

Single-Step Implementation of Universal Quantum Gates

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We construct optimized implementations of the controlled-NOT and other universal two-qubit gates that, unlike many of the previously proposed protocols, are carried out in a single step. The new protocols require tunable interqubit couplings but, in return, show a significant improvement in the quality of gate operations. We make specific predictions for coupled Josephson junction qubits and compare them with the results of recent experiments.

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According to one of the central results of quantum information theory, an arbitrarily complex quantum protocol can be decomposed into a sequence of single-qubit rotations and two-qubit gates [1]. However, despite its providing a convenient means of designing logical circuits, in practice such a decomposition may not necessarily achieve the shortest possible times of operation and, consequently, the lowest possible decoherence rates. In any practical implementations, however, the latter are crucially important, for any realistic qubit system would always suffer a detrimental effect of its dissipative environment.

Recently, there have been various attempts to improve the performance of universal quantum gates by searching for their optimal implementations among the entire class of two-qubit Hamiltonians with the most general time dependent coefficients. However, a typical outcome of such a tour-de-force variational search [2] tends to be a complicated sequence of highly irregular pulses whose physical content often remains obscure.

Conceivably, a significantly simpler alternative to this approach would be a straightforward implementation of a given unitary transformation in the smallest possible number of steps, during each of which the Hamiltonian remains constant. A well known example of this kind is provided by the two-qubit SWAP gate which can be readily implemented (up to a global phase) with the use of the spin-rotationally invariant Heisenberg interqubit coupling that remains constant during the gate operation.

In this Letter, we construct one-step implementations of some frequently used universal two-qubit gates. In contrast to the previous works where a constant decoherence rate was assumed and therefore the overall loss of coherence accumulated during a gate operation would be evaluated solely on the basis of its total duration, we quantify the adverse effect of the environment by actually solving the corresponding master equation for the density matrix of the coupled qubits. In this way, we account for the fact that the decoherence rates generally depend upon (and vary with) the adjustable parameters of the Hamiltonian.

In the case of interest, the Hamiltonian

$$\hat{H} = \sum_{i=1,2} \hat{\sigma}_i [\vec{B}_i(t) + \vec{h}_i(t)] + \sum_{a=x,y,z} J_a(t) \hat{\sigma}_1^a \hat{\sigma}_2^a \quad (1)$$

operates on a direct product of the Hilbert spaces of two (pseudo)spins labeled by $i = 1, 2$ and spanned by the eigenstates $|\uparrow, \downarrow\rangle_1 \otimes |\uparrow, \downarrow\rangle_2$ of the operators $\hat{\sigma}_{1,2}^z$.

The tunable local fields $\vec{B}_i = (\Delta_i, 0, \epsilon_i)$ encode tunneling amplitudes $\Delta_{1,2}(t)$ and biases $\epsilon_{1,2}(t)$ of the individual qubits, while their random (and uncorrelated, $\langle h_1(t)h_2(t') \rangle = 0$) counterparts $\vec{h}_i = (0, 0, h_i)$ represent the noisy environment in the worst-case scenario of two independent dissipative reservoirs. Contrary to the opposite limit of two strongly correlated reservoirs (collective decoherence), in this case no decoherence-free subspace exists for $J_a = 0$.

In order to facilitate the analysis of a decohering effect of the environment, in what follows we assume the Ohmic nature of the dissipative reservoirs described by the spectral function $S(\omega) = \int dt e^{i\omega t} \langle h_{1,2}(t)h_{1,2}(0) \rangle = \alpha \omega \times \coth(\omega/2T) \Theta(\omega_c - \omega)$ of dimensionless strength $\alpha \ll 1$ and bandwidth ω_c (we discuss the relevance of this type of noise for superconducting qubits below).

