Physical Origins of Gate Errors in Transmon Qubits

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We derive a physical model for single-qubit gates on superconducting transmon qubits of the type found in IBM Quantum Experience devices, incorporating angle, phase and off-resonance errors. We show how to leverage the model to experimentally determine these errors using novel techniques on IMBQ OpenPulse-enabled backends instructions. This allows us to calculate more precisely the major source of error in specific circuits, rather than using averaged approximations to gate fidelity from Randomized Benchmarking experiments. We present some applications and compare to experimental data to examine whether Pauli gates give an accurate representation of gate fidelities in a quantum device.

I. INTRODUCTION

The field of Quantum Computing has recently emerged as a practical realisation of decades of research in Quantum Information Theory, promising us algorithms that can suppress time complexity exponentially for certain problems [1], and provide smaller speedups for wider classes of problems [2]. In this sense, Quantum Computers threaten to revolutionize computing in academic contexts and beyond.
Superconducting Quantum Computing (SQC) is one of the more promising contemporary efforts to implement a physical Quantum Computer, a so-called Noisy Intermediate-Scale Quantum Computer (NISQ). In this paper, we examine the Hamiltonian of a widely-studied implementation of SQC, using transmon qubits driven by AWG microwaves pulses acting as the gates.
This work represents the first cohesive analytic account of the manifestation of gate error from physical miscalibration of a quantum device; it necessary to understand and accurately predict the error in common gates from first principles. We shall show gate errors can vary significantly over gate parameters in surprising ways; this furthers the work of [3] to cast doubt on the ability of Randomized Benchmarking (RB) to reliably assess the fidelity of particular circuits.

II. THEORETICAL RESULTS

A. Background

Single qubit gates on transmon qubits are implemented with a periodic monochromatic microwave drive pulse with angular frequency ω_d and phase offset γ; wlog take the electric field component to be

$$\mathbf{E}(\mathbf{t}) = \mathbf{E_0}(\mathbf{t})\cos(\omega_\mathbf{d}\mathbf{t} + \gamma), \tag{1}$$

where $\mathbf{E_0}(\mathbf{t}) \in \mathbb{R}^\mathbf{3}$.
The theoretical ideal drive pulse Hamiltonian in the Rotating Wave Approximation (RWA) is then easily derived as in the open-source Qiskit textbook [4]

$$\hat{H} = \frac{\hbar\delta\omega}{2}\hat{\sigma}_z + \frac{\hbar\Omega_R(t)}{2}(\cos(\gamma)\hat{\sigma}_x + \sin(\gamma)\hat{\sigma}_y), \tag{2}$$

where:

- $\Omega_R(t) \propto \|\mathbf{E_0}(\mathbf{t})\|_\mathbf{2}$ is known as the *Rabi Frequency.*
- $\delta\omega := \omega_{01} - \omega_d$, where $\omega_{01} = E(|0\rangle \to |1\rangle)/\hbar$.
- $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ are the Pauli operators.

By varying γ, we can implement an arbitrary U_2 gate. This leaves us to choose ω_d and $\Omega_R(t)$ (via $\mathbf{E_0}(\mathbf{t})$), as well as the total duration of the pulse, to maximise gate fidelity. From recent theory, we should choose $\omega_d = \omega_{01}$, a short pulse duration (to minimise circuit duration, and hence time-dependent errors) and $\Omega_R(t)$ as a DRAG pulse. This is for purposes of minimising *leakage* to higher energy states[5][6]. For ease of calculation, let's assume $\Omega_R(t)$ is constant, so that

$$\theta := 2E_C\left(\frac{E_J}{8E_C}\right)^{1/4}\int_0^T \Omega_R(t)\mathrm{d}t \tag{3}$$

$$= 2E_C\left(\frac{E_J}{8E_C}\right)^{1/4}\Omega T \tag{4}$$

where E_C and E_J are the Cooper Box and Josephson Junction energies respectively. In general, θ is calibrated [7][8][9] Then an ideal single resonant pulse with no errors

