Towards ultra-high fidelity quantum operations: SQiSW gate as a native two-qubit gate

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We propose SQiSW, the matrix square root of the standard iSWAP gate, as a native two-qubit gate for superconducting quantum computing. We show numerically that it has potential for an ultra-high fidelity implementation as its gate time is half of that of iSWAP, but at the same time it possesses powerful information processing capabilities in both the compilation of arbitrary two-qubit gates and the generation of large-scale entangled W-like states. Even though it is half of an iSWAP gate, its capabilities surprisingly rival and even surpass that of iSWAP or other incumbent native two-qubit gates such as CNOT. To complete the case for its candidacy, we propose a detailed compilation, calibration and benchmarking framework. In particular, we propose a variant of randomized benchmarking called interleaved fully randomized benchmarking (iFRB) which provides a general and unified solution for benchmarking non-Clifford gates such as SQiSW. For the reasons above, we believe that the SQiSW gate is worth further study and consideration as a native two-qubit gate for both fault-tolerant and noisy intermediate-scale quantum (NISQ) computation.

I. INTRODUCTION

Quantum computation offers the promise of tackling classically intractable computational problems with careful manipulation of quantum mechanical systems. However, practical quantum computational devices usually suffer from various sources of error and imprecision, precluding us from obtaining meaningful results from computational processes since the results are dominated by meaningless noise. One of the major challenges in quantum hardware design, fabrication and calibration is to implement the basic elements of quantum computation with very high precision. Not only does this improve the performance of Noisy Intermediate Scale Quantum (NISQ) algorithms1 running on bare physical qubits, but it is also a crucial step in realizing fault-tolerant quantum computation. Among the different basic elements of quantum computation, the two-qubit gate operation is the most error-prone as it acts upon a composite quantum system in which more complex errors can occur. It is therefore a high priority to theoretically design and experimentally realize an ultra-high fidelity two-qubit gate.

Many candidates for which two-qubit gate we should use have been proposed. In superconducting quantum computing, these include the cross-resonance gate2–4, the dynamically decoupled CZ gate5–8, the fSim gates9, the CPHASE family gates10–12 and the iSWAP family gates1–18. The square root of the iSWAP gate,

$$\text{SQiSW} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

is in the iSWAP family and its properties in compilation was studied in10,15,19,24. Note that we choose this particular square root since it can be physically implemented by halving the iSWAP gate. This halving of gate time also implies that SQiSW suffers from less $T_1$ and $T_2$ errors, the usual bottlenecks in gate fidelity, as well as well-known $ZZ$ errors19,25. It can therefore be realized with higher fidelities. Moreover, there is evidence that the SQiSW gate is still a very useful two-qubit gate. For example, it is a perfect entangler, that is, it maps a certain product state to a maximally entangled state; indeed, it is the smallest fraction of iSWAP with that property26. Despite these hints of promise, few works have systematically studied the information processing capabilities of SQiSW or its detailed experimental implementation, calibration and benchmarking, both of which we aim to accomplish in this work.

To this end, we propose SQiSW as a native two-qubit gate, highlighting its ultra-high-fidelity implementation and its information processing capabilities in several gate and circuit compilation tasks. We show that the SQiSW gate outperforms the incumbent native two-qubit gates such as CNOT and iSWAP on many tasks, both with a higher fidelity and sometimes even a lower gate count. More specifically, the central results of the report can be summarized as follows:

a. Ultra-high-fidelity implementation. Taking into account decoherence, stray coupling between qubits, and the instrumental limitations on experimental control parameters, we conduct a detailed numerical simulation showing that the SQiSW gate can be realized in the ultra-high fidelity regime ($\geq 99.9\%$ average gate fidelity). Based on experimentally achievable circuit parameters and decoherence times, we estimate that we can implement the SQiSW gate with an error of about $5 \times 10^{-4}$.
b. **Superior information processing capability.** We prove that an arbitrary two-qubit gate can be compiled using at most three uses of the SQiSW gate interleaved with arbitrary single-qubit gates, and we give explicit algorithms compiling an arbitrary gate with the optimal number of SQiSW gates. Moreover, we prove that 79% of two-qubit gates (under the Haar measure) can be generated using only two uses of the SQiSW gate. As a comparison, only a zero-measure set of two-qubit gates can be generated using two uses of common two-qubit gates such as CPHASE family gates, SWAP family gates or the iSWAP gate. Furthermore, we prove that in the task of generating certain W-like states, we need strictly less SQiSW gates compared to iSWAP or CNOT gates. These results suggest that while SQiSW is the square root of iSWAP, its information processing capabilities can rival and even surpass that of iSWAP and CNOT in multiple meaningful aspects.

c. **Calibration and benchmarking.** We develop a framework for efficiently calibrating and benchmarking the SQiSW gate. In particular, we introduce a variant of the randomized benchmarking framework [27], which we call **interleaved fully randomized benchmarking (iFRB)**, in order to benchmark the performance of an arbitrary, possibly non-Clifford, gate. The iFRB framework is based on the original proposal for randomized benchmarking using Haar random gates [27], which we refer to as fully randomized benchmarking (FRB), that characterizes the average noise level in a quantum system and the interleaved randomized benchmarking framework (iRB) [28] that characterizes the noise level associated to a particular target Clifford gate. Compared to previous approaches, iFRB does not require the target gate to lie in the Clifford group or exhibit any particular group structure. Using the scheme to compile arbitrary two-qubit gates using SQiSW, iFRB can readily be used to benchmark the SQiSW gate. In general, it is applicable whenever an efficient compilation scheme of an arbitrary gate is available.

In [22], the problem of generating two-qubit gates from a fixed set of native two-qubit gates and arbitrary single qubit gates was systematically studied using the monodromy polytope theory. They showed that the set of two-qubit gates generated with a fixed number of native two-qubit gates can always be characterized as a finite union of polytopes with respect to a certain parameterization. This makes such sets much easier to study, leading to many results regarding the CPHASE gate family and the iSWAP gate family. However, as pointed out in [22], it is not clear how their results can be translated to efficient compilation algorithms in general, or whether such an algorithm exists at all. In our paper, we focus on the SQiSW gate, and provide efficient and explicit compilation algorithms. These algorithms makes the SQiSW gate practically useful in scenarios where arbitrary two-qubit gates, or families of two-qubit gates, are needed.

The rest of the report proceeds as follows. In Section II we show how the SQiSW gate can be physically implemented on a superconducting quantum computing device and provide numerical evidence that it can be performed with ultra-high fidelity (≥ 99.9%). Section III focuses on SQiSW’s information processing capabilities such as compilation and generating entanglement (that is, W-like states). Section V provides proposals for calibrating and benchmarking the SQiSW gate, including our iFRB technique. We summarize the results and give a brief discussion of future work in Section V.

II. SQiSW: ULTRA-HIGH FIDELITY IMPLEMENTATION

In this section, we give numerical evidence that we can implement SQiSW on superconducting platforms with ultra-high fidelity.

Two-qubit gates in the iSWAP family can be implemented by tuning two superconducting qubits with transversal coupling into resonance. This can be demonstrated in a two-qubit system such as two tunable transmons or tunable fluxoniums capacitively coupled directly or through a bus resonator. Such an implementation suffers from possible stray longitudinal coupling (ZZ interaction), inaccurate flux tuning and decoherence [25, 29, 30]. Here we show how these errors will affect the fidelity of implementation.

First we will investigate the coherent error in the gate. Without loss of generality, we consider a two-qubit system with YY coupling [31], with only the lowest two levels of each qubit included. The relevant Hamiltonians near resonance are given by

\[
H_1 = \begin{bmatrix} 0 & 0 \\ 0 & \omega \end{bmatrix} \otimes I_2;
\]

\[
H_2 = I_1 \otimes \begin{bmatrix} 0 & 0 \\ 0 & \omega + \Delta \end{bmatrix};
\]

\[
H_c = \frac{1}{4} \left( g_{yy} \sigma_{y1} \otimes \sigma_{y2} + g_{zz} \sigma_{z1} \otimes \sigma_{z2} \right);
\]

\[
H = H_1 + H_2 + H_c = \begin{bmatrix} g_{zz}/4 & 0 & 0 & -g_{yy}/4 \\ 0 & \omega + \Delta - g_{zz}/4 & -g_{yy}/4 & 0 \\ 0 & -g_{yy}/4 & \omega - g_{zz}/4 & 0 \\ -g_{yy}/4 & 0 & 0 & 2\omega + \Delta + g_{zz}/4 \end{bmatrix},
\]

where \( H_1 \) and \( H_2 \) are the single-qubit Hamiltonians, \( H_c \) is the coupling term, \( H \) is the Hamiltonian of the whole two-qubit system, \( \omega \) and \( \omega + \Delta \) are frequencies of two qubits, and \( g_{yy} \) and \( g_{zz} \) are the corresponding coupling strengths. \( g_{yy} \) is the term
that contributes to the iSWAP family gate. \( \Delta \) and \( g_{zz} \) are introduced to account for inaccurate flux tuning and stray longitudinal coupling, respectively. We move into the frame rotating with both qubits at frequency \( \omega \). The rotating frame transformation \( R(t) \) and the rotated Hamiltonian \( H^R(t) \) are given by
\[
R(t) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & e^{-i\omega t} & 0 & 0 \\ 0 & 0 & 0 & e^{-i\omega t} \\ 0 & 0 & e^{-i\omega t} & 0 \end{bmatrix},
\]
\[
H^R(t) = R(t)H(t)R(t) + i\frac{\partial R(t)}{\partial t}R(t) = \begin{bmatrix} g_{zz}/4 & 0 & 0 & e^{-i2\omega t}g_{yy}/4 \\ 0 & \Delta - g_{zz}/4 & g_{yy}/4 & 0 \\ 0 & g_{yy}/4 & -g_{zz}/4 & 0 \\ e^{i2\omega t}g_{yy}/4 & 0 & 0 & \Delta + g_{zz}/4 \end{bmatrix}.
\]
Assuming \( \omega \) is much larger than any other frequency in the Hamiltonian, we can take the rotating wave approximation and eliminate all fast-oscillation terms with \( e^{i2\omega t} \) since the time-average is approximately zero. We thus have an approximate time-independent Hamiltonian of the system given by
\[
H_R \approx \begin{bmatrix} g_{zz}/4 & 0 & 0 & 0 \\ 0 & \Delta - g_{zz}/4 & g_{yy}/4 & 0 \\ 0 & g_{yy}/4 & -g_{zz}/4 & 0 \\ 0 & 0 & 0 & \Delta + g_{zz}/4 \end{bmatrix}.
\]
The time evolution operator corresponding to this Hamiltonian is
\[
U(t) = e^{-iH_R t}.
\]
It is easy to verify that when all error terms are zero, that is \( \Delta = 0 \) and \( g_{zz} = 0 \), \( U(t) \) is given by the well-known form of iSWAP family gate:
\[
U(t) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & -i\sin(\theta) & 0 \\ 0 & -i\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.
\]
\[
U(t = \pi/g_{yy}) = \text{SQiSW}^\dagger = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix};
\]
\[
U(t = 2\pi/g_{yy}) = \text{iSWAP}^\dagger = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},
\]
where \( \theta = t g_{yy}/4 \). Note that we assume above \( g_{yy} > 0 \) since the gate time must be positive. When \( g_{yy} < 0 \), we instead implement \( U(t = -\pi/g_{yy}) = \text{SQiSW} \). Note that SQiSW is equivalent to SQiSW\(^\dagger\) under local unitaries: we have SQiSW\(^\dagger\) = (\( Z \otimes I \))SQiSW(\( Z \otimes I \)). The properties of the two gates are very similar despite minor sign differences in compilation. In the subsequent sections we will consider the SQiSW gate even though SQiSW\(^\dagger\) is more common in physical implementations.

