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Resonant cancellation of off-resonant effects in a multilevel qubit

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Off-resonant effects are a significant source of error in quantum computation. This paper presents a group-theoretic proof that off-resonant transitions to the higher levels of a multilevel qubit can be completely prevented in principle. This result can be generalized to prevent unwanted transitions due to qubit-qubit interactions. A simple scheme exploiting dynamic pulse control techniques is presented that can cancel transitions to higher states to arbitrary accuracy.

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Successful quantum computation depends on the accurate manipulation of the quantum states of the qubits [1]. In practice, qubits are subject to many sources of quantum errors, including thermal fluctuations of the environment [2], unwanted qubit-qubit interactions [3], and the effect of the higher levels in many practical qubit designs [4–6]. This paper proposes a dynamic pulse control technique that efficiently eliminates unwanted off-resonance transitions.

Various schemes to protect the qubit from qubit errors have been proposed that can be divided into two categories. The first one is the quantum error correcting codes [7–14] where the qubit state is encoded by redundant qubits. Different errors project the redundant system into different subspaces that can be determined by measuring the extra qubits. By applying a transformation according to the measurement, the correct qubit state can be restored. This approach relies on large numbers of extra qubits to keep the errors from propagating. The second approach exploits ''bang-bang'' control techniques [15,16] where the dynamics of the qubit and its environment are manipulated by fast pulses that flip the qubit state. As the influence of the environment is averaged out, the qubit evolves in the error-free subspace. This method relies on the ability to apply the pulses rapidly compared with the correlation time of the environment. This is an open loop control method.

A particularly important form of intrinsic qubit errors comes from the off-resonant transitions to the higher levels of a qubit during gate operation. Real qubits are not $S=1/2$ spins that are perfect two-level systems; additional levels always exist that affect the information content of the qubit. The gate operation that is introduced to couple the lowest two states of a qubit almost always induces unwanted couplings between the lowest two states and the higher levels. When the interaction is applied with the frequency $\omega=\omega_2-\omega_1$, resonant transition occurs between the lowest two states; meanwhile, off-resonant transitions to the higher states are also switched on. These transitions deviate the phase and amplitude of the qubit state from perfect Rabi oscillation. Numerical simulations on the superconducting persistent current qubit (pc-qubit) [4,17] show that this deviation can be severe when the unwanted couplings are of the same order as the Rabi frequency.

In this Rapid Communication, we study the effect of the higher levels on qubit dynamics during qubit operation by a group-theoretic approach. We prove that the errors can be completely avoided by applying a time-varying operation Hamiltonian. Then we generalize this result to the qubit-qubit interaction problem, which can be mapped exactly onto the first problem. Extending the idea of dynamic pulse control [15], we design a pulse sequence that cancels the leakage to the higher levels to arbitrary accuracy with $O(N)$ number of pulses, N being the number of higher levels.

The proposed method for protecting quantum information is complementary to quantum error correcting codes and the ''bang-bang'' technique mentioned above. Like the bang-bang method, it has the advantage that it does not require extra qubits to enact. The proposed method protects against a different class of errors from those corrected by the methods of [15], however. Dynamic pulse control can be used in conjunction with quantum error correcting codes and the bang-bang decoupling method.

The off-resonant leakage during gate operation has two significant characteristics. First, unlike the environmental fluctuations that affect the qubit only slightly (less than 10^{-4}) within one operation, the leakage changes the qubit dynamics by an amplitude of roughly ω_{Rabi}/ω_0 and on a time scale $1/\omega_0$ that is much shorter than qubit operation time (about $1/\omega_{Rabi}$). Conventional quantum error correcting codes correct errors that occur with small probability and are not a suitable strategy to cancel these strong off-resonant transitions. Neither can we use the bang-bang method to average this effect out [18] simply by flipping the qubit states, as the flipping pulses induce the same transitions as well. Second, ignoring all interactions with external variables, the leakage is coherent, although the coherent oscillation will collapse since the revival time is too long to be observed due to the large number of transitions of different frequencies [19]. As will now be shown, the coherent nature of the leak-

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age implies that this type of error can be corrected by applying a control sequence that coherently modifies the qubit dynamics.

Consider an N-level quantum system with Hamiltonian $\mathcal{H}_0$, the lowest two states of which are chosen as the qubit states $|\uparrow\rangle$ and $|\downarrow\rangle$. The unitary transformations on this N-dimensional Hilbert space form the N^2-dimensional compact Lie group U(N). Without other interaction, the trajectory of the qubit follows the Abelian subgroup $\{e^{-i\mathcal{H}_0 t}, t \in R\}$.

