be zero, its fluctuation \( \delta \epsilon_d \) breaks the DFS and causes leakage. It has been shown that the fluctuation of quadrupolar detuning control parameter is smaller than \( \delta \epsilon_d \) and is thus neglected. Now we focus on the influence of \( \delta \epsilon_d \) on the CQ qubit operations. Noise spectrum of \( \delta \epsilon_d \) is dominated by low-frequency fluctuations which are slow in comparison with gate operations [21]. Therefore \( \delta \epsilon_d \) is assumed to remain constant during a given gate operation [19, 22]. As a result, unitary operators for \( x \) and \( z \) rotations can be given by

\[
U_x(g, \delta \epsilon_d, \theta) = \exp\{-i[H_x(g) + H_{\text{leak}}(\delta \epsilon_d)]\theta/2g\},
\]

\[
U_z(\epsilon_q, \delta \epsilon_d, \varphi) = \exp\{-i[H_z(\epsilon_q) + H_{\text{leak}}(\delta \epsilon_d)]\varphi/\epsilon_q\},
\]

with arbitrary angles \( \theta \) and \( \varphi \). In the bang-bang limit where the control pulses switch instantaneously between two values, the angles are associated with the corresponding bang-bang gate time intervals \( t_x \) and \( t_z \), which are \( \theta = t_x(\epsilon_q/\delta \epsilon_d), \varphi = t_z(2g/\epsilon_q) \). As shown by Eq. (5), rotation operators are obviously polluted by \( \delta \epsilon_d \). Below, we will explain our exact solution to this problem.

A set of \( su(2) \) generators, finite rotations, exact elimination of leakage. To suppress the fluctuation \( \delta \epsilon_d \) in \( U_x(g, \delta \epsilon_d, \theta) \), we start with the following three matrices

\[
M_1 = \left( \begin{array}{ccc}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0
\end{array} \right), \quad M_2 = \left( \begin{array}{ccc}
0 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{array} \right), \quad M_3 = \left( \begin{array}{ccc}
0 & 0 & -i \\
0 & 0 & 0 \\
i & 0 & 0
\end{array} \right).
\]

It can be shown that their commutation relations satisfy

\[
[M_1, M_2] = iM_3, \quad [M_2, M_3] = iM_1, \quad [M_3, M_1] = iM_2,
\]

indicating that these operators generate an \( su(2) \) algebra. An arbitrarily given finite rotation can be represented in an exponential form [25]

\[
\exp[i(\gamma_1 M_1 + \gamma_2 M_2 + \gamma_3 M_3)],
\]

where \( \gamma_1, \gamma_2, \gamma_3 \) are three continuous parameters and a linear combination of \( M_i (i = 1, 2, 3) \) indicates a specific rotation axis and the corresponding angle. On the other hand, the finite rotation can also be expressed by three Euler's angles \( \phi_1, \phi_2, \) and \( \phi_3 \),