In realistic systems \( g_{zz} \) and \( \Delta \) are generally not zero. This causes a nonzero error, which we can quantify using the average fidelity \( F \) between two unitary matrices \( U, V \) [32]:
\[
F(U, V) = \frac{|\text{Tr}(V^\dagger U)|^2 + d}{d(d+1)}
\]
where \( d = 4 \) is the dimension of our matrices. We can estimate the infidelity \( E = 1 - F \) between the simulated physical implementation of SQiSW\(^\dagger\) with \( U(t = \pi/g_{yy}) \) and the ideal SQiSW\(^\dagger\) unitary induced by a specific error term by turning on the given error while turning off all others.

We find that the infidelity induced by the ZZ interaction \( g_{zz} \) and detuning \( \Delta \) can be written as a power series of \( g_{zz}/g_{yy} \) and \( \Delta/g_{yy} \) respectively, assuming each error term is small:
\[
E_{ZZ} \approx \frac{\pi^2}{20} \left( \frac{g_{zz}}{g_{yy}} \right)^2;
\]
\[
E_{\Delta} \approx \frac{8 + \pi^2}{10} \left( \frac{\Delta}{g_{yy}} \right)^2.
\]

(1)
Therefore, the infidelity of SQiSW scales quadratically with the ratio of ZZ to YY coupling and the ratio of $\Delta$ to YY coupling. We also expect there to be a cross-interaction between these two errors, and this is investigated below. To include the decoherence of the system, we perform numerical simulations to estimate the effect of $T_1$ and $T_\phi$ on the fidelity. The time evolution is based on the Lindblad master equations:

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H(t), \rho(t)] + \sum_{j=1,2} \left( \Gamma_{1,j} \mathcal{L}[\sigma_j^-] + \frac{1}{2} \Gamma_{\phi,j} \mathcal{L}[\sigma_j^z] \right) \rho(t)$$

where $\rho(t)$ is the time-dependent density matrix, $H(t)$ is the time-dependent Hamiltonian, $\Gamma_{1,j}$ is the dissipation rate of $j$-th qubit, $\Gamma_{\phi,j}$ is the dephasing rate of $j$-th qubit, and $\mathcal{L}[c] \rho = c \rho c^\dagger - \frac{1}{2} (\rho c^\dagger c - c^\dagger c \rho)$ is the Lindblad superoperator. Note this model includes only the Markovian noise. The gate fidelity is affected little by the non-Markovian noise when the gate time is short \cite{33}, so we neglected the non-Markovian noise in the discussion. We can then compute the average gate fidelity via the process fidelity and $\chi$-matrix as follows \cite{32}:

$$F_p(\chi_1, \chi_2) = \text{Tr}(\chi_1 \chi_2);$$

$$F(\chi_1, \chi_2) = \frac{dF_p(\chi_1, \chi_2) + 1}{d + 1} = \frac{\text{Tr}(\chi_1 \chi_2)d + 1}{d + 1}.$$

We choose the following range of parameters, which can be experimentally realized in fabricated fluxonium qubits, to perform the numerical simulations. For simplicity, we assume $T_1 = T_{1,1} = T_{1,2}$ and $T_\phi = T_{\phi,1} = T_{\phi,2}$.

- $g_{yy} / h = 25MHz$, corresponds to a SQiSW gate time of 20ns
- $g_{zz} / h \in [-0.6, +0.6]$ MHz
- $\Delta / h \in [-0.4, +0.4]$ MHz
- $T_1 \geq 25\mu$s
- $T_\phi \geq 25\mu$s

We check the effect of nonzero temperature as the thermal population of the first excited state $|e\rangle$ may be large. However, we find no major difference between the infidelity at zero temperature and that of a typical fluxonium system ($T = 50mK$ and frequency $\omega_{ge} = 2\pi \times 1GHz$). After computing the infidelity via numerical simulation, we perform a polynomial regression up to 2nd order in the different parameters to identify the error sources (3rd order polynomial regression does not add any new important terms as shown in Fig. 2). In particular, $g_{zz}$, $\Delta$, $\Gamma_1$ and $\Gamma_\phi$, are features in the regression as they are expected to increase the infidelity linearly or quadratically. The regression accuracy is plotted in Fig. 1. The polynomial regression works very well in this case: the root mean square error of the regression is on the order of $10^{-9}$.

To identify the key error sources contributing to the infidelity, we check the permutation feature importance as shown in Fig. 2. There are 5 dominant features in the polynomial regression. The infidelity depends linearly on $\Gamma_\phi$ and $\Gamma_1$, which is a general behavior of decoherence. And the infidelity also depends quadratically on $g_{zz}$ and $\Delta$, which agrees with the symbolic results in eq. (1). Finally, an additional term $g_{zz} \Delta$ emerges, which is the cross-term between $g_{zz}$ and $\Delta$. This term makes it unclear what the error contributions are due to $g_{zz}$ and $\Delta$ individually. In our experiments, $g_{zz}$ is fixed at the design stage and $\Delta$ is microwave tunable, so we can choose an optimal $\Delta$ in the experiments to minimize the infidelity contributed by the terms $c_{\Delta} \Delta^2$, $c_{g_{zz}} g_{zz} \Delta$, $c_{g_{zz}^2} g_{zz}^2$. This isolates the contribution to the infidelity from $g_{zz}$. This optimal $\Delta$ will be our operating point. However, the precision of the frequency is limited by our instruments, and there is an error caused by the deviation from the optimal point which we call $\Delta_p$. Overall, we define the infidelity from each error source as follows:

- $c_{\Delta} \Delta^2 + c_{g_{zz}} g_{zz} \Delta + c_{g_{zz}^2} g_{zz}^2$ at the optimal $\Delta$ as the error from the stray coupling $g_{zz}$;
- $c_{\Delta} \Delta_p^2$ as the error from the instrumental limitation of the frequency $\Delta_p$;
- $c_{\Gamma_1} \Gamma_1$ and $c_{\Gamma_\phi} \Gamma_\phi$ as the error from the decoherence processes.

These errors are plotted for both SQiSW and iSWAP in Fig. 2. Note that because we are working at the optimal $\Delta$, the above errors add up to the total error.

Considering the recent progress on fluxonium fabrication \cite{34} and the precision of the arbitrary wave generator, we compute for a realistic set of parameters $g_{yy} / h = 25MHz$, $T_1 = 100\mu$s, $T_\phi = 100\mu$s, $g_{zz} / h = -0.3MHz$, $\Delta_p / h = 0.18MHz$, which is what we take as input for the results in Fig. 2. SQiSW can be realized with about $5 \times 10^{-4}$ infidelity.
FIG. 1: Infidelity via polynomial regression against simulated infidelity of SQiSW gates. The black dashed line is the $x = y$ line for visual effect. The root mean square error of the regression is on the order of $10^{-9}$.

FIG. 2: Left: The permutation feature importance for the polynomial regression in Fig. 1. Only features with importance $> 0.01$ are included in the figure. Right: Comparison of features’ contributions to the infidelity of SQiSW and iSWAP with the parameters $g_{yy}/h = 25$MHz, $T_1 = 100\mu s$, $T_\phi = 100\mu s$, $g_{zz}/h = -0.3$MHz, $\Delta_p/h = 0.18$MHz.

III. SQiSW: INFORMATION PROCESSING CAPABILITIES

In this section, we first show some basic mathematical properties of the SQiSW gate and then study the information processing capabilities of the SQiSW gate, in particular its ability to compile two-qubit and higher operations. Specifically, we prove that an arbitrary two-qubit gate can be decomposed into at most three applications of the SQiSW gate interleaved by single qubit rotations and give explicit decompositions for certain families of two-qubit rotations. The CNOT gate and the iSWAP gate also generate all two-qubit gates with three applications; however we prove that a majority ($\sim 79\%$) of two-qubit gates, under the Haar measure, can be generated using only two uses of the SQiSW gate, whereas gates generated by two uses of the CNOT gate or the iSWAP gate only spans zero-measure sets. We lastly prove that SQiSW has an advantage over the CNOT and iSWAP gates in the task of preparing W-like states.

A. Basic mathematical properties

We summarize some useful mathematical properties of the SQiSW gate. Besides being the square root of the iSWAP gate, SQiSW satisfies the following properties:

- SQiSW lies in the third level of the Clifford hierarchy: just like the $T$ gate and the Controlled-$S$ gate, the SQiSW gate conjugates Pauli matrices to Clifford matrices. Also, it is not in the second level of the Clifford hierarchy, meaning that it
itself is not a Clifford gate.

- SQiSW is a perfect entangler, that is, it maps a product state into a maximally entangled state. Explicitly,
  \[ \text{SQiSW}|01\rangle = \frac{1}{\sqrt{2}}(|01\rangle + i|10\rangle). \]

- SQiSW is an excitation number preserving gate, meaning that for all \( \theta \), \([\text{SQiSW}, Z_\theta \otimes Z_\theta] = 0\).

To explore further properties, we first introduce some mathematics.

1. KAK decomposition and the Weyl chamber

The KAK decomposition and Weyl chamber provide mathematical tools to characterize two-qubit gates up to single qubit gates. That is, they give the “non-local” information of a two-qubit gate. In particular, the KAK decomposition characterizes equivalence classes of two-qubit unitaries, or elements in the group \( SU(4) \), under actions by single-qubit rotations in \( SU(2) \otimes SU(2) \) before and after. This perspective is particularly useful when we can experimentally regard single qubit local operations as free resources that introduce little error compared to two-qubit gates. We here directly state the results and refer the reader to \([26, 35]\) for more detailed expositions.

**Theorem 1** (KAK decomposition \([26]\)). For an arbitrary \( U \in SU(4) \), there exists a unique \( \bar{\eta} = (x, y, z) \), \( \frac{\pi}{4} \geq x \geq y \geq |z| \), single qubit rotations \( A_0, A_1, B_0, B_1 \in SU(2) \) and a global phase \( g \in \{1, i\} \) such that
  \[ U = g \cdot (A_1 \otimes A_2) \exp\{i\bar{\eta} \cdot \bar{\Sigma}\} (B_1 \otimes B_2), \]
where \( \bar{\Sigma} \equiv [\sigma_X \otimes \sigma_X, \sigma_Y \otimes \sigma_Y, \sigma_Z \otimes \sigma_Z] \). The tuple \( (g, \bar{\eta}, A_0, A_1, B_0, B_1) \) is called the KAK decomposition of the unitary \( U \).

Define the magic basis change matrix \( M \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & i \\ 0 & i & 1 & 0 \\ 0 & i & -1 & 0 \\ 1 & 0 & 0 & -i \end{bmatrix} \). The KAK decomposition theorem can be equivalently stated as follows:

\[ M^\dagger UM = g \cdot A \cdot K \cdot B, \]

where \( A, B \in SO(4) \) and

\[ K = \begin{bmatrix} e^{i(x-y+z)} & 0 & 0 & 0 \\ 0 & e^{i(x+y-z)} & 0 & 0 \\ 0 & 0 & e^{i(-x-y-z)} & 0 \\ 0 & 0 & 0 & e^{i(-x+y+z)} \end{bmatrix} \]

is a diagonal matrix.