The Ohmic noisy environment can be treated in the standard Bloch-Redfield (i.e., weak-coupling and Markovian) approximation. In the basis of the eigenstates of the noiseless part of the Hamiltonian (1), the Bloch-Redfield equation for the reduced two-qubit density matrix reads [3]

$$\dot{\rho}_{nm}(t) = -i\omega_{nm}\rho_{nm}(t) - \sum_{k,l} R_{nmkl}\rho_{kl}(t), \quad (2)$$

where $\omega_{nm} = (E_n - E_m)/\hbar$, $n, m = 1, \dots, 4$, are the transition frequencies between the unperturbed (i.e., for $\alpha = 0$) eigenstates of Eq. (1), and the relaxation tensor $R_{nmkl} = \delta_{lm} \sum_r \Lambda_{nrrk} + \delta_{nk} \sum_r \Lambda_{lrrm}^* - \Lambda_{lmnk} - \Lambda_{knml}^*$ is computed in terms of the partial transition rates whose real parts describe the effect of decoherence $\text{Re}\{\Lambda_{lmnk}\} = \frac{1}{4\pi} S(\omega_{nk}) \times [\sigma_{1,lm}^z \sigma_{1,nk}^z + \sigma_{2,lm}^z \sigma_{2,nk}^z]$, whereas $\text{Im}\{\Lambda_{lmnk}\}$ yield the Lamb shifts of the energy levels E_n .

As a customary measure of the coupled qubits' performance, we use the gate purity $P(t)$ [4]. The gate purity provides a convenient measure of decoherence, for in the case of a unitary evolution $P(t)$ remains equal to unity.

Below, we restrict our analysis to the Hamiltonians that remain constant, $\hat{H}(t) = \hat{H}_0 \theta(t) \theta(t_0 - t)$, for the entire

duration t_0 the gate operation and therefore commute at all times ($[\hat{H}(t), \hat{H}(t')] = 0$). We then demonstrate that within this class of quasistationary Hamiltonians, the problem of constructing an optimized (coherence-wise) implementation of a given universal gate allows for a rather simple and physically transparent solution.

To that end, we utilize the mechanism of decoherence suppression proposed in Ref. [5] where the decoherence properties (decay rate) of any initial state of an idling pair of coupled qubits (“quantum memory”) were shown to be related to the spectral properties of the noiseless Hamiltonian. In particular, it was demonstrated in Ref. [5] that the relaxation-related component of the overall decoherence can be significantly reduced by tuning the Hamiltonian parameters toward the point in the parameter space where a pair of the lowest eigenvalues of the quasistationary Hamiltonian (1) becomes degenerate (see also the more recent Ref. [6] for corroborating results).

The underlying (energy exchange-based) mechanism of the suppression of relaxation is based on the observation that near a degeneracy point and at low temperatures the relaxation rates R_{nmkl} appear to be given by linear combinations of the transition frequencies $\sum_{i \neq j} c_{ij} |\omega_{ij}|$, where the coefficients c_{ij} are essentially independent of ω_{ij} [5]. Therefore, the relaxation rates attain their minimum values at those points in the parameter space where the largest possible number of the transition frequencies vanish due to degeneracy. By contrast, a contribution from the other, pure dephasing processes is generally unavoidable and can be suppressed only by lowering the temperature of the reservoirs.

In order to further illustrate the above point, in Fig. 1 we plot the absolute value of the purity decay rate $|dP/dt|$ (which, if computed in the Markovian approximation, remains approximately constant at the times much shorter than the decoherence time) as a function of the components of the interqubit coupling J_x and J_y , while keeping the single-qubit fields \vec{B}_i constant and the length of the vector $J = \sqrt{J_x^2 + J_y^2 + J_z^2}$ fixed. On physical grounds, the latter constraint is justified by the fact that in any realistic qubit

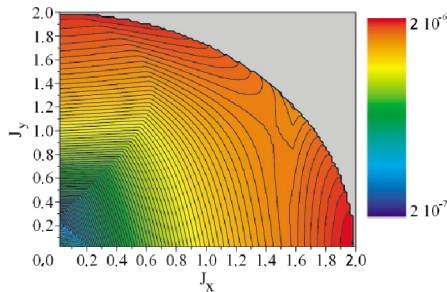


FIG. 1 (color online). Decay rate of the gate purity $|dP/dt|$ as a function of the interqubit couplings J_x and J_y at $\epsilon_1 = \epsilon_2 = 0$, $\Delta_1 = \Delta_2 = \Delta$, $\Delta = 1$ (in units of \hbar/t_0), $\alpha = 0.01$, and $T = 0.1\Delta$ (see text).

system an unlimited increase of J would eventually result in an unwanted leakage from the designated two-qubit Hilbert subspace.