\[
\exp[i\phi_1 M_2] \exp[i\phi_2 M_1] \exp[i\phi_3 M_2],
\]
The relation between the two sets of parametrizations can be found by setting
\[
\exp[i\phi_1 M_2] \exp[i\phi_2 M_1] \exp[i\phi_3 M_3] = \exp[i(\gamma_1 M_1 + \gamma_2 M_2 + \gamma_3 M_3)],
\]
where the two sets \( \phi_i \) and \( \gamma_i \) \((i = 1, 2, 3)\) are in one-to-one correspondence. In our cases \((5)\), we can set \( \gamma_1 = \alpha \alpha \), \( \gamma_2 = \alpha b \), \( \gamma_3 = 0 \), where \( a^2 + b^2 = 1 \). It is easy to verify that the powers of \( M_i \) satisfy
\[
M_i^{2n} = I - \Delta(i), \quad M_i^{2n+1} = M_i,
\]
\[
(aM_1 + bM_2)^2n = (aM_1 + bM_2)^2, \quad (aM_1 + bM_2)^2n+1 = aM_1 + bM_2,
\]
where \( n \) is a positive integer, \( I \) is the three dimensional identity matrix, and \( \Delta(i) \) is a matrix with \( \Delta(i)_{i,j} = 1 \), \( \Delta(i)_{j,k} = 0 \) for \( j \neq i \) or \( k \neq i \). Based on the above properties, we can derive an exact matrix equation \((9)\) representing a system of nine nonlinear equations of which only three equations are independent. These independent equations determine \( \phi_1 = \phi_3 \) and
\[
\cos \phi_2 = 1 + a^2(\cos \alpha - 1), \\
\sin \phi_2 \sin \phi_1 = ab(1 - \cos \alpha), \\
\sin \phi_2 \cos \phi_1 = a \sin \alpha.
\]
Therefore angles \( \phi_1 \) and \( \phi_2 \) can be expressed in terms of \( \alpha, a \) and \( b \). Substituting Eq. \((8)\) to \( U_x(g, \delta \epsilon, \theta) \), we obtain
\[
U_x(g, \delta \epsilon, \theta) = \exp(i\beta_1 H_{\text{leak}}) \exp(i\beta_2 X_g) \exp(i\beta_1 H_{\text{leak}}),
\]
with parameter constraints
\[
a = -\theta/2\alpha, \quad b = -\theta \delta \epsilon/2g, \quad \alpha = (\theta/2g) \sqrt{g^2 + \delta \epsilon^2},
\]
\[
\beta_1 = \pm \arcsin[ab(1 - \cos \alpha)]/\sin \beta_2/\delta \epsilon, \quad \beta_2 = \pm \arccos[1 - a^2(1 - \cos \alpha)]/g,
\]
which are obtained from the first two Eqs. \((10)\). The sign of \( \beta_1 \) and \( \beta_2 \) can be further determined by checking the parameter solutions with the third Eq. \((10)\). By reversing Eq. \((11)\) we obtain the ideal gate operator with respect to \( x \) axis,
\[
U_{xx}(g, -2g \beta_2) = \exp[-iH_x(g)(-2g \beta_2)]/2g
\]
\[
= \exp(-i\beta_1 H_{\text{leak}}) U_x(g, \delta \epsilon, \theta) \exp(-i\beta_1 H_{\text{leak}}).
\]
and eliminate the leakage \( H_{\text{leak}} \). The unitary operator \( \exp(-i\beta_1 H_{\text{leak}}) \) is the special case of the imperfect gate \( U_x(0, \delta \epsilon, 2g \beta_1) \) which is experimentally feasible by microwave pulses in semiconducting dots.

**Parameter settings.**— For a CQ qubit under noise \( \delta \epsilon \), an ideal \( x \) rotation with angle \( -2g \beta_2 \) is generated by experimental parameters \( \beta_1, \theta, g \) and \( \delta \epsilon \) in terms of the constraints \((12)\). In semiconducting quantum dots, gate operations are implemented by microwave pulses so that \( \theta \) can be modulated by the pulse width, and \( g \) is determined by tunnel couplings \( t_{A,B} \). The spectrum of the noise \( \delta \epsilon \) in range of 5 kHz to 1 MHz has been shown by Hahn echo curves \([21]\). Here our derivation suggests a new perspective to look into the noise \( \delta \epsilon \). An estimation of \( \delta \epsilon \) can be done by following steps: (i) prepare an initial state, for example \([0]\). (ii) perform the three operations on the right side of Eq. \((13)\) with given \( g, \beta_1 \) and \( \theta \) which has no limitation. The resultant operation in the logical subspace is an ideal \( x \) rotation. (iii) measure the output state, and then \( \beta_2 \) can be given. (iv) substitute \( g, \beta_1, \theta \) and the measurement result of \( \beta_2 \) to Eq. \((12)\), then \( \delta \epsilon \) are estimated. In experiments on semiconducting quantum dots, state initialization and read-out take about 4 ms to 5 ms, and state manipulation needs about 1 ms \([21]\). Therefore our estimation is allowed to be performed and repeated for several times and an effective strength curve of \( \delta \epsilon \) in the time domain can be concluded. Based on the noise spectrum as shown in Ref. \([21]\), the strength of \( \delta \epsilon \) oscillates and the effective strength curve shows a periodicity. As a result, an effective \( \delta \epsilon \) at a desired operation time and its periodic extension can be given by the curve.