The equivalence class of a unitary \( U \) under local unitaries is characterized by the interaction coefficients \( \eta(U) \), which lives in a 3-dimensional tetrahedron called the Weyl chamber \([59]\)

\[ W \equiv \{ \pi/4 \geq x \geq y \geq |z| \text{ and } z \geq 0 \text{ if } x = \frac{\pi}{4} \mid (x, y, z) \in \mathbb{R}^3 \}. \]

We say that two unitaries \( U, V \in SU(4) \) are locally equivalent, or \( U \sim V \), if \( \eta(U) = \eta(V) \). We give the interaction coefficients for some common gates:

- \( I : \eta(I) = (0, 0, 0) \);
- \( \text{SWAP} : \eta(\text{SWAP}) = (\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}) \);
- \( \text{CNOT, CZ} : \eta(\text{CNOT}) = \eta(\text{CZ}) = (\frac{\pi}{4}, 0, 0) \). Note that CNOT \( \sim \text{CZ} \) by a local Hadamard conjugation on the target qubit;
- \( \text{iSWAP} : \eta(\text{iSWAP}) = (\frac{\pi}{4}, \frac{\pi}{4}, 0) \);
- \( B \in [35] : \eta(B) = (\frac{\pi}{4}, \frac{\pi}{4}, 0) \);
I \left( 0, 0, 0 \right)

\text{SWAP} \left( \frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4} \right)

\text{SQiSW} \left( \frac{\pi}{4}, \frac{\pi}{4}, 0 \right)

i\text{SWAP} \left( \frac{\pi}{4}, \frac{\pi}{4}, 0 \right)

\text{B}

\text{SQiSW} \left( \frac{\pi}{8}, \frac{\pi}{8}, 0 \right)

\text{CNOT} \left( \frac{\pi}{4}, 0, 0 \right)

\text{SWAP} \left( \frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4} \right)

\text{FIG. 3: An illustration of the Weyl chamber and the positions of common gates. Note that SQiSW lies in the midpoints of the identity and iSWAP. The point SWAP}^\dagger \text{ is to be identified with the point SWAP but is drawn separately for easier visualization.}

- SQiSW : \eta(\text{SQiSW}) = \left( \frac{\pi}{8}, \frac{\pi}{8}, 0 \right).

These gates and their positions in the Weyl chamber is given in Fig. 3.

\textbf{Definition 1.} Let \( L(x, y, z) \equiv \exp \left( i [x, y, z] \cdot \vec{\Sigma} \right) \) be the canonical element of the equivalence class.

We have \( U \sim L(\eta(U)) \) for all \( U \in \text{SU}(4) \).

2. \textbf{Local invariants and the character polynomial}

The KAK decomposition geometrically characterizes the equivalence class of a unitary \( U \in \text{SU}(4) \); however, it requires diagonalization of matrices and thus can sometimes be difficult to study analytically. Local invariants \([37]\) characterizes the equivalence class of the unitary \( U \), while still being easy to solve. There are many different choices of local invariants. We choose ours to be the degree-4 polynomial

\[ F_U(t) = \det \left[ \Re[M^\dagger U M] + t \cdot \Im[M^\dagger U M] \right], \]

where \( \Re[\cdot] \) and \( \Im[\cdot] \) represent the (element-wise) real and imaginary part of a matrix. We call this the \textit{character polynomial}. To see that the polynomial is locally invariant, we first observe \( U \sim V \iff \exists O_1, O_2 \in \text{SO}(4), O_1 M^\dagger U O_2 = M^\dagger V M \). Then

\[ F_U(t) = \det \left[ \Re[M^\dagger U M] + t \cdot \Im[M^\dagger U M] \right] = \det \left[ \Re[O_1 M^\dagger V M O_2] + t \cdot \Im[O_1 M^\dagger V M O_2] \right] = \det \left[ O_1 \Re[M^\dagger V M] O_2 + t \cdot O_1 \Im[M^\dagger V M] O_2 \right] = \det \left[ O_1 \Re[M^\dagger V M] + t \cdot \Im[M^\dagger V M] \right] \det[O_2] = \det \left[ \Re[M^\dagger V M] + t \cdot \Im[M^\dagger V M] \right] = F_V(t). \]

The polynomial is a complete characterization of the equivalence classes as the zeros of the polynomial are \( -\cot(x - y + z), -\cot(x + y - z), -\cot(-x - y + z) \) and \( -\cot(-x + y + z) \) by evaluating it on the canonical element. Hence, one only needs to check the corresponding character polynomial coefficients in order to determine whether two unitaries are locally equivalent. Furthermore,

\[ F_U(i) = \det[M^\dagger U M] = 1, F_U(-i) = \det[M^\dagger U^* M] = 1, \]
since $U, U^* \in SU(4)$, leaving the character polynomial with three free coefficients. For $U$ with interaction coefficients $(x, y, z)$, we have

$$F_U(t) = (t^2 + 1)(Ct^2 + Bt + A) - t^2,$$

where

$$A = \cos(x + y - z) \cos(x - y + z) \cos(-x - y + z) \cos(-x + y + z),$$

$$B = -\sin 2x \sin 2y \sin 2z,$$

$$C = \sin(x + y - z) \sin(x - y + z) \sin(-x - y + z) \sin(-x + y + z).$$

3. Effective target size

An interesting way to quantify how easy it is to realize a two-qubit gate with quantum control is its effective target size, as put forth in [38]. Intuitively, the effective target size is the invariant volume of the region around a two-qubit gate that corresponds to a small perturbation of its interaction coefficients. We show in this section that the effective target size of $\text{SQiSW}$ is larger than that of $\text{CNOT}$ and $\text{iSWAP}$, having a target size that scales with the perturbation better than any other common two-qubit gate, save for the $B$ gate.

Let $U \in SU(4)$ and its interaction coefficients $\eta(U) = (x, y, z) \in W$. Furthermore, let $U$ be the neighborhood of $\eta(U)$ given by a box with edge length $a$ centered on $\eta(U)$ and with sides parallel to the $x, y, z$ axes. Then, the effective target size of $U$ is defined as

$$T(U) \equiv \int_{(SU(2) \otimes SU(2)) \times U \times (SU(2) \otimes SU(2))} d\mu = \int_{U} d\mu_W$$

where $d\mu$ is the Haar measure over $SU(4)$ and

$$d\mu_W \equiv M_W(x, y, z) dx \land dy \land dz = \frac{3}{\pi} [\cos 2x \cos 4y + \cos 2y \cos 4z + \cos 2z \cos 4x - \cos 2x \cos 4z - \cos 2y \cos 4x - \cos 2z \cos 4y] dx \land dy \land dz$$

is the normalized Haar measure over $W$.

We note that the effective target size is the same for mirror gates (differ by a SWAP) since its definition is symmetric under exchanging which qubits we deem as the first and the second. Now, the Weyl coordinates of $\text{SQiSW}$ is $(\pi/8, \pi/8, 0)$. Its mirror gate has coordinates (e.g. see [39])

$$(\pi/4 - 0, \pi/4 - \pi/8, 1 \times (\pi/8 - \pi/4)) = (\pi/4, \pi/8, -\pi/8) \\
\sim (-\pi/4, \pi/8, -\pi/8) \\
\sim (\pi/4, \pi/8, \pi/8),$$

where the first equivalence follows by subtracting $\pi/2$ from the first coordinate and the second follows from flipping the signs of the first and third coordinates [35]. Hence, the effective target size of $\text{SQiSW}$ is the same as that of its mirror gate $(\pi/4, \pi/8, \pi/8)$ which is given [60] in (47) of [38]:

$$T(\text{SQiSW}) = \frac{1}{2\pi} [3\cos(a) - 3\cos(3a) - 4a \sin(3a)]$$

$$= 4a^4/\pi + O(a^6) \text{ as } a \to 0.$$  

This is a larger area than that of $\text{CNOT}$ and $\text{iSWAP}$ [38]:

$$T(\text{CNOT}) = T(\text{iSWAP})$$

$$= \frac{1}{2\pi} [8a + 7a \cos(3a) - 15a \cos(a) - 9 \sin(3a) + 12 \sin(2a) + 3 \sin(a)]$$

$$= 4a^5/\pi + O(a^7) \text{ as } a \to 0.$$  

Note that the effective target sizes of $\text{CNOT}$ and $\text{iSWAP}$ are the same since they are mirror gates up to local equivalence.
B. Compiling two-qubit gates into SQiSW and single-qubit rotations

We first study the problem of compiling arbitrary two-qubit gates. In particular, we prove the following theorem.

**Theorem 2.** Every two-qubit unitary can be expressed by at most 3 SQiSW gates interleaved by single qubit gates.

The proof of the theorem will consist of two steps. We first completely characterize the set $W(S_2)$ of all two-qubit gates that can be generated using only 2 uses of the SQiSW gate. We second show how to decompose a gate outside of $W(S_2)$ into one use of SQiSW and one use of a gate in $W(S_2)$. This completes the proof. We end by providing an explicit decomposition algorithm.

1. Weyl chamber region spanned by two SQiSW gates

We now study the region in the Weyl chamber that can be generated by two SQiSW gates interleaved with single qubit rotations. This will later help us establish compilation schemes of arbitrary two-qubit gates using SQiSW and single qubit rotations.

**Lemma 1.** The Weyl chamber region spanned by two SQiSW gates is the region described by the inequalities $\frac{\pi}{4} \geq x \geq y \geq |z| \wedge x \geq y + |z|$.

**Proof.** Denote the subset of the Weyl chamber spanned by two SQiSW gates $W(S_2)$ and

$$W' \equiv \left\{ \frac{\pi}{4} \geq x \geq y \geq |z| \wedge x \geq y + |z| \mid (x, y, z) \in W \right\}.$$

The proof proceeds in two steps: We first prove that $W' \subset W(S_2)$ by giving an analytical solution to the interleaving single qubit rotations for a general element in $W'$, and then prove that $W(S_2) \subset W'$ by investigating the character polynomial coefficients associated to a general element in $W(S_2)$.

$W' \subset W(S_2)$: We prove this statement constructively by giving explicit analytical forms for the interleaving single qubit rotations: For $(x, y, z) \in W'$, consider the following gate in $W(S_2)$:

$$U(\alpha, \beta, \gamma) \equiv S \cdot \left( \begin{bmatrix} e^{i\gamma} \cos \alpha/2 & i \sin \alpha/2 \\ i \sin \alpha/2 & e^{-i\gamma} \cos \alpha/2 \end{bmatrix} \otimes \begin{bmatrix} \cos \beta/2 & i \sin \beta/2 \\ i \sin \beta/2 & \cos \beta/2 \end{bmatrix} \right) \cdot S,$$

where

$$\alpha = \arccos \left( \cos 2x - \cos 2y + \cos 2z + 2\sqrt{C} \right),$$

$$\beta = \arccos \left( \cos 2x - \cos 2y + \cos 2z - 2\sqrt{C} \right),$$

$$\gamma = \arccos \left( \text{sgn}(z) \cdot \sqrt{\frac{4 \cos^2 x \cos^2 z \sin^2 y}{4 \cos^2 x \cos^2 z \sin^2 y + \cos 2x \cos 2y \cos 2z}} \right).$$

(6) (7) (8)

Here we define $\text{sgn}(z) = 1$ if $z \geq 0$ and is otherwise $-1$. Note that $C$ in terms of $x, y, z$ was given in eq. (4). One can verify that all operations including the square root and the inverse cosine functions are legal when $(x, y, z) \in W'$, and one can also verify that the interaction coefficient associated to $U(\alpha, \beta, \gamma)$ is indeed $(x, y, z)$ by comparing the coefficients in the character polynomial.