The color plot of Fig. 1 demonstrates that $|dP/dt|$ does attain its absolute minimum at the points characterized by the incidence of double degeneracy between the eigenvalues of the noiseless part of Eq. (1) [see Eq. (5) below]. Furthermore, albeit being somewhat less effective than its double counterpart, the onset of even a single degeneracy between the two lowest eigenvalues appears to provide a relative improvement, as compared to the generic (nondegenerate) situation. Even in this case, the two-dimensional degenerate ground state gets protected by the energy gap separating it from the rest of the spectrum that gives rise to the exponential suppression of relaxation at low temperatures. Considering the challenge of a high-precision tuning of the qubits’ couplings in any realistic setup, the possibility of improving the gate quality with such a more relaxed constraint on the Hamiltonian parameters should be of a particular interest for practical realizations of robust quantum gates.

Having identified the conditions required for a suppression of decoherence, we can now attempt to satisfy them in the cases of some popular universal gates.

First, we impose the less stringent condition of a single degeneracy between the lowest pair of energy levels, while looking for a one-step implementation of the standard controlled-NOT (CNOT) gate $\hat{X}_{\text{CNOT}} = \text{diag}([1 \ 0 \ 0 \ 0] \times [0 \ 1 \ 0 \ 0][0 \ 0 \ 0 \ 1][0 \ 0 \ 1 \ 0])$ (hereafter all the universal gates are presented in the basis of the eigenstates of $\hat{\sigma}_1^z \otimes \hat{\sigma}_2^z$).

In the noiseless case, this goal can be accomplished by directly computing the matrix-valued logarithm of the unitary matrix \hat{X}_{CNOT} . It turns out, however, that the latter features a high degree of ambiguity:

$$\hat{H}_{\text{CNOT}} = i(\hbar/t_0) \ln(\hat{X}_{\text{CNOT}}) = C(A + B)C^{-1}, \quad (3)$$

where $A = \text{diag}([0 \ 0 \ 0 \ 0][0 \ 0 \ 0 \ 0][0 \ 0 \ -\pi/2 \ \pi/2] \times [0 \ 0 \ \pi/2 \ -\pi/2]) + \phi_0 \hat{E}$, a possible “mismatch” phase ϕ_0 entering with the unity matrix \hat{E} , and $B = 2\pi n_1 \times \text{diag}([1 \ 1 \ 0 \ 0][1 \ 1 \ 0 \ 0][0 \ 0 \ 1 \ 1][0 \ 0 \ 1 \ 1]) + 2\pi n_2 \times \text{diag}([0 \ 0 \ 1 \ 1][0 \ 0 \ 1 \ 1][1 \ 1 \ 0 \ 0][1 \ 1 \ 0 \ 0]) + 2\pi n_3 \hat{E}$ [observe that $[A, B] = 0$ and $C = \text{diag}([e^{i\phi_0} \hat{\sigma} \ 0] \times [0 \ e^{i\phi_1} \sigma_x])$].

Equation (3) manifests the multivaluedness of the matrix logarithm of the CNOT gate which can be obtained by exponentiating \hat{H}_{CNOT} for an arbitrary choice of the integer $(n_{1,2,3})$ as well as continuous $(\vec{\phi}, \phi_1)$ parameters, respectively. The existence of such an extensive invariant subspace within the equivalence class of CNOT (see below) is a special property of this particular gate.

A straightforward analysis reveals that the CNOT gate can indeed be reproduced up to a global phase $\phi_0 = -\pi/4$ [so that $\hat{X}_{\text{CNOT}} = \exp(-i\pi/4 - it_0 \hat{H}_0/\hbar)$] under the condition of a single spectral degeneracy ($E_1 = E_2 = -0.875$,

$E_3 = 0.625$, $E_4 = 1.125$) with the following choice of the parameters in Eq. (3): $\Delta_1 = J_x = J_y = 0$, $\Delta_2 = 1.5$, $\epsilon_1 = -0.25$, $\epsilon_2 = J_z = -0.66$ (hereafter all the energies are measured in units of \hbar/t_0).