Now apply to the qubit the perturbation $\mathcal{H}_I$, $[\mathcal{H}_0,\mathcal{H}_I] \neq 0$, to induce a desired transformation of the qubit. In most physical systems, unwanted transitions to the higher levels are simultaneously induced. For example, in the pc-qubit [4] operation, $(\mathcal{H}_I)_{mn}=2\pi\delta f\langle m|\sin(2\phi_m+2\pi f)|n\rangle\cos\omega t$, when the bias flux is modulated with rf components of amplitude δf and frequency ω. This perturbation has couplings between all the energy levels. By successive commutation of $\mathcal{H}_0$, $\mathcal{H}_I$ and their commutators until no independent operator appears, a Lie algebra $\mathcal{A}_I$ is created. In almost all cases, $\mathcal{A}_I = \mathrm{u}(N)$ [20], u(N) being the Lie algebra of U(N). The only exception occurs in a zero measure subspace of u(N) when $\mathcal{H}_I$ and $\mathcal{H}_0$ are both in the same subalgebra of u(N). Thus, with almost all perturbations, the evolution operator can be any element in U(N); and transitions to higher levels are unavoidable, with an initial state that only occupies the lowest two levels.

To prevent transitions to the higher states at time t means to restrict the evolution operator $\mathcal{U}(t)$ to the submanifold of $\mathrm{U}(2)\oplus\mathrm{U}(N-2)$, U(2) being the unitary group on $\{|\uparrow\rangle,|\downarrow\rangle\}$ and U($N-2$) on the remaining $N-2$ states. This applies $4(N-2)$ real domain restrictions on $\mathcal{U}(t)$: $\mathcal{U}(t)_{1k},\mathcal{U}(t)_{2k}=0, k=3,\ldots,N$. In contrast to a perfect qubit operation during which $\mathcal{U}(t)$ remains in the subspace $\mathrm{U}(2)\oplus\mathrm{U}(N-2)$ all the time, the qubit is allowed to stray away from this subspace as far as it can go back to this subspace at the designated time t. The qubit dynamics can be manipulated by varying the strength and phase of the perturbation with time. As the N^2-dimensional Lie group U(N) is compact, any transformation can be reached at time t by adjusting the N^2+1 parameters in the following process [20]:

$$\mathcal{U}(t)=e^{-i\alpha\mathcal{H}_I t_{N^2}}e^{-i\alpha\mathcal{H}_0 t_{N^2-1}}\cdots e^{-i\alpha\mathcal{H}_0 t_1}, \qquad (1)$$

where α is introduced to ensure that $t=\Sigma t_i$. By playing with the N^2+1 real parameters, the $4(N-2)$ real numbers in $\mathcal{U}(t)_{1k},\mathcal{U}(t)_{2k}$ can be set to zero so that the state of the qubit stays in the $\{\uparrow,\downarrow\}$ space without leakage. Hence by turning the perturbation on and off $O(N^2)$ times, the lowest two states are completely decoupled from the higher states. $O(N^2)$ pulses give a sufficient condition that is required to achieve arbitrary transformation. As will be shown later in this Rapid Communication, with the proper arrangement, we can design a pulse sequence of $O(N)$ pulses to cancel the transitions to the higher levels. Furthermore, these pulses can be superposed to make a single shaped pulse, as in [21,16], that average out the unwanted transitions. For a given driven power per unit frequency, the length of the shaped pulse is independent of the number of higher levels. Unlike that in the quantum Zeno effect [22] where measurement is used to prevent the system from evolving, the dynamics in this process is described completely by unitary evolutions.

As the unwanted transitions are off-resonant transitions whose amplitudes decrease roughly as γ_{ij}/ω_i (ω_i is the energy of the ith level, γ_{ij} the coupling between level i and j), the influence of the levels with $\omega_i/\omega_0 \gg 1$ can be ignored. In the pc-qubit [4] the energies of the lower levels increase fast enough ($\omega_{10} > 10\omega_0$) that levels beyond $|10\rangle$ can be ignored. The energy of the ith level of the charge state qubit [5] increases as i^2; fewer levels affect the qubit dynamics than that in the pc-qubit. Hence the number N of the higher states involved in the qubit dynamics in real designs can be reasonably small. As a result, the number of pulses in the previous analysis is also reasonable.

One question to ask is whether there is any fundamental difference between the errors due to transitions to the higher levels and those due to the fluctuations of environmental variables. Putting it in another way: what is the difference between the intraqubit coupling in a multilevel qubit and the qubit-external-system coupling? In the following we will show that the N-level qubit can be mapped into interacting subsystems, and vice versa.