$W(S_2) \subset W'$: Up to local equivalence, a general element in $W(S_2)$ can be parameterized by six parameters:

$$U(\alpha, \beta, \gamma_1, \gamma_2, \delta_1, \delta_2) = S \cdot \left( \begin{bmatrix} e^{i\gamma_1} \cos \alpha & e^{i\delta_1} \sin \alpha \\ -e^{-i\delta_1} \sin \alpha & e^{-i\gamma_1} \cos \alpha \end{bmatrix} \otimes \begin{bmatrix} e^{i\gamma_2} \cos \beta & e^{i\delta_2} \sin \beta \\ -e^{-i\delta_2} \sin \beta & e^{-i\gamma_2} \cos \beta \end{bmatrix} \right) \cdot S,$$

where $S$ is shorthand for SQiSW. The corresponding coefficient $C$ in the character polynomial associated to it is then

$$C = \frac{1}{16} \left( \cos 2\alpha - \cos 2\beta \right)^2.$$

(9)

Combining eq. (9) with eq. (4), we have

$$C = \sin(x + y - z) \sin(x - y + z) \sin(-x - y - z) \sin(-x + y + z) \geq 0,$$
The region $W' = W(S_2)$ spanned by 2 SQISW gates. It is a pyramid with vertices $I$, CNOT, $(\frac{\pi}{4}, \frac{\pi}{8}, \frac{\pi}{8})$, iSWAP, and $(\frac{\pi}{4}, \frac{\pi}{8}, -\frac{\pi}{8})$.

In Fig. 5 we show the region $W' \subset W$. We also show a schematic of how an element of $W(S_2)$ can be decomposed in Fig. 5.

where $(x, y, z) = \eta(U(\alpha, \beta, \gamma_1, \gamma_2, \delta_1, \delta_2))$. Since $(x, y, z) \in W$ ensures that $\sin(x + y - z), \sin(x + y + z) \geq 0$, we know that

$$\sin(x - y + z) \sin(x - y - z) \geq 0 \Rightarrow |z| \leq x - y$$

when $\frac{\pi}{4} \geq x \geq y \geq |z| \geq 0$. Combining this constraint with the ones from $W$ gives us

$$\frac{\pi}{4} \geq x \geq y \geq |z| \wedge x \geq y + |z| \Rightarrow W(S_2) \subset W'$$

In Fig. 4 we show the region $W' \subset W$. We also show a schematic of how an element of $W(S_2)$ can be decomposed in Fig. 5.

2. Decomposing arbitrary two-qubit gate into $\leq 3$ SQISW gates

We now consider unitaries whose interaction coefficients lie outside of the region $W'$. Those gates include the SWAP family $(x, x, \pm x)$, the Sycamore fSim gates and so on. We show below that a third SQISW gate is sufficient to span the whole Weyl chamber.

Given that all gates in the Weyl chamber region $W'$ can be generated using 2 SQISW gates by Lemma 1, it suffices to prove the following.

**Lemma 2.** For all $(x, y, z) \in W \setminus W'$, $L(x, y, z)$ can be generated with one use of some $L(x', y', z')$ and one $L(\frac{\pi}{8}, \frac{\pi}{8}, 0) \sim$ SQISW, where $(x', y', z') \in W'$.

**Proof.** Before proceeding to the proof, we first visualize the constraints imposed by region $W$ and $W'$ in terms of the eigenphases
\{a_0, a_1, a_2, a_3\} of \(L(x, y, z)\), where

\[
\begin{align*}
    a_0 &= x + y - z, \\
    a_1 &= x - y + z, \\
    a_2 &= -x + y + z, \\
    a_3 &= -x - y - z.
\end{align*}
\]

The constraint that \((x, y, z) \in W\) can be equivalently stated as

\[
a_0 \geq a_1 \geq a_2 \geq a_3, \quad \sum_i a_i = 0, a_0 + a_1 \leq \frac{\pi}{2}.
\]

It can be deduced that \(a_0 \geq 0 \geq a_3\). \((x, y, z) \in W'\) imposes an additional constraint:

\[
a_0 \geq a_1 \geq 0 \geq a_2 \geq a_3, \quad \sum_i a_i = 0, a_0 + a_1 \leq \frac{\pi}{2}.
\]

Assuming that \(z = \frac{1}{2}(a_1 + a_2) \geq 0\) (the other case can be reduced to this by observing that \(\text{SQiSW} \sim \text{SQiSW}^\dagger\) and \(L(x, y, z) \sim L(x, y, -z)\), \((x, y, z) \in W \setminus W'\) indicates that this additional constraint is violated via the sign violation \(a_2 > 0\). We show that the following is true: we can always select \(a_i, a_j, i \neq j\) append on them phases \(\frac{\pi}{2}, -\frac{\pi}{2}\) such that \(b_0 \geq b_1 \geq b_2 \geq b_3\) being the sorted permutation of \((a_i + \frac{\pi}{4}, a_j - \frac{\pi}{4}, a_k, a_i), \{i, j, k, l\} \in \{0, 1, 2, 3\}\) satisfies

\[
b_0 \geq b_1 \geq 0 \geq b_2 \geq b_3, \quad \sum_i b_i = 0, b_0 + b_1 \leq \frac{\pi}{2}.
\]

This indicates that there is a way of decomposing \(L(x, y, z)\) to \(L(x', y', z')\) associated to the eigenphases \((b_0, b_1, b_2, b_3)\) and \(L(\frac{\pi}{8}, \frac{\pi}{8}, 0)\). Explicitly, we argue via the following two cases. We also give a visual argument in Fig. 6.

1. \(x \leq \frac{\pi}{8}\). Then \(a_2 \leq x \leq \frac{\pi}{8}\). One can take

\[
\{b_0, b_1\} = \left\{a_0 + \frac{\pi}{4}, a_1\right\}, \quad \{b_2, b_3\} = \text{sort} \left\{a_2 - \frac{\pi}{4}, a_3\right\},
\]

where “sort” means the set is sorted in descending order. One has \(a_0 + \frac{\pi}{4} \geq a_1 \geq 0, a_2 - \frac{\pi}{4}, a_3 \leq 0, a_0 + a_1 + \frac{\pi}{4} = 2x + \frac{\pi}{4} \leq \frac{\pi}{2}\).

2. \(x > \frac{\pi}{8}\). Then \(a_3 = -2x - a_2 < -\frac{\pi}{4}\) and \(a_2 \leq x \leq \frac{\pi}{4}\). One can take

\[
\{b_0, b_1\} = \{a_0, a_1\}, \quad \{b_2, b_3\} = \text{sort} \left\{a_2 - \frac{\pi}{4}, a_3 + \frac{\pi}{4}\right\}.
\]

One has \(a_0 \geq a_1 \geq 0, a_2 - \frac{\pi}{4}, a_3 + \frac{\pi}{4} \leq 0, a_0 + a_1 \leq \frac{\pi}{4}\).

Note that when an eigenphase crossing happens, i.e. that \(a_2 - \frac{\pi}{4} < a_3\) in case 1 and \(a_2 - \frac{\pi}{4} < a_3 + \frac{\pi}{4}\) in case 2, additional single qubit gates need to be applied to switch the two-qubit unitary to the canonical form for compilation purposes, see Algorithm \[\] 1.

3. Decomposition algorithms for two-qubit gates into SQiSW gates

The full decomposition algorithm for an arbitrary two-qubit gate into sequences of single qubit rotations and the SQiSW gate is summarized in Algorithm 1 and visualized in Fig. 7. We also list compilation schemes of some common two-qubit gates or gate families into SQiSW below and summarize the results in Fig. 8.

In this section and throughout the rest of the paper, we use \(\|\) to denote the concatenation of two quantum gates. For example, \(A\|B\) represents a composite quantum gates where \(A\) is applied before \(B\), resulting an overall operation of \(B \cdot A\).

Before proceeding, note that \([R_z(\alpha) \otimes R_z(\alpha), \text{SQiSW}] = 0\) for all \(\alpha\). This introduces gauge freedom in compilation of the circuit and enables us to choose the single qubit gates with the simplest form in our compilation.
(a) Eigenphases without sign violation of $a_2$.

(b) $a_2$ has a sign violation and $x \leq \frac{\pi}{8}$.

(c) $a_2$ has a sign violation and $x > \frac{\pi}{8}$.

FIG. 6: Illustration of the eigenphases $a_0 \geq a_1 \geq a_2 \geq a_3$. Being in $W$ requires that $x \leq \frac{\pi}{4}$, and $a_0, a_1$ and $a_2, a_3$ lie symmetrically with respect to $x$ and $-x$ respectively. Fig. 6a corresponds to no sign violation of $a_2$ and hence can be generated using 2 SQiSW gates. Fig. 6b and Fig. 6c are possible value assignments corresponding to the two eigenphase modifications corresponding to case 1 and 2 in the proof, respectively.

Special orthogonal gates $(x, y, 0)$ All gates locally equivalent to special orthogonal gates in $SO(4)$, i.e. gates that lie in the I–CNOT–iSWAP plane can be generated with two SQiSW gates. Moreover, the expressions of $\alpha, \beta, \gamma$ can be simplified as

$$\alpha = 0,$$

$$\beta = 2 \arccos \sqrt{\cos 2x + 2 \sin^2 y},$$

$$\gamma = \arccos \sqrt{4 \cos^2 x \sin^2 y}.$$
FIG. 7: Visualization of the full compilation scheme. When a gate is outside of the region $W'$, there are eight cases corresponding to different circuit compilations, indicated by three inequalities. (a) $x > \frac{\pi}{8}$, the $>$ case indicated in green. This corresponds to the two cases considered in the proof. (b) $z < 0$, the $<$ case indicated in blue. The proof only deals with the case $z > 0$, where the case $z < 0$ follows similarly with appropriate inversions. (c) Whether there is eigenphase crossing, i.e. whether the order of $a_0, \ldots, a_3$ is preserved after the phase modification. The purple region shows when it isn’t, and a corresponding correction needs to be made in order to transform the gate to its canonical form. (d) The corresponding modifications are the green $R_z$-conjugations around the SQiSW gate, the violet $R_x$-conjugations around the $L(x',y',z')$ in red, and the cyan $Z$ gates on the first qubit.