In Fig. 2 we contrast the resulting optimized gate against the standard CNOT protocol consisting of a series of non-overlapping pulses (see, e.g., [7]):

$$\hat{X}_{\text{CNOT}} = \exp\left(-i\frac{\pi}{2}\frac{\sigma_2^x + \sigma_2^z}{\sqrt{2}}\right)\exp\left(-i\frac{\pi}{2}\sigma_1^z\right)\exp\left(-i\frac{\pi}{2}\sigma_2^z\right) \\ \times \exp\left(-i\frac{\pi}{4}\sigma_1^z\sigma_2^z\right)\exp\left(-i\frac{\pi}{2}\frac{\sigma_2^x + \sigma_2^z}{\sqrt{2}}\right). \quad (4)$$

In order to compare the quality of the two protocols, we solve the corresponding Bloch-Redfield Eq. (2) in the presence of a weak ($\alpha \ll 1$) noise in both cases. As a result, we find that the single-step implementation, where both the two- and one-qubit operations are carried out simultaneously, takes about 15% of the time of and appears to be approximately 10 times (in terms of the gate purity) better than the standard protocol (4).

Next, we attempt to impose the double degeneracy condition that, if at all attainable, is expected to result in an even better performance. Although this more stringent condition may not necessarily allow for a construction of an arbitrary two-qubit gate, one can still elect to settle for a more readily achievable goal of constructing a gate X' which is equivalent (i.e., $X' = U_1 \otimes U_2 X U_1' \otimes U_2'$, where $U_{1,2}$ and $U_{1,2}'$ are single-qubit rotations), albeit not necessarily identical, to a target gate X . It should be noted, however, that in practice such a substitute solution might only be acceptable if all the one-qubit rotations can be performed sufficiently quickly, thus contributing negligibly towards the overall loss of coherence.

Formally, the equivalence between a pair of gates is established on the basis of a coincidence of their Makhlin's invariants G_1, G_2 (see, e.g., [7]). A straightforward analysis shows that in the presence of a double spectral degeneracy G_1 always turns out to be a real number, which in fact severely restricts the set of gates that can be constructed this way. One example of a gate incompatible with the

double degeneracy condition is provided by the $\sqrt{\text{SWAP}}$ gate with $G_1 = -i/4$. By contrast, the CNOT equivalence class (albeit not the original CNOT gate itself) with the invariants $G_1 = 0, G_2 = 1$ can be readily attained under the condition of double degeneracy.

The above theoretical findings can be of an immediate relevance to such a viable candidate to the role of robust two-qubit gates as a pair of charge/flux Josephson junction qubits. Therefore, in what follows we specifically discuss this particular realization and focus on its most coherence-friendly regime (dubbed ‘‘quantonium’’ in Ref. [8]) where the individual qubits are tuned to their optimal points $\epsilon_{1,2} = 0$ and coupled together capacitively [8] and/or inductively [9].

At the optimal point, the eigenvalues of the noiseless part of Eq. (1) assume a particularly simple form:

$$E_{1,2} = J_x \mp \sqrt{(\Delta_1 + \Delta_2)^2 + (J_y - J_z)^2}, \quad E_{3,4} = -J_x \pm \\ \sqrt{(\Delta_1 - \Delta_2)^2 + (J_y + J_z)^2}. \quad \text{Considering, for the sake of} \\ \text{simplicity, the case of two identical qubits } (\Delta_{1,2} = \Delta), \\ \text{one can readily show that the double degeneracy condition} \\ (E_1 = E_4, E_2 = E_3) \text{ is achieved at}$$

$$J_x = 0, \quad J_y J_z = \Delta^2, \quad (5)$$

in complete agreement with Fig. 1.

Thus, in order to implement a transformation that belongs to the CNOT equivalence class under the double degeneracy condition, it suffices to use a single rectangular interaction pulse with the parameters $\vec{J}_{\text{CNOT}} = [0, (\sqrt{J^2 + \Delta^2} - \sqrt{J^2 - \Delta^2})/\sqrt{2}, (\sqrt{J^2 + \Delta^2} - \sqrt{J^2 - \Delta^2})/\sqrt{2}]$.