**An arbitrary rotation without leakage.**— An arbitrary leakage-free gate can be generated by three ideal \( x \) and \( z \) rotations. While the ideal \( x \) rotation is given by \((13)\), in what follows, we will first show how to generate the ideal \( z \) rotation. Let us start with the experimentally available \( U_z(\epsilon, \delta \epsilon, \phi) \) in Eq. \((5)\). By using the commutation relation \([H_z, H_{\text{leak}}] = 0\), \( U_z \) can be simply decomposed into
\[
U_z(\epsilon, \delta \epsilon, \phi) = \exp[-iH_z(\epsilon, \phi)/\epsilon] \exp[-iH_{\text{leak}}(\delta \epsilon, \phi)/\epsilon].
\]
Consequently, the leakage-free \( z \) rotation can be realized.
by

\[
U_{ix}(\epsilon_q, \varphi) = \exp[-iH_z(\epsilon_q)\varphi/\epsilon_q] = U_z(\epsilon_q, \delta\epsilon_d, \varphi)U_x(0, \delta\epsilon_d, -\varphi),
\]

(15)

where \(\varphi' = \varphi\epsilon_q\). Eq. (15) shows that only two different gates with the same \(\delta\epsilon_d\) are needed for the implementation of an ideal \(z\) rotation. It does not require the detail of \(\delta\epsilon_d\) as well.

In general, it is well-known that an arbitrary leakage-free rotation for a single qubit can be implemented by combining \(U_{ix}\) and \(U_{iz}\), i.e., three experimentally-available rotations for \(x\) axis and two for \(z\) axis, as sketched in Fig. (2).

\[\text{FIG. 2. Circuits for generating } U_{ix} \text{ and } U_{iz}. \text{ The magnitude of applied pulses are } \epsilon_q \text{ and } g. \text{ The operation time } t_z(t_z') \text{ are given through angle } \varphi(\varphi') \text{ and detuning parameter } \epsilon_q \text{ and } t_2 \text{ and } t_4 \text{ are given by angles } \beta_1, \beta_2 \text{ and the coupling parameter } g. \text{ The sign of angle parameters can be adjusted by setting the pulse width according to rotation period } 2\pi.\]

**Numerical Results.**— Let us start with the initial state \(|\psi_0\rangle = (|C\rangle + |E\rangle)/\sqrt{2}\), or its corresponding density matrix \(\rho_0\)

\[
\rho_0 = |\psi_0\rangle \langle \psi_0| = \begin{pmatrix}
1/2 & 1/2 & 0 \\
1/2 & 1/2 & 0 \\
0 & 0 & 0
\end{pmatrix}.
\]

(16)

The time evolution of \(\rho(t)\) by the propagator \(U(t)\) is \(\rho(t) = U(t)\rho_0 U(t)^\dagger\) for a noise channel. The dynamics of \(\rho(t)\) will remain in the logical states and the matrix element \(\rho_{23}(t) = 0\) if the propagator \(U(t)\) does not contain leakage errors. If there are leakage errors in \(U(t)\), where \(\rho(t)\) is thus required to be an average over different noise channels denoted by \(\delta\epsilon_d\), we can use \(\rho_{23}\) (or \(\rho_{32}\)) to characterize the errors.

Figs. 3 show the dynamics of \(|\rho_{23}(t)|\) for the propagators \(U_{ix}\) and \(R_{xxs}\), where the latter is defined as in Ref. [19]. Note that we set parameters in \(R_{xxs}\) such that it acts the same as \(U_{ix}\). The semiconducting dot experiments [19, 26] suggest that we can set \(g/h\) to be 3.0 GHz and the evolution time from 0 ns to 0.6 ns. \(\delta\epsilon_d\) is a random number and is supposed to range from 0.2 GHz to 0.5 GHz. The top subfigure is the case when \(\delta\epsilon_d\) remains a constant for a given channel, where the gate \(U_{ix}\) is perfect since leakage is fully eliminated. The bottom illustrates the dynamics of \(|\rho_{23}(t)|\) when \(\delta\epsilon_d\) is completely random over the course of time, i.e., the time-dependent noise. The two subfigures may imply two bounds of leakage effects, the time-independent bound and full time-dependent bound. The time-independent noise is more realistic as shwon in Ref. [21]. It is noticeable that the present exact circuit performs perfectly even for full time-dependent noise.

**Conclusion.**— We provide an exact solution to elimination of leakage errors in a three-level quantum model using simple circuits of gates. The model comprises of two logical states and a leakage state, which can be used to describe a triple quantum dot system supporting a DFS. DFS is a well-known strategy in error suppression for quantum computation, which attracts significant attentions because of its minimal overhead requirements. The concatenation of DFS and the exact circuits promises to give this approach a twofold resilience, against decoherence and stochastic leakage errors. Numerical simulation shows that the exact circuits perform perfectly even in the presence of full time-dependent noise, indicating the stability and fault-tolerance of these circuits. Furthermore we propose an estimation of dipolar detuning control fluctuation to extract precise strength information of noise. The feasibility of our approach is ensured by the development of sophisticated experimental techniques [19, 20].

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