Therefore, one can check by applying the gauge freedom that

$$L(x, y, 0) \sim \text{SQiSW} \cdot (I \otimes B) \cdot \text{SQiSW},$$

where

$$B = R_z(\gamma)R_x(\beta)R_z(\gamma) = \begin{bmatrix} 2 \cos x \sin y - i \sqrt{\cos 2x \cos 2y} & i \sqrt{\cos 2y - \cos 2x} \\ i \sqrt{\cos 2y - \cos 2x} & 2 \cos x \sin y + i \sqrt{\cos 2x \cos 2y} \end{bmatrix}.$$ 

In the case of special orthogonal gates, the single qubit corrections can be solved analytically. Let

$$\xi \equiv - \arcsin \left( \sin y \cdot \sqrt{\frac{2 \cos 2x}{\cos 2x + \cos 2y}} \right),$$

$$\phi \equiv \arccos \left( \frac{- \cos y \cdot \sqrt{2 \cos 2x}}{\cos 2x + \cos 2y} \right),$$

$$\psi \equiv - \arccos (\cot(x) \tan(y)).$$

Then

$$L(x, y, 0) = (R_z(\xi) \otimes R_z(\phi)R_z(\psi)) \cdot \text{SQiSW} \cdot (I \otimes B) \cdot \text{SQiSW} \cdot (R_z(\xi) \otimes R_z(\psi))R_z(\phi - \pi)).$$

Specific examples of special orthogonal gates include:
Algorithm 1 Decomposing an arbitrary two-qubit gate into a sequence of single qubit rotations and the SQiSW gate.

1: procedure DECOMP(U) \(\triangleright\) Decompose U into single qubit gates and the SQiSW gate
2: \(g, (x, y, z), A_1, A_2, B_1, B_2 \leftarrow \text{KAKDECOMP}(U)\) \(\triangleright\) 2 SQiSW gates needed
3: if \(|z| \leq x - y\) then
4: \(C_1, C_2 \leftarrow \text{INTERLEAVING SINGLE QUBIT ROTATIONS}(x, y, z)\)
5: \(V \leftarrow \text{SQiSW}(C_1 \otimes C_2)\)
6: \(g', (x, y, z), D_1, D_2, E_1, E_2 \leftarrow \text{KAKDECOMP}(V)\) \(\triangleright\) L(x, y, z) = \((1/g')(D_1^\dagger \otimes D_2^\dagger)\text{SQiSW}(C_1 \otimes C_2)\text{SQiSW}(E_1^\dagger \otimes E_2^\dagger)\)
7: return \(E_1^\dagger B_1 \otimes E_2^\dagger B_2||\text{SQiSW}||C_1 \otimes C_2||\text{SQiSW}||A_1 D_1^\dagger \otimes A_2 D_2^\dagger\) \(\triangleright\) Global phases \(g, g'\) omitted
8: else
9: \((x', y', z'), F_1, F_2, G_1, G_2, H_1, H_2 \leftarrow \text{CANONICALIZE}(x, y, z)\)
10: \(\triangleright L(x, y, z) = (F_1 \otimes F_2)L(x', y', z')(G_1 \otimes G_2)\text{SQiSW}(H_1 \otimes H_2), x', y', z' \in W'\)
11: \(C_1, C_2 \leftarrow \text{INTERLEAVING SINGLE QUBIT ROTATIONS}(x', y', z')\)
12: \(V \leftarrow \text{SQiSW}(C_1 \otimes C_2)\)
13: \(g', (x', y', z'), D_1, D_2, E_1, E_2 \leftarrow \text{KAKDECOMP}(V)\) \(\triangleright\) L(x', y', z') = \((1/g')(D_1^\dagger \otimes D_2^\dagger)\text{SQiSW}(C_1 \otimes C_2)\text{SQiSW}(E_1^\dagger \otimes E_2^\dagger)\)
14: return \(H_1 B_1 \otimes H_2 B_2||\text{SQiSW}||E_1^\dagger G_1 \otimes E_2^\dagger G_2||\text{SQiSW}||C_1 \otimes C_2||\text{SQiSW}||A_1 F_1^\dagger \otimes A_2 F_2^\dagger D_2^\dagger\)
15: end if
16: end procedure
17: procedure INTERLEAVING SINGLE QUBIT GATES(x, y, z) \(\triangleright\) Output the single qubit rotations given the interaction coefficients
18: \((x, y, z) \in W'\) when sandwiched by two SQiSW gates
19: \(C \leftarrow \sin(x + y - z)\sin(x - y + z)\sin(-x + y - z)\sin(-x + y + z)\)
20: \(\alpha \leftarrow \arccos(\cos 2x - 2\cos 2y + 2\cos 2z + 2\sqrt{C})\)
21: \(\beta \leftarrow \arccos(\cos 2x - 2\cos 2y + 2\cos 2z - 2\sqrt{C})\)
22: \(\gamma \leftarrow \arccos(\text{sgn}z \cdot \frac{4\cos^2 z \cos^2 y \sin^2 y}{4\cos^2 z \cos^2 y + 4\cos^2 z \cos 2y})\)
23: return \(R_x(\gamma)R_x(\alpha)R_x(\beta)\)
24: end procedure
25: procedure CANONICALIZE(x, y, z) \(\triangleright\) Decompose an arbitrary gate into one SQiSW and one L(x', y', z') where \((x', y', z') \in W'\) and output the coefficients \((x', y', z')\) and the interleaving single qubit rotations
26: \(A_0 \leftarrow I, A_1 \leftarrow I, B_1 \leftarrow R_y(-\frac{\pi}{2}), B_2 \leftarrow R_y(\frac{\pi}{2}), C_1 \leftarrow R_y(-\frac{\pi}{2}), C_2 \leftarrow R_y(\frac{\pi}{2}), s \leftarrow \text{sgn}(z), x' \leftarrow x, y' \leftarrow y, z' \leftarrow |z|\)
27: if \(x > \frac{\pi}{4}\) then
28: \(y' \leftarrow y' - \frac{\pi}{4}, z' \leftarrow z' - \frac{\pi}{4}, B_1 \leftarrow R_x(\frac{\pi}{2})B_1, B_2 \leftarrow R_x(-\frac{\pi}{2})B_2, C_1 \leftarrow C_1 R_x(-\frac{\pi}{2}), C_2 \leftarrow C_2 R_x(\frac{\pi}{2})\)
29: else
30: \(x' \leftarrow x' + \frac{\pi}{4}, z' \leftarrow z' - \frac{\pi}{4}\)
31: end if
32: if \(|y'| < |z'|\) then \(\triangleright\) Eigenphase crossing
33: \(y', z' \leftarrow -z', -y', A_1 \leftarrow R_x(\frac{\pi}{2}), A_2 \leftarrow R_x(-\frac{\pi}{2}), B_1 \leftarrow R_x(-\frac{\pi}{2})B_1, B_2 \leftarrow R_x(\frac{\pi}{2})B_2\)
34: end if
35: if \(s < 0\) then \(\triangleright\) Half rotation
36: \(z' \leftarrow -z', A_1 \leftarrow Z A_1 Z, B_1 \leftarrow Z B_1 Z, C_1 \leftarrow Z C_1 Z\)
37: end if
38: return \((x', y', z'), A_1, A_2, B_1, B_2, C_1, C_2\)
39: end procedure

- The CPHASE family \((x, 0, 0)\), where \(B = Z R_y(2 \arcsin(2\sqrt{2} \sin x))\);
- The super-controlled gate family\(^{[40]}\) \(\left(\frac{\pi}{4}, y, 0\right)\), where \(B = R_x(2 \arccos(2\sqrt{2} \sin y))\);
- The iSWAP family \((x, 0, 0)\), where \(B = R_z(4x - \frac{\pi}{2})\).

**Improper orthogonal gates** \((\frac{\pi}{4}, y, z)\) Half of the improper orthogonal gate family can be generated by 2 SQiSW gates when \(y + |z| \leq \frac{\pi}{4}\). In this case, one has

\[
\alpha = \arccos \left(\cos 2z - \cos 2y + \sqrt{\frac{\cos 4z + \cos 4y}{2}}\right),
\]

\[
\beta = \arccos \left(\cos 2z - \cos 2y - \sqrt{\frac{\cos 4z + \cos 4y}{2}}\right),
\]

\(\gamma = 0\).
Therefore,

\[ L\left(\frac{\pi}{4}, y, z\right) \sim \text{SQiSW} \cdot (R_x(\alpha) \otimes R_x(\beta)) \cdot \text{SQiSW}. \]

In this case we can also explicitly solve for the single qubit corrections. Let

\[ \phi = -\arccos\sqrt{\frac{1 + \tan(y - z)}{2}}, \psi = \arccos\sqrt{\frac{1 + \tan(y + z)}{2}}, \]

then

\[ L\left(\frac{\pi}{4}, y, z\right) = (R_x(\phi + \psi) \otimes R_x\left(\frac{\pi}{2}\right) R_x(\phi - \psi)) \cdot \text{SQiSW} \cdot (R_x(\alpha) \otimes R_x(\beta)) \cdot \text{SQiSW} \cdot (R_x(\phi + \psi) \otimes R_x(\phi - \psi) R_x\left(-\frac{\pi}{2}\right)). \]

Decomposition for the other half of the improper orthogonal gates can be obtained by first decomposing it into one SQiSW and a gate in \( W(S_2) \), then decomposing the gate in \( W(S_2) \) by observing that it is an improper orthogonal gate.

4. Comparison with other two-qubit gates

It can be observed from the visualization in Fig. 4 that \( W' \) takes up 1/2 of the entire Weyl chamber, similar to the set of all perfect entanglers \[26\]. However, the measure in the Weyl chamber does not reflect the Haar measure of the unitary group \( SU(4) \) \[38\]. Indeed, the probability that a Haar random element in \( SU(4) \) can be decomposed with two SQiSW gates can be calculated as

\[ \int_{(x,y,z) \in W'} d\mu_W = \frac{7}{8} - \frac{4}{15\pi} \approx 79\%. \]

It is well known that the B gate with interaction coefficients \( \left(\frac{\pi}{2}, \frac{\pi}{2}, 0\right) \) spans the whole Weyl chamber with only two uses \[36\]. It is also well known that many two-qubit gates, including the CNOT, iSWAP gate and the other gates in the super controlling gate family, generates the whole Weyl chamber with three uses \[41\]. We find that SQiSW lies in-between: although it cannot generate the whole Weyl chamber, it generates a unitary subset of a nonzero measure. Although this holds for general two-qubit gates \[22\], we show that two uses of standard gates such as CNOT, iSWAP or the SWAP family actually generate a subset of the Weyl chamber with zero measure, even though three uses of either gate span the whole Weyl chamber.

**FIG. 8:** Summary of compilations of common two-qubit gates into SQiSW gates
Corollary 1. For any two gates \( U_1, U_2 \in SU(4) \) in the CPHASE gate family \( \eta(U_1) = (x_1, 0, 0) \), \( \eta(U_2) = (x_2, 0, 0) \) and any two single qubit gates \( A_1, A_2 \in SU(2) \), define the gate
\[
V \equiv U_1(A_1 \otimes A_2)U_2.
\]
Then the last element in \( \eta(V) \) is always zero. Equivalently, \( V \) must lie in the I-CNOT-iSWAP plane in the Weyl chamber.

Proof. Let \( \eta(V) = (x', y', z') \). It can be checked from the characteristic polynomial \( F_V(t) \) that the corresponding polynomial coefficient
\[
B = \sin 2x' \sin 2y' \sin 2z' = 0,
\]
regardless of how \( U_1, U_2, A_1, A_2 \) are chosen. This indicates that \( z' = 0 \) given \( \frac{\pi}{4} \geq x \geq y \geq |z| \).