Let the initial state of an N-level qubit be $|\Psi_0\rangle=\alpha_1^{(0)}|1\rangle+\alpha_2^{(0)}|2\rangle$, $|1\rangle$ and $|2\rangle$ being the lowest two states. To map the qubit into two subsystems, we divide the N states into two subspaces SP_1 and SP_2 by adding the vacuum states $|V_1\rangle$ and $|V_2\rangle$ to the respective subspaces as $SP_1=\{|V_1\rangle,|1\rangle,|2\rangle\}$ and $SP_2=\{|V_2\rangle,|3\rangle,\ldots,|N\rangle\}$. Now the N-dimensional Hilbert space of the original qubit is embedded in the $3(N-1)$-dimensional direct product space $SP_1\otimes SP_2$. The states in the expanded space are $|\Psi\rangle=\Sigma_{i,j}\beta_{i,j}|b_i^{(1)}\rangle|b_j^{(2)}\rangle$, where $b_i^{(1)}$ and $b_j^{(2)}$ are the bases of the two subspaces, respectively. The initial state is $|\Psi_0\rangle=(\alpha_1^{(0)}|1\rangle+\alpha_2^{(0)}|2\rangle)|V_2\rangle$ in the expanded form. The unitary transformations in this expanded space form the group U($3(N-1)$).

Perturbation introduces couplings between different states. When mapped to the expanded space, the perturbation $\overline{\mathcal{H}_I}$ connects states in the N-dimensional subspace spanned by $\{|1\rangle|V_2\rangle,|2\rangle|V_2\rangle,|V_1\rangle|3\rangle,\ldots,|V_1\rangle|N\rangle\}$. So $\overline{\mathcal{H}_I}$ and $\overline{\mathcal{H}_0}$ create N^2-dimensional subalgebra u(N) in the expanded space. Under the perturbation, the wave function in the expanded space can be described as $|\overline{\Psi}\rangle=(\alpha_1|1\rangle+\alpha_2|2\rangle)|V_2\rangle+\Sigma_{i=3}^{N}\alpha_i|V_1\rangle|i\rangle$, where α_i are time-dependent parameters evolving with the perturbation.

From this analysis, the higher levels in the qubit form an effective environment that interferes *strongly* with the lowest two levels. Interaction strength and spectrum density are the major differences between this effective environment and a real one [4]. The couplings between SP_1 and SP_2 are strong and comparable to the Rabi coupling that realizes qubit operation. In contrast, the interactions between the environmental oscillators and the qubit are weak due to the $O(1/\sqrt{V})$ factor that originates from the normalization of the extended modes [2]. So the thermal fluctuations are not enslaved to the qubit dynamics and can be treated classically. The strong

interaction with the higher levels also explains why the error due to leakage occurs at such a short time that a particular strategy other than the bang-bang technique is required to correct this error. The spectrum density of a real environment is continuous with macroscopic degrees of freedom, while for the higher states, the spectrum is discrete. Another thing to mention is that this effective environment only comes with qubit operation, while the real environment affects the qubit all the time. Hence we worry about the leakage only during qubit operation and choose to correct the leakage by controlling the operation process.

Note that interacting qubits can be modeled as one multilevel quantum system by reversing the above mapping. This implys that errors due to qubit-qubit interactions [3] can be treated with the proposed method. Off-resonant effects are significant in existing NMR quantum computers, and techniques analogous to the ones suggested have been developed to correct unwanted transitions [21]. Although the number of levels grows exponentially with the number of qubits [23], because the two-qubit couplings in NMR are relatively weak, effective decoupling procedures only require that the number of pulses be polynomial in the number of qubits and the complexity of a single shaped pulse also be polynomial in the number of qubits.

To illustrate the general idea of dynamic pulse control, we give an example of a pulse sequence that completely cancels the transitions to the higher levels with $O(N)$ pulses. Let us start from a three-level system with eigenvalues ω_i, $i=1,2,3$. The energy difference between level i and j is ω_{ij}. An interaction $\mathcal{H}_I$ that couples level i and j by γ_{ij} is applied to the qubit. When the third level is not present, γ_{12} is the Rabi frequency of the lowest two states. For simplicity, we ignore the diagonal couplings γ_{ii} as $\gamma_{ii} \ll \omega_i$. As will become clear, the effectiveness of the designed pulse sequence depends on the condition $|\gamma_{ij}/\omega_{ij}| \ll 1$, which is satisfied in most qubit designs.