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($\delta\omega = 0$) gives the gate

$$U = e^{-i\hat{H}(\delta\omega=0)} \text{ by TDSE} \tag{5}$$
$$= e^{-i\frac{\theta}{2}\left(\cos(\gamma)\hat{\sigma}_x + \sin(\gamma)\hat{\sigma}_y\right)} \tag{6}$$
$$= \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2)e^{-i\gamma} \\ -i\sin(\theta/2)e^{i\gamma} & \cos(\theta/2) \end{pmatrix} \text{ up to a phase} \tag{7}$$
$$= Z(\gamma)\cdot X(\theta)\cdot Z(-\gamma), \tag{8}$$

where we take $\hbar = 1$ wlog, and $X(\cdot), Z(\cdot)$ are the Pauli rotations; considering (ufactors) from this perspective, this demonstrates that U is universal for single-qubit gates [10].

B. General Theoretical Results

C. Noise Results

Then the noisy version of this gate, adding in errors $\delta\theta$ and $\delta\gamma$ (henceforth referred to as *angle error* and *phase error* respectively), is

$$\tilde{U}(\gamma) = e^{-\frac{i}{2}\left[\delta\omega\hat{\sigma}_z + (\theta+\delta\theta)\left(\cos(\gamma+\delta\gamma)\hat{\sigma}_x + \sin(\gamma+\delta\gamma)\hat{\sigma}_y\right)\right]} \tag{9}$$

Now let

$$\boldsymbol{\rho}(\gamma) := \begin{pmatrix} (\theta+\delta\theta)\cos(\gamma+\delta\gamma) \\ (\theta+\delta\theta)\sin(\gamma+\delta\gamma) \\ \delta\omega \end{pmatrix}, \text{ so that} \tag{10}$$
$$\tilde{U}(\gamma) = e^{-i\frac{\boldsymbol{\rho}(\gamma)\cdot\boldsymbol{\sigma}}{2}} \tag{11}$$
$$= \cos\left(\frac{\Delta}{2}\right)\mathbb{1}_2 - i\sin\left(\frac{\Delta}{2}\right)\hat{\boldsymbol{\rho}}(\gamma).\boldsymbol{\sigma}, \tag{12}$$

Where we have set $\boldsymbol{\rho}(\gamma) = \Delta\hat{\boldsymbol{\rho}}(\gamma)$, for $\Delta = \sqrt{(\theta+\delta\theta)^2 + \delta\omega^2}$ independent of γ and $\left\|\hat{\boldsymbol{\rho}}(\gamma)\right\| = 1$.
Now observe that the Pauli combination in (9) is in the Lie Algebra $\mathfrak{su}(2)$ so $\tilde{U}(\gamma) \in SU(2)$, and by connectedness of $SU(2)$ and hence the surjectivity of $\exp : \mathfrak{su}(2) \to SU(2)$, we may write

We give more explicit results in Appendix A.

D. An Optimality Result

We now note that in (8), we can physically implement the γ rotations easily by configuration of the AWG, but θ requires careful calibration via a Rabi Experiment[7][8][9].
Although this procedure effectively provides calibration data for all values of θ [**?**], in real quantum devices we often use just a single value out of practical concerns. We thus examine the necessary and optimal conditions for universal single-qubit computation in this regime.

Theorem 1. *For the noiseless pulse-implemented X-Z* gate sandwich *detailed in (8) with a single calibrated value of* θ*,*

(i) $\theta = \frac{(2k+1)\pi}{n} \in (0, 2\pi)$ *(for some positive integers* $k < n$ *) is necessary to achieve universal single-qubit computation.*

(ii) For this θ*,* $n \geq 2$ *such pulses are necessary and sufficient for the most general single-qubit gate.*

Proof. (i) Suppose we wish to implement $X(\pi)$ starting from $|0\rangle$ on the Bloch Sphere. Clearly any such implementation may not have any Z rotations in its *X-Z gate sandwich*. Hence we require $X(\theta)^n \equiv X(\pi)$ up, whence $\theta = \frac{(2k+1)\pi}{n}$, where we take $k < n$ to keep $\theta \in (0, 2\pi)$ and $\gcd(2k+1, n) = 1$ wlog.