Two CPHASE family gates only generates a two dimensional submanifold because they are \( U(1) \)-covariant, or “leaky” \([22, 42]\); we have
\[
[R_Z(\theta_1) \otimes R_Z(\theta_2)]\text{diag}(1, 1, e^{-i \phi}, e^{i \phi}) = \text{diag}(1, 1, e^{-i \phi}, e^{i \phi})[R_Z(\theta_1) \otimes R_Z(\theta_2)]
\]
for all \( \theta_1, \theta_2 \) and \( \phi \). By commuting the Z-rotations, the interleaving single qubit gates, which can each be decomposed into a \( Z - X - Z \) sequence of rotations, can only generate a two-dimensional manifold in the Weyl chamber, as illustrated in Fig. 9.

By making use of the properties of mirror gates, we can extend this result to gates on the iSWAP − SWAP line as well. The results are visualized in Fig. 10.

Corollary 1. For any two gates \( U_1, U_2 \in SU(4) \) such that
\[
\eta(U_1) = (\frac{\pi}{4}, \frac{\pi}{4}, x_1), \eta(U_2) = (\frac{\pi}{4}, \frac{\pi}{4}, x_2)
\]
and any two single qubit gates \( A_1, A_2 \in SU(2) \), define the gate
\[
V \equiv U_1(A_1 \otimes A_2)U_2.
\]
Then the last element in \( \eta(V) \) is always zero.

Corollary 2. For any two gates \( U_1, U_2 \in SU(4) \) such that
\[
\eta(U_1) = (\frac{\pi}{4}, \frac{\pi}{4}, x_1), \eta(U_2) = (x_2, 0, 0)
\]
and any two single qubit gates \( A_1, A_2 \in SU(2) \), define the gate
\[
V \equiv U_1(A_1 \otimes A_2)U_2.
\]
Then the first element in \( \eta(V) \) is always \( \frac{\pi}{2} \), i.e. the gate \( V \) always lies inside the CNOT − iSWAP − SWAP plane of the Weyl chamber.

We can also prove a result for the case when we have two gates in the SWAP family. This result is visualized in Fig. 11.

Proposition 2. For any two gates \( U_1, U_2 \in SU(4) \) such that
\[
\eta(U_1) = (x_1, x_1, x_1), \eta(U_2) = (x_2, x_2, x_2)
\]
and any two single qubit gates \( A_1, A_2 \in SU(2) \), define the gate
\[
V \equiv U_1(A_1 \otimes A_2)U_2.
\]
Then \( (x', y', z') \equiv \eta(V) \) must satisfy \( y' = x' \) or \( y' = |z'| \). Equivalently, \( V \) must either lie in the I − CNOT − SWAP plane, or the I − SWAP \( ^\dagger \) − SWAP plane in the Weyl chamber.
FIG. 10: The area spanned by 2 CPHASE family gates or their mirror gates. Two gates on the I–CNOT line, or the SWAP†–SWAP line, spans the red area, whereas one gate on each line spans the green area.

FIG. 11: The area spanned by 2 SWAP family gates. Two gates on the SWAP†–I–SWAP line spans either the red area (I–SWAP–SWAP†) or the green area (I–SWAP–CNOT or I–SWAP†–CNOT).

Proof. Let \( \eta(V) = (x', y', z') \). It can be checked that the character polynomial \( F_V(t) \) has a zero with multiplicity two:

\[
(t \cdot \sin(x_1 + x_2) + \cos(x_1 + x_2))^2 \quad | \quad F_V(t),
\]

regardless of how \( U_1, U_2, A_1, A_2 \) are chosen. This indicates that there must be at least one equality in the inequalities \( x' + y' - z' \geq x' - y' + z' \geq -x' + y' + z' \geq -x' - y' - z' \), or equivalently, one equality in \( x' \geq y' \geq \lvert z' \rvert \).

C. Compilation of circuits with more than two qubits

To further demonstrate the information processing superiority of SQiSW, we prove a linear separation between the number of gates needed to generate an \( n \)-qubit W-like state from the product state \( \lvert 0 \rangle \otimes^n \) using the CNOT gate and the SQiSW gate. Considering the corresponding family of circuits with the SQiSW gates, our proof extends to a linear separation between the gate counts in the task of compiling this family of circuits using the SQiSW gate and the CNOT gate. (Note that iSWAP is equivalent to CNOT for this purpose, since they are mirror gates up to local equivalence.) Throughout we consider single qubit rotations as free resources.

The \( n \)-qubit W state is defined as

\[
\lvert W_n \rangle = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \lvert 0 \rangle \otimes^{(i-1)} \otimes \lvert 1 \rangle \otimes \lvert 0 \rangle \otimes^{(n-i)} \right).
\]

An interesting property of the W state is that it is robust against the disposal of qubits [33]: even after tracing out any subset of \( n - 2 \) qubits, the marginal state of the remaining two qubits is still an entangled state. In contrast, the most common multipartite
generalization of maximally entangled states, the $n$-qubit GHZ state $|\text{GHZ}_n\rangle = (|0\rangle^\otimes n + |1\rangle^\otimes n) / \sqrt{2}$, does not satisfy this condition when $n \geq 3$. This special property of the W state can be abstracted as follows:

**Definition 2.** An $n$-partite state $|\Psi\rangle$ is W-like if the marginal state on any two subsystems is an entangled bipartite state.

It is easy to see that $n$-qubit states of the form

$$\sum_{i=1}^{n} \alpha_i \left( |0\rangle^\otimes (i-1) \otimes |1\rangle \otimes |0\rangle^\otimes (n-i) \right), \quad \alpha_i > 0, \quad \sum_{i=1}^{n} |\alpha_i|^2 = 1 \tag{10}$$

are special cases of W-like states. Now, in order to generate any $n$-qubit W-like state from $|0\rangle^\otimes n$, it takes at least $n - 1$ two-qubit gates, since the generating circuit as a graph needs to be at least connected. Surprisingly, $n - 1$ SQiSW gates is also sufficient to generate a particular W-like state of the form in eq. (10): it can be verified that

$$\text{SQiSW}_{n-1,n} \cdots \text{SQiSW}_{2,3}\text{SQiSW}_{1,2}X_1 |0\rangle^\otimes n$$

is a state of the above form where $\alpha_i = 2^{-i/2}$ for $i \leq n - 1$, and $\alpha_n = \alpha_{n-1}$.

In contrast, we show that two-qubit gates that are equivalent to a diagonal gate up to local unitaries, such as CNOT $\sim$ CZ, are ill-suited for generating any W-like state. We have the following result.

**Theorem 3.** An $n$-qubit W-like state cannot be generated using single qubit gates and less than $\frac{15n-3}{4}$ CNOT gates.

**Proof.** The proof is somewhat involved and we give it in Appendix A. \qed

This is evidence that SQiSW has better information processing capabilities beyond just compiling two-qubit gates, but it is unclear how general a statement can be made.

### D. Numerical Experiments

The information processing capabilities of SQiSW we have proved all point to its superiority in actual experimental realizations. To strengthen this claim, in this section we conduct a series of numerical experiments comparing SQiSW to iSWAP with respect to different metrics under a noisy setting. For simplicity we assume a simple depolarizing noise model.

#### 1. Fidelity of Compiling Two-Qubit Gates

In our first experiment we compare SQiSW to iSWAP by computing the fidelity of generating arbitrary two-qubit gates in a noisy setting. An arbitrary two-qubit gate is compiled using SQiSW according to algorithm 1 and using iSWAP according to [40]. We consider a simple error model: each gate is followed by a depolarizing channel with error rate $p_{\text{iswap}} = 2p_{\text{sqisw}} = 0.005$, $p_{\text{single}} = 0.0005$. For the two-qubit gates, each of the qubits undergo a depolarizing channel of the corresponding error rate.

As the family of all two-qubit unitaries SU(4) has 15 real degrees of freedom, we choose one element from each Weyl chamber coordinate, appending it with randomly chosen single-qubit gates. The results we find show that the errors are dominated by the two-qubit gates. We use an interleaved version of Fully Randomized Benchmarking, or iFRB [44] to compute the fidelity value for each Weyl chamber coordinate (please refer to Section [IV B 1] for more details on iFRB). The corresponding results are shown in fig. 12.

It can be seen from the figure that, under this particular noise model, all gates can be compiled using SQiSW with an error rate below 1.8%. Meanwhile, although gates in the $I$-CNOT-iSWAP plane can be compiled with 2 applications of the iSWAP gate, reaching an error rate of about 2%, general gates requiring 3 applications of the iSWAP gate has error rate about 3%. This significant difference indicates an appreciable advantage to using SQiSW for compiling quantum algorithms.

#### 2. Achievable Quantum Volume

Quantum volume [39] is a measure of the largest random quantum circuit of equal width and depth that a quantum computer can successfully implement. It is an all-around measure, taking into account gate fidelities, expressibility of native gate sets, quality of compilers, and even qubit connectivity. We conduct numerical experiments computing the quantum volume that directly compares using SQiSW to using iSWAP as the native two-qubit gate, ceteris paribus, under different noise levels and
FIG. 12: iFRB fidelity value projected onto the Weyl chamber. Data points are taken where $\eta_x$ are multiples of $\pi/20$, and $\eta_y$ and $\eta_z$ are multiples of $\pi/60$. Each data point is collected using iFRB on a gate with the Weyl chamber coordinate, with a randomly chosen set of single-qubit operations applied before and after. For demonstration, we consider a simple error model: each gate is followed by a depolarizing channel with error rate $p_{\text{swap}} = 2p_{\text{qisw}} = 0.005$, $p_{\text{single}} = 0.0005$. It can be seen from the figure that the effects of the randomly chosen single-qubit operations are negligible as the predominant error sources are the two-qubit gates.

FIG. 13: A random circuit used to evaluate quantum volume. The number of qubits and the number of cycles of permutation plus random two-qubit gates are both $d$. Connectivities. Note that unlike compiled two-qubit gate fidelity, this compares the gates in a multi-qubit setting beyond just two qubits.

For the sake of being self-contained, we repeat here the definition of quantum volume. Given the number of qubits and depth $d$, we generate a random circuit of the form shown in fig. 13. The $SU(4)$ box indicates a Haar-random two-qubit unitary, while the $\pi$ box indicates a uniformly randomly chosen permutation. The circuit as a whole defines an overall unitary $U \in SU(2^d)$.

We first numerically compute the probability distribution over bit strings $x \in \{0, 1\}^d$ measured if we implement $U$ on $|0\rangle^\otimes d$:

$$p_U(x) \equiv |\langle x | U |0\rangle^\otimes d|^2.$$  

Using this, we can define the heavy outputs as the bit strings whose probability is higher than the median:

$$H_U \equiv \{x \in \{0, 1\}^d | p_U(x) > p_{\text{med}}\},$$

where $p_{\text{med}}$ is the median of the probabilities of the bit strings. Next, we compute the probability distribution obtained using imperfect gates, compilation and such: $q_U(x)$ [61]. We then define

$$h_U \equiv \sum_{x \in H_U} q_U(x).$$
FIG. 14: $h_d$ as a function of $d$ for different depolarizing noise rates assuming we use SQiSW or iSWAP as our native two-qubit gate. We assume here a complete connectivity graph.

FIG. 15: $h_d$ as a function of $d$ for different depolarizing noise rates assuming we use SQiSW or iSWAP as our native two-qubit gate. We assume here a 1-D chain connectivity graph.