By solving the Bloch-Redfield equations, we find that corresponding protocol outperforms the CNOT-equivalent gate constructed with the use of the Heisenberg interqubit coupling [10], as far as both the duration (≈ 2.3 shorter) and robustness (≈ 10.5 times lower purity decay rate) are concerned, thereby resulting in ≈ 25 times lower overall loss of purity $1 - P(t_0)$.

For most part, the ubiquitous CNOT gate owes its high popularity to the fact that a generic two-qubit gate requires no more than three CNOT applications complemented by local single-qubit rotations [11]. Recently, the authors of Ref. [7] put forward an alternative gate (dubbed as the ‘‘B’’ gate) with the invariants $G_1 = G_2 = 0$. Unlike CNOT, however, the B gate needs to be used only twice in order to implement an arbitrary two-qubit gate (up to a single-qubit rotation).

With an eye on the possibility of a further optimization, we find that our approach, which takes a full advantage of the double degeneracy condition, offers a superior realization of the B -gate universality class, too. Namely, by choosing the gate parameters in accordance with the above double degeneracy conditions, $\Delta_{1,2} = 1$, $\epsilon_{1,2} = J_x = 0$, $J_y = 0.58$, $J_z = 1.71$ (in units of \hbar/t_0), we arrive at the one-step implementation of the equivalent of the B gate which takes only $\approx 56\%$ of the duration of the protocol of Ref. [7] and results in a much improved (≈ 4.5 times

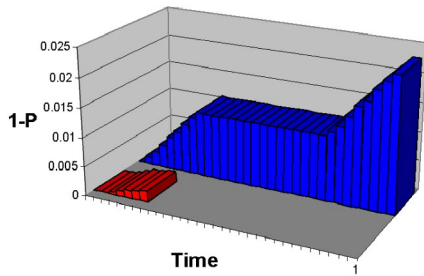


FIG. 2 (color online). Loss of the gate purity $1 - P$ as a function of time [in units of t_0 , where t_0 is the duration of the standard protocol given by Eq. (4)] for the standard five-step (blue or dark gray) and the optimized one-step (red or gray) implementations of the CNOT gate.

slower) purity decay rate, thus decreasing the purity loss $1 - P(t_0)$ by a factor of ≈ 8 .

Finally, we apply our theoretical analysis to the two-qubit Josephson junction setups of Ref. [12] with the parameters $\Delta \sim 10$ GHz and $J \sim 20$ GHz. To that end, we use the experimentally reported single-qubit relaxation rate $1/T_1 = \frac{\pi}{2} S(\Delta)$, which, at the optimal point, was found to be of order ≈ 0.1 GHz [12], thus providing a pertinent value of the dissipative coupling $\alpha \sim 0.01$.

With these parameters at hand, we estimate the loss of purity occurring in the course of implementing the above equivalent of the B gate as $1 - P_B(t_0) \approx 0.03$. However, this estimate would hold only for temperatures above ~ 0.1 K (albeit smaller than Δ), since at still lower temperatures decoherence is believed to be dominated by the non-Ohmic (most likely, $1/f$) noise which, in contrast to the Ohmic one, can not be treated within the Bloch-Redfield approach [3].

In the case of the before mentioned equivalent of the CNOT gate, one would obtain $1 - P_{\text{CNOT}}(t_0) \approx 0.15$, which compares favorably with the experimental result $1 - P_{\text{CNOT}}(t_0) \approx 0.27$ reported in Ref. [12]. However, our theoretical prediction still falls too short of the maximally acceptable error rate $\sim 10^{-4}$, which can be tackled with the existing error-correction codes. Therefore, we surmise that a further significant improvement would be impossible without making a conscience effort towards the engineering of a coherence-friendly environment and reducing the parameter α itself.

In the context of the superconducting qubits, achieving the latter goal requires an aggressive suppression of the Ohmic noise in measuring circuits by eliminating stray inductive and capacitive couplings, avoiding accidental environmental resonances, and attaining the lowest operating temperatures. Moreover, real progress would be unlikely without further advances in materials preparation with the aim at quenching the local fluctuators (e.g., bistable trapped charges) believed to be the source of the $1/f$ -noise.