The Hamiltonian in the interaction picture is $\mathcal{H}_{int} = e^{i\mathcal{H}_0 t}\mathcal{H}_I e^{-i\mathcal{H}_0 t}\cos(\omega t+\phi)$, ω being the pulse frequency. The wave function $\Psi(t)=[u\ v\ w]^T$ evolves according to the equation $i[\partial\Psi(t)/\partial t]=\mathcal{H}_{int}\Psi(t)$. When the perturbation is weak, this equation is integrated order by order as:

$$\Psi(t)=\Psi(0)+\int_0^t dt'\mathcal{H}_{int}(t')\Psi(0) + \int_0^t dt'\int_0^{t'} dt''\mathcal{H}_{int}(t')\mathcal{H}_{int}(t'')\Psi(0)+\cdots. \quad (2)$$

The cosine function is used in the rf pulse instead of a single frequency wave. In many systems, no physical correspondence of the circularly polarized wave exists. For example, the circuit of the pc-qubit is biased by z direction magnetic flux and the perturbation is high-frequency modulation of the z flux.

Our strategy to reduce the unwanted transitions is to divide the qubit operation into short intervals of t_0 and attach additional pulses to each operation pulse to correct errors from this short interval. The operation pulse is in resonance with ω_{21} of the lowest two states. Besides rotating the qubit between the level 1 and 2, it brings up off-resonant transitions between the third level and these two levels by the couplings γ_{13} and γ_{23}. Then the same perturbation is applied in two other pulses with different frequencies, amplitudes, and phases as $\alpha_{31}\mathcal{H}_I\cos(\omega_{31}t+\phi_{31})$ and $\alpha_{32}\mathcal{H}_I\cos(\omega_{32}t+\phi_{32})$, both for time t_0, to cancel the unwanted transitions to the third level. This three-piece sequence is repeated τ_{op}/t_0 times to finish the qubit operation. The time t_0 satisfies $1/\omega \ll t_0 \ll 1/\gamma_{ij}, i,j=1,2,3$, with both $1/\omega_{21}t_0$ and $\gamma_{ij}t_0$ being small parameters of the same order. Thus we have two small parameters in this procedure. This is crucial for this simple pulse sequence to work.

Starting with an initial wave function $\Psi(0)=[u_0\ v_0\ w_0]^T$, $w_0=0$, after the ω_{21} pulse, the third level has the component

$$w = u_0\left(\frac{\gamma_{13}^*(e^{-i(\omega_{21}-\omega_{31})t_0}-1)}{\omega_{21}-\omega_{31}} - \frac{\gamma_{13}^*(e^{i(\omega_{21}+\omega_{31})t_0}-1)}{\omega_{21}+\omega_{31}}\right) + v_0\left(\frac{\gamma_{23}^*(e^{-i(\omega_{21}-\omega_{32})t_0}-1)}{\omega_{21}-\omega_{32}} - \frac{\gamma_{23}^*(e^{i(\omega_{21}+\omega_{32})t_0}-1)}{\omega_{21}+\omega_{32}}\right) + u_0\theta_u + v_0\theta_v, \quad (3)$$

where θ_u and θ_v are of third order. The main components in w are second-order terms that depend on the initial condition u_0 and v_0 linearly. With t_0 satisfying $e^{2i\omega_{21}t_0}=1$, u and v have third-order deviations from the desired two-level rotation. The other two pulses are applied to cancel the w component. The ω_{31} pulse induces a resonant transition between levels one and three to cancel the u_0 term; the ω_{32} pulse induces a resonant transition between levels two and three to cancel the v_0 term. The amplitudes and phase shifts of these two pulses can be expanded in ascending order as

$$\alpha_{31}e^{i\phi_{31}} = \alpha_{31}^{(1)}e^{i\phi_{31}^{(1)}} + \alpha_{31}^{(2)}e^{i\phi_{31}^{(2)}} + \cdots, \qquad \alpha_{32}e^{i\phi_{32}} = \alpha_{32}^{(1)}e^{i\phi_{32}^{(1)}} + \alpha_{32}^{(2)}e^{i\phi_{32}^{(2)}} + \cdots. \quad (4)$$