We average over unitaries $U$ according to the above distribution to obtain

$$h_d \equiv \int_U dU h_U.$$

The quantum volume is defined as

$$V_Q \equiv 2^{\max\{d \mid h_d > \frac{2}{3}\}}.$$

In our particular case, we generate $q_U(x)$ as follows. As before, an arbitrary two-qubit gate is compiled using SQiSW according to algorithm [1] and using iSWAP according to [40]. The two-qubit gates are then subject to depolarizing noise with rate $p_{iSWAP} = 2p_{SQiSW}$, and the single-qubit gates with rate $5 \times 10^{-4}$.

We now show the results of our numerical experiments, conducted using the quantum volume module in Cirq [45]. $h_d$ is approximated by averaging over 1001 different $U$ for increasing $d$ (We find numerically that $h_U$ is approximately the same for all 1001 samples.), under different noise levels and connectivities. In fig. 14 a complete graph is assumed and fig. 15 assumes a 1-D chain graph. The chain case is done by computing a list of SWAP gates needed to implement the random permutations using the corresponding function in the quantum volume module of Cirq. Finally, in the figures we only compute even $d$ for simplicity — the odd values show a similar trend. We see that for all the error rates we consider, SQiSW clearly outperforms iSWAP, consistently achieving a higher quantum volume. This indicates that simply changing from iSWAP to SQiSW can appreciably change the quantum volume boasted by a quantum computer.

IV. SQiSW: CALIBRATION AND BENCHMARKING

In this section, we provide detailed experimental procedures for calibrating and benchmarking the SQiSW gate for a superconducting circuit architecture. In particular, we give a variant of the interleaved randomized benchmarking framework, which we call iFRB for interleaved fully randomized benchmarking, in order to benchmark non-Clifford target gates. We then apply the new framework to the benchmarking of the SQiSW gate, which is not in the Clifford group. Throughout this section we will need to consider compiling circuits with SQiSW and arbitrary single qubit gates. As noted in [8], SQiSW does not commute with single qubit Z rotations, and therefore common techniques to implement Z rotations such as frame updates [46] are not applicable. To address this, we use the single qubit compiling scheme in [47], which is applicable for any two-qubit gate. We choose to use this instead of specialized schemes such as that of [8] to make our framework more general beyond just the SQiSW gate [62]. Indeed, our iFRB framework can be applied to any two-qubit gate.
A. Calibration of the SQiSW gate

When physically implementing the SQiSW gate, there is a variety of phase errors that can occur from different processes, including the phase accumulation due to each individual qubit’s static Hamiltonian (−ωZ, where ω is the qubit frequency), phase acquired during flux tuning, and even two-qubit phase errors via unwanted ZZ coupling. Since we know the phase errors for each SQiSW in the quantum circuit before compilation, we can correct for the phase errors at compile time by compiling the single qubit gates in the circuit with the appropriate corrections.

The procedure is as follows. For generality, we consider a two-qubit gate \( U \) in the iSWAP family, that is, of the form

\[
U = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \theta & -i \sin \theta & 0 \\
0 & -i \sin \theta & \cos \theta & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}.
\]

Common sources of single qubit phase errors transform it into [19]

\[
U' = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & e^{-i(\xi + \zeta)} \cos \theta & -ie^{-i(\xi - \zeta)} \sin \theta & 0 \\
0 & -ie^{-i(\xi + \zeta)} \sin \theta & e^{-i(\xi - \zeta)} \cos \theta & 0 \\
0 & 0 & 0 & e^{-i2\xi}
\end{bmatrix}.
\]

Note we omit the two-qubit phase error [63] since that cannot be corrected by single qubit gates. The relationship between \( U \) and \( U' \) can be summarized as

\[
U' = (Z_{\lambda_+} \otimes Z_{\lambda_-}) U (Z_{\kappa} \otimes Z_{-\kappa}),
\]

where \( \lambda_\pm \equiv \pm (\zeta - \chi)/2 \) and \( \kappa \equiv (\zeta + \chi)/2 \).

We now give the overall phase correcting compilation algorithm. Consider a quantum circuit consisting of arbitrary single qubit gates and an iSWAP family gate \( U \). We can represent this as a directed graph \( G = (V, E) \) with vertices corresponding to qubits and edges corresponding to instances of \( U \) between pairs of qubits. We also impose a total order on the edges corresponding to the order in which the \( U \) gates are implemented (for simultaneous gates we assign an arbitrary total order). We give the pseudocode for the algorithm in algorithm 2 where throughout we will refer to different compilation schemes named in [47] to compile arbitrary single qubit gates and for conciseness we denote \( P(\sigma, \phi) \equiv Z_{-\phi}X_\sigma Z_\phi \).

**Algorithm 2 Phase correction compilation algorithm**

1. **procedure** PHASECORRECT(G = (V, E))

2. for \( e = (v_0, v_1) \in E \) do

3. \( U_0, U_1 \leftarrow \) single qubit gates immediately prior to \( e \) on \( v_0, v_1 \)

4. \( Z_{C_0}, Z_{C_1} \leftarrow \) phase carried on qubits \( v_0, v_1 \)

5. Compile \( U_0 \) using virtual Z compilation scheme \( Z_{\phi_0} X_{\pi/2} Z_{\phi_0} X_{\pi/2} Z_{\omega_0} \)

6. Implement \( P(\pi/2, \phi_0 + \omega_0 - F_0) P(\pi/2, \omega_0 - F_0) \) on \( v_0 \)

7. in terms of paulis, this is \( Z_{-\phi_0 - \omega_0 + F_0} X_{\pi/2} Z_{\phi_0} X_{\pi/2} Z_{\omega_0 - F_0} \)

8. Compile \( U_1 \) using three-pulse compilation scheme \( P(\pi/2, \phi_1 + \omega_1 - F_1) P(\pi, \phi_1) P(\pi/2, \omega_1) \)

9. Implement \( P(\pi/2, -x - \kappa + \theta_1) P(\pi, 2\phi_1 - x - \kappa - F_1)/2 P(\pi/2, \omega_1 - F_1) \) on \( v_1 \)

10. in terms of paulis, this is \( Z_{x + \kappa - \phi_1 - \omega_1 - F_1} X_{\pi/2} Z_{\phi_1 - \omega_1} X_{\pi/2} Z_{\omega_1 - F_1} = Z_{x + \kappa} P(\pi/2, \theta_1) P(\pi, \phi_1) P(\pi/2, \omega_1) Z_{-F_1} \)

11. in terms of paulis, this is \( Z_{x + \kappa - \phi_1 - \omega_1 - F_1} X_{\pi/2} Z_{\phi_1 - \omega_1} X_{\pi/2} Z_{\omega_1 - F_1} = Z_{x + \kappa} P(\pi/2, \theta_1) P(\pi, \phi_1) P(\pi/2, \omega_1) Z_{-F_1} \)

12. Phases carried on \( v_0, v_1 \leftarrow Z_{x + \lambda_+}, Z_{x + \lambda_-} \)

end procedure

B. Benchmarking of the SQiSW gate

We now give a variant of the interleaved randomized benchmarking (iRB) framework [28] for benchmarking the SQiSW gate. The iRB framework was first proposed to benchmark the average fidelity of a target gate given the ability to implement arbitrary Clifford gates with high fidelity. However, under the iRB framework, the target gate, i.e. the gate to be benchmarked, needs to be Clifford too. For this reason, the iRB framework is usually used on two-qubit gates such as the iSWAP gate or the CNOT gate, but not on non-Clifford gates such as the Controlled-S gate, much of the fSim gate family, the matchgates [48], or SQiSW. Our
variant, called interleaved fully randomized benchmarking (iFRB), relies on the efficient implementation of Haar random gates as the reference gate set. Compared to Clifford-based iRB, the iFRB scheme is readily applicable to benchmarking of arbitrary quantum gates (not necessarily Clifford) and especially useful when benchmarking on a small quantum system where efficiency of implementing Haar random gates is not an issue.

1. Fully randomized benchmarking

Before introducing iFRB, we first briefly recall the vanilla randomized benchmarking (RB) and the iRB frameworks. Randomized benchmarking [27] was first proposed to study the amplitude of the gate-independent, time-independent, average noise level in a quantum system, while isolating out the errors caused by imperfect state preparation and measurement (SPAM error). The experimental protocol goes as follows: for a d-dimensional quantum system, choose an appropriate gate sequence length \( m \), choose \( m \) gates \( U_1, \ldots, U_m \) i.i.d. from the Haar random distribution and compute \( U_{m+1} \) the recovery gate such that \( U_{m+1} U_m \cdots U_1 = I \) assuming there are no errors. The gate sequence \( U_1 || U_2 || \cdots || U_m || U_{m+1} \) is then performed on an initial state \( |0\rangle \) and subsequently measured in the computational basis. A survival probability \( p_{m,j} \) of measuring 0 is estimated from repeated experiments with sequence \( j \) of length \( m+1 \). By averaging over many different sequences with the same length and collecting data over several different gate sequence lengths, one can extract the average gate fidelity \( r = 1 - (1 - u)(d - 1)/d \), where \( d \) is the dimension of the system (\( 2^n \) for an \( n \)-qubit system) and \( u \) is obtained from fitting the curve

\[
\mathbb{E}_j[p_{m,j}] = A \cdot u^m + B.
\]

Here, the parameters \( A \) and \( B \) are supposed to capture the SPAM error, leaving \( u \) represent solely the imperfection in gate implementation. The requirement for Haar randomness was subsequently found to be unnecessary and unscalable to larger sized quantum systems and is relaxed to a unitary 2-design, most commonly a uniform distribution on the Clifford gates [49]. To avoid confusion, we refer to the Haar random benchmarking as fully randomized benchmarking (FRB) and the Clifford-based one RB.

After the first proposal of FRB, follow-up works flourished [28, 49–54], most of which were based on the Clifford gate set. In particular, interleaved randomized benchmarking [28] was proposed to benchmark the average fidelity of a specific gate, referred to as the target gate, with the hope to exclude not only the SPAM error, but the errors of other gates in a gate set. An iRB experiment consists of two parts. The first part is an ordinary RB protocol on a gate set, referred to as the reference gate set. The second part performs RB with interleaved sequences. Given a target gate \( T \), a random gate sequence of length \( m, U_1, U_2, \ldots, U_m \), is generated i.i.d. from the Clifford group, but the final recovery gate is chosen to be \( U_{m+1} = (T \cdot U_m \cdot T \cdot \cdots \cdot T \cdot U_2 \cdot T \cdot U_1)^\dagger \), and the gate sequence \( U_1 || T || U_2 || T || \cdots || T || U_m || T || U_{m+1} \) is then performed as in the RB experiment. A different error quantity \( v \) can be calculated from the decay rate of the average survival probability with respect to the sequence length, similar to \( u \) in the ordinary RB experiment. The average fidelity of the target gate can then be calculated as

\[
r_T = 1 - \frac{(1 - v/u)(d - 1)}{d}.
\]

In order to be able to carry out the iRB experiment, it is crucial that the final recovery gate, \( U_{m+1} \), lies in the reference gate set, i.e. the Clifford group. Although this holds when the target gate itself lies in the Clifford group, this is not true for many common gates. That the iRB framework cannot be applied for non-Clifford gates is a serious outstanding issue as a non-Clifford gate is necessary for universal quantum computing, by the Gottesman-Knill Theorem [55]. Several alternatives have been proposed, including choosing different finite groups other than the Clifford group [54]. Altogether different benchmarking experiments were also proposed [9, 56], but these alternatives either rely on extensive algebraic studies of the target gate or lack a rigorous theoretical framework for analyzing their interpretation and applicability.