(ii) Consider the most general single-qubit gate $U3 \in \mathrm{PU}(2) \cong \mathrm{SO}(3)$, where the isomorphism is apparent when considering the action of the gate on the Bloch sphere. We adopt the parameterization

$$U3(\phi,\chi,\psi) = \begin{pmatrix} \cos(\frac{\phi}{2}) & -e^{i\psi}\sin(\frac{\phi}{2}) \\ e^{i\chi}\sin(\frac{\phi}{2}) & e^{i(\chi+\psi)}\cos(\frac{\phi}{2}) \end{pmatrix} \tag{13}$$

This group has three real degrees of freedom, but suppose we were to implement k such gates in succession. Then via the factorization

$$U3(\phi,\chi,\psi) = Z(\chi)X(\frac{\pi}{2})Z(\pi+\phi)X(\frac{\pi}{2})Z(\psi+\pi), \tag{14}$$

we see that for adjacent gates, one free parameter from each gate may be combined into a single Z gate, collapsing to one effective degree of freedom. The final Z-gate in the final $U3$ does not affect the measurement statistics for a Pauli-Z measurement. Hence each gate has 2 effective degrees of freedom, and each pulse from 8 has 1, so $n \geq 2$ is necessary. This is also sufficient for $n = 2$ by 14, and for higher values of n by the following construction. ¡¡Insert here¿¿

□

Corollary 1. *Suppose we have calibrated* $\theta = \{\alpha_1, \alpha_2, ..., \alpha_k\}$*. Then the existence of* $n_i \in \boldsymbol{N}$ *such that* $\sum_{i=1}^{k} n_i\alpha_i = \pi$ *is a necessary condition for universal quantum computation.*

We also make the following remark for the case $\theta = \frac{\pi}{2}$, which is the *optimal* value in the above sense.

Remark 1. *The following are the only factorizations of* $U3$ *into the* $X(\frac{\pi}{2})Z(\cdot)$ sandwich*, and hence define all implementations of* $U3$ *with pulses of the form* $U(\gamma)$

$$U3^{(1)}(\phi,\chi,\psi) = Z(\chi+\pi)X(\frac{\pi}{2})Z(\phi+\pi)X(\frac{\pi}{2})Z(\psi) \tag{15}$$

$$U3^{(2)}(\phi,\chi,\psi) = Z(\chi)X(\frac{\pi}{2})Z(\pi-\phi)X(\frac{\pi}{2})Z(\psi+\pi) \tag{16}$$

Proof is constructive, and in Appendix B.

E. Implementation-Specific Noise Results

We now develop the theory for implementation on real quantum devices under some assumptions.
The errors $\delta\theta, \delta\omega$ depend on calibration experiments which are subject to errors. If we assume θ is calibrated to some constant value, and observe that $\delta\omega = \omega_{01} - \omega_d$ where ω_d is calibrated to some fixed value and ω_{01} does not drift quickly from the value measured at the time of calibration, we may assume that **assume that $\delta\theta$ and $\delta\omega$ are constant** over a sufficiently short time period.
The error $\delta\gamma$ can only be caused by a miscalibration of the AWG responsible for the drive pulse; correspondingly $\delta\gamma$ should be much smaller, and we can safely assume it is caused by a *systematic bias* rather than stochastic noise; correspondingly, we **also assume $\delta\gamma$ is constant**.

F. Gate Error Results

Assume we now have some fixed $\theta = \alpha$. Under the assumptions above, We calculate $\tilde{\mathcal{P}}(\alpha)$, the noisy probability of measuring $|0\rangle$ from $\tilde{U}(\gamma_1) \cdot \tilde{U}(\gamma_2)|0\rangle$

1. $U2(\phi)$

We adopt the following parameterization

$$U2(\phi, \chi) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{i\chi} \\ e^{i\phi} \\ e^{i(\phi+\chi)} \end{pmatrix} \tag{17}$$

So that we may implement $X\left(\frac{\pi}{2}\right)$ as $\tilde{U}(0)$. The probability of measuring $|0\rangle$ after $2n$ applications is then

$$\tilde{X}\left(\frac{\pi}{2}\right) \tag{18}$$

In particular, the error on

2. $U3(\phi)$

The following error probabilities arise from defining pulse schedules using equations (15) - (16) respectively:

$=$

$=$

3. X(ϕ)

We have that $X(\phi) = U3(\phi, -\frac{\pi}{2}, \frac{\pi}{2})$ only. We implement $\tilde{X}(\phi)$ by the 2 possible decompositions from (15) and (16):

$$\tilde{X}^{(1)}(\phi) = \tilde{U}\left(\frac{\pi}{2} - \phi\right)\tilde{U}\left(-\frac{\pi}{2}\right) \tag{19}$$

$$\tilde{X}^{(2)}(\phi) = \tilde{U}\left(\phi - \frac{\pi}{2}\right)\tilde{U}\left(\frac{\pi}{2}\right) \tag{20}$$

Giving ϕ-dependent error probabilities $\cos^2(\phi/2)\delta\alpha \pm \frac{2\sin(\phi)}{\pi}\delta\omega$ to first order, respectively.

4. $Y(\phi)$

III. EXPERIMENTAL RESULTS

We now demonstrate experimental evidence for the above, as well as a novel use of our results to measure error sources experimentally.

A. Non-Uniform Errors in $X(\phi)$

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B. Angle Error via Fourier Transforms

We use the result in [11] that sufficiently small ORRs are correctable.

C. Errors in Repeated X-gates

Appendix A: Derivation of $\tilde{U}$

We obtain an explicit element-wise expression for $\tilde{U}$ and a Taylor series in $\delta\theta$ and $\delta\omega$ to illustrate the perturbative effects of error

$$\tilde{U}_{11}(\gamma) = \cos\left(\frac{\Delta}{2}\right) - i\frac{\delta\omega}{\Delta}\sin\left(\frac{\Delta}{2}\right) \tag{A1}$$

$$= U_{11} - \left[\frac{\sin(\theta/2)}{2}\delta\theta + \frac{\sin(\theta/2)}{\theta}\delta\omega i\right] \tag{A2}$$

$$- \left[\frac{\sin(\theta/2)}{8}\delta\omega^2 + \frac{\cos(\theta/2)}{8}\delta\theta^2 + \left(\frac{\cos(\theta/2)}{2\theta} - \frac{\sin(\theta/2)}{\theta^2}\right)\delta\theta\delta\omega i\right] \tag{A3}$$

$$- \dots$$

$$\tilde{U}_{12}(\gamma) = (\theta+\delta\theta)\sin\left(\frac{\Delta}{2}\right)e^{-i\left(\gamma+\delta\gamma+\frac{\pi}{2}\right)} \tag{A4}$$

$$= U_{12}e^{-i\delta\gamma} \tag{A5}$$

$$+ \cos(\theta/2)\delta\theta e^{-i\left(\gamma+\delta\gamma+\frac{\pi}{2}\right)} \tag{A6}$$

$$- \left[\left(\frac{\sin(\theta/2)}{\theta^2} - \frac{\cos(\theta/2)}{2\theta}\right)\delta\omega^2 + \frac{\sin(\theta/2)}{4}\delta\theta^2\right]\frac{e^{-i\left(\gamma+\delta\gamma+\frac{\pi}{2}\right)}}{2} \tag{A7}$$

$$+ \dots$$

For the remaining terms, recall $\tilde{U}(\gamma) \in SU(2)$ (**??**) and hence

$$\tilde{U}_{11}(\gamma) = \tilde{U}_{22}(\gamma)^* \tag{A8}$$

$$\tilde{U}_{12}(\gamma) = -\tilde{U}_{21}(\gamma)^* \tag{A9}$$

In the case $\theta = \frac{\pi}{2}$ used in many IBMQ backends this simplifies (A2) - (A7) to:

$$\tilde{U}_{11}(\gamma) = U_{11}$$

$$- \sqrt{2}\left[\frac{\delta\theta}{4} + \frac{i}{\pi}\delta\omega\right] \tag{A10}$$

$$- \sqrt{2}\left[\frac{\delta\omega^2+\delta\theta^2}{16} + \left(\frac{i(\pi-4)}{2\pi^2}\right)\delta\theta\delta\omega\right] \tag{A11}$$

$$- \dots$$

$$\tilde{U}_{12}(\gamma) = U_{12} \tag{A12}$$

$$+ \frac{e^{-i\left(\gamma+\delta\gamma+\frac{\pi}{2}\right)}\delta\theta}{\sqrt{2}} \tag{A13}$$