The first-order coefficients cancel the second-order terms in w and modify the higher-order terms θ_u and θ_v when

$$\alpha_{31}^{(1)}e^{i\phi_{31}^{(1)}} = \frac{e^{-i(\omega_{21}-\omega_{31})t_0}-1}{i(\omega_{21}-\omega_{31})t_0} - \frac{e^{i(\omega_{21}+\omega_{31})t_0}-1}{i(\omega_{21}+\omega_{31})t_0}, \qquad \alpha_{32}^{(1)}e^{i\phi_{32}^{(1)}} = \frac{e^{-i(\omega_{21}-\omega_{32})t_0}-1}{i(\omega_{21}-\omega_{32})t_0} - \frac{e^{i(\omega_{21}+\omega_{32})t_0}-1}{i(\omega_{21}+\omega_{32})t_0}. \quad (5)$$

It turns out that the nth-order terms of w after the correction pulses include linear terms of $\alpha_{31}^{(n-1)}$ and $\alpha_{32}^{(n-1)}$ and complicated terms that depend on $\alpha_{3i}^{(k)}e^{i\phi_{3i}^{(k)}}$ $[k=1,\ldots,(n-2)]$. So, for any n, $\alpha_{31}^{(n-1)}$ and $\alpha_{32}^{(n-1)}$ can be determined by the lower-order components of α_{31} and α_{32} to cancel the nth order of w. As a result, transitions to the third level can be completely erased. The parameters α_{31} and α_{32} do not depend on the initial condition u_0 and v_0. This is similar to solving the wave function in the perturbation theory where the higher-order terms are derived after the lower-order ones.

After the kth pulse sequence, with $w=0$, the wave function is

$$\begin{bmatrix} u_{k+1} \\ v_{k+1} \end{bmatrix} = \begin{bmatrix} \cos\bar{\varphi}+\bar{s}_u & -i\sin\bar{\varphi}+\bar{t}_u \\ -i\sin\bar{\varphi}+\bar{t}_v & \cos\bar{\varphi}+\bar{s}_v \end{bmatrix} \begin{bmatrix} u_k \\ v_k \end{bmatrix}, \quad (6)$$

where $\bar{\varphi}=\gamma_{12}t_0$ is the phase rotation of the two-level qubit; the $\bar{s}$ and $\bar{t}$ terms are of third-order. As $w=0$, this is a unitary transformation that deviates from Rabi oscillation by third order corrections. The matrix can be written as $\mathcal{U}(t_0)=\exp[-i(\gamma_{12}\sigma_x+\delta_0+\Sigma_i\delta_i\sigma_i)t_0]$, where δ_i are third-order small numbers that can be determined by known parameters and do not depend on the index k. This is a renormalization of the qubit operation γ_{12} with the third level decoupled.

This correction strategy is easily generalized to the $N(N\geqslant 3)$ level system. By applying rf pulses with frequencies ω_{i1},ω_{i2}, $i=3\ldots N$, the transitions to the higher levels are completely erased. Assuming no particular symmetry between the states, $2(N-2)$ pulses are required in this process.

One may wonder why this simple pulse sequence works so well to correct the off-resonant transitions to the higher states. For $N-2$ higher levels, to decouple these levels is to exert $4(N-2)$ real domain restrictions on the transformation matrix: $\mathcal{U}_{1i},\mathcal{U}_{2i}=0$, $i=3,\ldots,N$. Our tools are the Hamiltonians $\mathcal{H}_0$ and $\mathcal{H}_I$ that create the whole u(N) algebra by commutation. Our pulse sequence $\mathcal{U}(t_0)=\Pi_{i,\beta}P(\alpha_{i\beta},\phi_{i\beta})\exp(-i\int\mathcal{H}_I\cos\omega_{21}t'dt')$ $(i=3,\ldots,N$ and $\beta=\uparrow,\downarrow)$, $P(\alpha_{i\beta},\phi_{i\beta})=\exp[-i\int\mathcal{H}_I\alpha_{i\beta}\cos(\omega_{i\beta}t'+\phi_{i\beta})dt']$, contents $4(N-2)$ free parameters. By choosing proper pulse sequences, we can achieve the decoupling with proper pulse parameters.

In conclusion, we discussed the errors due to unwanted transitions to the higher states of a qubit during qubit operation. It was shown by a group-theoretic argument that these errors can be completely prevented in principle. Then we generalized the result to the errors due to qubit interactions, which can also be prevented when the number of coupled qubits is not too large. A simple pulse sequence that modifies the qubit dynamics and cancels off-resonant transitions to arbitrary accuracy with $O(N)$ pulses was proposed to illustrate the general analysis. Our results showed that the idea of dynamic pulse control [15] also works for the fast gate errors due to off-resonant transitions to the higher states of a qubit. These results suggest that dynamic pulse control, together with conventional quantum error correcting codes, can function as a powerful tool for performing accurate quantum computation in the presence of errors.

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