It should be noted, however, that the authors of Ref. [12] attributed the loss of purity measured in their work solely to the errors in controlling the shape of the operation pulses (finite rise/fall time). In this regard, our optimized protocols take the advantage of a reduced (quadratic, as opposed to a generic linear) sensitivity on variations of the control parameters near the optimal value. In particular, we find that in order to keep $1 - P(t_0)$ under the 10^{-4} threshold the tolerance limit of (de)tuning of the optimized CNOT and B gates' parameters has to be better than 0.3% of their values.

Before concluding, it is worth mentioning that our approach differs from the previous proposals for constructing "supercoherent" qubits which, while being capable of providing an exponential suppression of decoherence, require at least four physical qubits which are governed by the Hamiltonian that conserves total spin [13]. Apart from a larger number of physical qubits required to encode a

logical one, the condition of spin-rotational invariance of the Hamiltonian is unlikely to be fulfilled in any realistic solid-state qubits where (contrary, e.g., to liquid-state NMR designs) the instantaneous values of the single- and two-qubit terms in Eq. (2) are often related, thus resulting in the local terms ($\vec{B} \neq 0$) which break the spin-rotational invariance.

To summarize, we present a systematic approach to constructing simplified (single-step) and highly robust implementations of various two-qubit universal gates. The increased stability against decoherence is achieved, thanks to the choice of the Hamiltonian parameters that provide for the degeneracies in the instantaneous energy spectrum, thereby resulting in the suppression of relaxation processes. Finally, we anticipate that due to a general nature of the energy exchange-related decoherence suppression mechanism exploited in this work it might be possible to extend our results to combinations of elementary two-qubit as well as irreducible many-qubit gates.

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- [1] D.P. DiVincenzo, Phys. Rev. A **51**, 1015 (1995); A. Barenco *et al.*, Phys. Rev. Lett. **74**, 4083 (1995); D. Deutsch, A. Barenco, and A. Ekert, Proc. R. Soc. A **449**, 669 (1995).
 - [2] A. O. Niskanen *et al.*, Phys. Rev. A **67**, 012319 (2003); A. O. Niskanen, J. J. Vartiainen, and M. M. Salomaa, Phys. Rev. Lett. **90**, 197901 (2003); J. J. Vartiainen *et al.*, Int. J. Quantum. Inform. **2**, 1 (2004).
 - [3] K. Blum, *Density Matrix Theory and Applications* (Plenum, New York, 1981); U. Weiss, *Quantum Dissipative Systems* (World Scientific, Singapore, 1999).
 - [4] J. F. Poyatos, J. I. Cirac, and P. Zoller, Phys. Rev. Lett. **78**, 390 (1997).
 - [5] I. A. Grigorenko and D. V. Khveshchenko, Phys. Rev. Lett. **94**, 040506 (2005).
 - [6] J. Q. You, Xuedong Hu, and Franco Nori, cond-mat/0407423 [Phys. Rev. B (to be published)]; M. J. Storz *et al.*, Phys. Rev. B **72**, 064511 (2005); Y. S. Weinstein and C. S. Hellberg, Phys. Rev. A **72**, 022331 (2005).
 - [7] Jun Zhang *et al.*, Phys. Rev. Lett. **91**, 027903 (2003); **93**, 020502 (2004); Phys. Rev. A **67**, 042313 (2003); **69**, 042309 (2004).
 - [8] D. Vion *et al.*, Science **296**, 886 (2002); C. Rigetti and M. Devoret, J. Low Temp. Phys. **139**, 175 (2005).
 - [9] J. E. Mooij *et al.*, Science **285**, 1036 (1999); I. Chiorescu *et al.*, Nature (London) **431**, 159 (2004).
 - [10] K. M. Romero, S. Kohler, and P. Hanggi, cond-mat/0409774 [Phys. Rev. Lett. (to be published)].
 - [11] Z.-W. Zhou *et al.*, Phys. Rev. Lett. **93**, 010501 (2004).
 - [12] Y. A. Pashkin *et al.*, Nature (London) **421**, 823 (2003); T. Yamamoto *et al.*, *ibid.* **425**, 941 (2003); O. Astafiev *et al.*, Phys. Rev. Lett. **93**, 267007 (2004).
 - [13] D. Bacon, K. R. Brown, and K. B. Whaley, Phys. Rev. Lett. **87**, 247902 (2001).