$$- \frac{e^{-i\left(\gamma+\delta\gamma+\frac{\pi}{2}\right)}}{\sqrt{2}}\left[\frac{4-\pi}{2\pi^2}\delta\omega^2 + \delta\theta^2\right] \tag{A14}$$

$$+ \dots$$

¡¡¡TO DELETE¿¿¿ We examine $\tilde{H}$, the matrix in square brackets in (9)

$$\tilde{H} = \begin{pmatrix} \delta\omega & (\theta+\delta\theta)\,e^{-i(\gamma+\delta\gamma)} \\ (\theta+\delta\theta)e^{i(\gamma+\delta\gamma)} & -\delta\omega \end{pmatrix} \tag{A15}$$

$$:= S \cdot J \cdot S^{-1}, \text{ where} \tag{A16}$$

$$S_{11} = \left(\delta\omega - \sqrt{\delta\omega^2 + (\theta+\delta\theta)^2}\right)e^{-i(\gamma+\delta\gamma)} \tag{A17}$$

$$S_{12} = \left(\delta\omega + \sqrt{\delta\omega^2 + (\theta+\delta\theta)^2}\right)e^{-i(\gamma+\delta\gamma)} \tag{A18}$$

$$S_{21} = S_{22} = \theta + \delta\theta \tag{A19}$$

$$J = \operatorname{diag}\left(-\sqrt{\delta\omega^2+(\theta+\delta\theta)^2}, \sqrt{\delta\omega^2+(\theta+\delta\theta)^2}\right). \tag{A20}$$

This gives the result

$$\tilde{H}_{11}^n = \begin{cases} \delta\omega\left(\delta\omega^2 + (\theta+\delta\theta)^2\right)^{\frac{n-1}{2}} & \text{if } n \text{ odd} \\ \left(\delta\omega^2 + (\theta+\delta\theta)^2\right)^{\frac{n}{2}} & \text{if } n \text{ even} \end{cases} \tag{A21}$$

$$\tilde{H}_{12}^n = \begin{cases} e^{-i(\gamma+\delta\gamma)}(\theta+\delta\theta)\left(\delta\omega^2 + (\theta+\delta\theta)^2\right)^{\frac{n-1}{2}} & \text{if } n \text{ odd} \\ 0 & \text{if } n \text{ even} \end{cases} \tag{A22}$$

We then expand $\tilde{U}$ as a series in $\tilde{H}^n$ to obtain the given expansion.

Appendix B: Construction of $U3$ in the case $\theta = \pi/2$

¡¡Add construction of $U3$ from pulses emphasising the restriction to 4 equivalent cases ¿¿

Appendix C: General Method for the Derivation of Probabilities

We additionally present Taylor series for (II F 2)

$$\tilde{\mathcal{P}}(\alpha) = \mathcal{P}(\alpha) \tag{C1}$$

$$+ \sin(\alpha)\left(\sin^2\left(\frac{\gamma_2-\gamma_1}{2}\right) - 3\cos(\alpha)\cos^2\left(\frac{\gamma_2-\gamma_1}{2}\right)\right)\delta\alpha \tag{C2}$$

$$+ \frac{[(1-\cos(\alpha)]\sin(\alpha)\sin(\gamma_2-\gamma_1)}{\alpha}\delta\omega \tag{C3}$$

$$+ \dots \tag{C4}$$

Where $\mathcal{P}(\alpha) = 1 - \sin^2(\alpha)\cos^2\left(\frac{\gamma_2-\gamma_1}{2}\right)$ is the error-free result. In particular, now proceeding with the optimal $\alpha = \frac{\pi}{2}$ for the remainder of the section,

$$\tilde{\mathcal{P}}\left(\frac{\pi}{2}\right) = \mathcal{P}\left(\frac{\pi}{2}\right) + \sin^2\left(\frac{\gamma_2-\gamma_1}{2}\right)\delta\alpha + \frac{2\sin(\gamma_2-\gamma_1)}{\pi}\delta\omega + \dots \tag{C5}$$

Where $\mathcal{P}\left(\frac{\pi}{2}\right) = \frac{1-\cos(\gamma_2-\gamma_1)}{2}$ is the error-free result.

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