To resolve this issue thorough iFRB, we simply apply iRB, except that instead of using random Clifford gates, we return to the original FRB proposal by using Haar random gates. As there are no restrictions on the recovery gate, iFRB applied to any gate. Since Haar random gates are trivially a unitary 2-design, iFRB carries the same theoretical guarantees of RB and iRB that the original FRB proposal by using Haar random gates. However, FRB/iFRB can still be a very useful tool to benchmark single qubit or two-qubit gates, or even unitaries acting on a small number of qubits. In superconducting systems, 1-qubit FRB/iFRB is readily realized via the virtual Z compilation scheme [46]. On two-qubit systems, the FRB/iFRB framework requires the efficient generation of arbitrary two-qubit unitaries from native two-qubit gates. Luckily, for many families of gates, such as the super-controlling gates [40] and the SQiSW gate, an efficient decomposition of arbitrary two-qubit gates into an optimal number of native two-qubit gate exists. Hence we can realize two-qubit FRB/iFRB in such cases.
Algorithm 3 Generating iFRB sequences

1: procedure GenRandSeq(m, t)  \Comment{Generate a random FRB sequence of length m, interleaved with SQiSW iff t is True}
2: \hspace{1em} U \leftarrow I
3: \hspace{1em} S \leftarrow ε
4: \hspace{1em} for i = 1, \ldots, m - 1 do
5: \hspace{2em} U_i, S_i \leftarrow GenRandGate()
6: \hspace{2em} if t == True then
7: \hspace{3em} U \leftarrow SQiSW \cdot U_i \cdot U
8: \hspace{3em} S \leftarrow S || S_i || SQiSW
9: \hspace{2em} else
10: \hspace{3em} U \leftarrow U_i \cdot U
11: \hspace{3em} S \leftarrow S || S_i
12: \hspace{2em} end if
13: \hspace{1em} end for
14: \hspace{1em} return S || Decom(U^\dagger)  \Comment{Append the recovery gate}
15: end procedure
16: procedure GenRandGate  \Comment{Generate a Haar random SU(4) gate and its corresponding decomposition into SQiSW sequence}
17: \hspace{1em} U \leftarrow GenHaarSU(4)
18: \hspace{1em} return U, Decom(U)  \Comment{Generate a Haar random element in SU(4)}
19: end procedure

V. SUMMARY AND FUTURE WORK

In this report, we investigated the properties of the square-root-iSWAP gate, or SQiSW for short. Being the matrix square root of the iSWAP gate, the SQiSW gate can be readily implemented on any quantum computing platform with the ability to implement the iSWAP gate. Moreover, taking only roughly half of the time of the iSWAP gate, the SQiSW gate can be implemented with ultra-high fidelity. At the same time, it surprisingly still possesses powerful compilation capabilities. The SQiSW gate outperforms both the iSWAP and the CNOT gates in terms of W-like state generation with respect to gate count and in other more standard compilation tasks if the higher fidelity of SQiSW is taken into account.

Our systematic study of SQiSW supports the use of the gate as a native two-qubit gate in both NISQ and fault-tolerant quantum computing. For example, the SQiSW gate is advantageous in compiling Haar random qubit gates compared to the more conventional iSWAP or CNOT gates, which could be useful for variational algorithms requiring a continuous family of quantum gates. Moreover, it takes the same number of SQiSW and iSWAP gates to compile a CNOT gate and a SWAP gate respectively. Taking into account the higher fidelity of SQiSW, this provides evidence that the SQiSW gate is more suitable than the iSWAP gate in realizing certain quantum error correction tasks. However, the analysis of the compilation properties of the SQiSW gate is far from thorough, as its applicability to specific NISQ algorithms or fault-tolerant computing tasks remains unclear.

The fully randomized benchmarking / interleaved FRB schemes are general schemes for benchmarking arbitrary gates, assuming that the gate can be implemented efficiently. Although such schemes face the same scale-up issues of ordinary Clifford-based
Lemma 3. Consider a tripartite system disposal of qubits: leads to Theorem 3. in Definition 4. Then in Appendix A 2 we will prove a lower bound for the number of edges in a good graph, which ultimately precise, we will show in Lemma 4 that the graph given by a circuit generates a W-like state only if it is a “good graph” defined in Definition 4. Then in Appendix A 2 we will prove a lower bound for the number of edges in a good graph, which ultimately leads to Theorem 5.

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Appendix A: Lower bound for the number of CNOT gates to generate W-like states

In this appendix, we will provide a proof to Theorem 3. In Appendix A 1 we will provide a graph theoretical perspective towards quantum circuits. We will first establish the limitations on the entangling power of CNOT gate in Lemma 3, which leads to nontrivial constraints on circuits that generate W-like states using CNOT gates and single-qubit gates. To be more precise, we will show in Lemma 5 that the graph given by a circuit generates a W-like state only if it is a “good graph” defined in Definition 5. Then in Appendix A 2 we will prove a lower bound for the number of edges in a good graph, which ultimately leads to Theorem 5.

1. Conversion to graph problem

The key observation is that entanglement generated by a lone diagonal two-qubit gate is inherently non-robust against the disposal of qubits:

**Lemma 3.** Consider a tripartite system ABC where AB is not entangled with C. If we apply a diagonal two-qubit gate between B and C and then immediately trace out B, then A will still not be entangled with C (i.e. the quantum state on system AC is a separable state).

**Proof.** Note that any diagonal two-qubit gate $U$ can be written in the block diagonal form

$$U = |0\rangle \langle 0| \otimes U_0 + |1\rangle \langle 1| \otimes U_1.$$

First we suppose that the initial state of the system $ABC$ is a product state $\rho_{AB} \otimes \rho_C$. Then after applying $U$ on BC and tracing out B, the state of AC becomes

$$\text{Tr}_B \left[(I_A \otimes U)(\rho_{AB} \otimes \rho_C)(I_A \otimes U_1^T)\right]$$

$$= \text{Tr}_B \left[(I_A \otimes |0\rangle \langle 0| \otimes U_0 + I_A \otimes |1\rangle \langle 1| \otimes U_1)(\rho_{AB} \otimes \rho_C)(I_A \otimes |0\rangle \langle 0| \otimes U_0^T + I_A \otimes |1\rangle \langle 1| \otimes U_1^T)\right]$$

$$= (I_A \otimes U_0)(|0\rangle_B \rho_{AB} |0\rangle_B \otimes \rho_C)(I_A \otimes U_0^T) + (I_A \otimes U_1)(|1\rangle_B \rho_{AB} |1\rangle_B \otimes \rho_C)(I_A \otimes U_1^T)$$

$$= (|0\rangle_B \rho_{AB} |0\rangle_B \otimes (U_0 \rho_C U_0^T) + (|1\rangle_B \rho_{AB} |1\rangle_B \otimes (U_1 \rho_C U_1^T),$$

which is a mixture of two product states between $A$ and $C$ and thus is not entangled. If the initial state of the system $ABC$ is a mixture of multiple product states between $AB$ and $C$, then the final state will become a mixture of such mixtures, so A and C are still not entangled.

**Corollary 3.** A 3-qubit W-like state cannot be generated with only 2 diagonal two-qubit gates.

**Proof.** If such a generation scheme exists, then without loss of generality we can assume that the first two-qubit gate is between qubits $A$ and $B$ and the second is between qubits $B$ and $C$, but Lemma 5 shows that after the second two-qubit gate, $A$ is still not entangled with $C$, and single-qubit gates thereafter will not help.
In fact, this argument can be generalized to give a non-trivial bound for any number of qubits.

Represent a circuit on \( n \) qubits by an undirected graph on \( n \) vertices with distinct edge weights. Larger edge weight means that an edge correspond to a two-qubit gate later in the circuit.

**Definition 3.** An edge \( C-D \) is considered a useful edge with respect to the vertices \( A \) and \( B \), if there exists a path \( C-D-D_1-D_2-\cdots-D_s \) such that all edges in the path have strictly increasing weights, and \( D_1 \in \{A, B\} \), and the same condition also holds for the other direction of the edge.

Note that if \( D \in \{A, B\} \) then the condition in one direction is automatically satisfied by \( t = 0 \). Also, \( D_1 \) can be the same as \( C \), but then by the strictly increasing condition there must be at least two edges between \( C \) and \( D \).

**Definition 4.** A graph is good if for all vertex pairs \( A \) and \( B \), there is a path between \( A \) and \( B \) that consists entirely of useful edges with respect to the vertices \( A \) and \( B \).

Note that this trivially implies a good graph must be connected.

**Lemma 4.** Consider a circuit on \( n \) qubits in which all two-qubit gates are diagonal. If that circuit can generate an \( n \)-qubit W-like state from \( |0\rangle^\otimes n \), then the corresponding graph must be good.

**Proof.** Consider any vertex pair \( A \) and \( B \) in the graph. Since the final state of the circuit is W-like, in the final state \( A \) and \( B \) must be entangled. We will show that this implies that \( A \) and \( B \) are connected by a path consisting entirely of useful edges (with respect to the vertices \( A \) and \( B \)).

First, we trace out all qubits except \( A \) and \( B \) from the final state to get the marginal state \( \rho_{AB} \). Then we remove some edges from the graph corresponding to the circuit in two sequential steps:

1. Any single-qubit gates followed immediately by a trace operator, as well as two-qubit gates followed by two trace operators on both qubits involved, can be removed without affecting the marginal state. Repeat this step until there are no more gates to remove.

2. Then, for each diagonal two-qubit gate \( U \) followed immediately by a trace operator on one of the qubits involved (say, the first qubit), we write \( U \) as \( |0\rangle \langle 0| \otimes U_0 + |1\rangle \langle 1| \otimes U_1 \). Similar to in the proof of Lemma 3, after tracing out the qubit, the final state can be written as a mixture of two components, in each component the two-qubit gate is replaced by two single-qubit operations. Therefore, we remove all edges corresponding to such gates from the graph. (Note that this step cannot be repeated because this step removes the trace operator, too.)

In what is left of the graph, there must still be a path connecting \( A \) and \( B \); otherwise, \( A \) and \( B \) will not be entangled in any of the components of the mixture, and thus they will not be entangled in \( \rho_{AB} \). It suffices to show that this path consists entirely of useful edges in the beginning.

In fact, consider any edge \( C-D \) left in the graph. Since this edge was not removed in the second step, either \( D \in \{A, B\} \) or there was at least one two-qubit gate on \( D \) between \( C-D \) and the final trace operator on \( D \). In the second case, let the last of those gates be \( D-D_1 \). This gate must have been removed in the second step since it is followed immediately by a trace operator on \( D \), but it must have not have been removed in the first step, either because \( D_1 \in \{A, B\} \) or because there was at least one other two-qubit gate on \( D_1 \) between it and the final trace operator on \( D_1 \). Repeating this argument, since there are a finite number of gates, we must end at some \( D_1 \in \{A, B\} \), which gives a path satisfying the condition in Definition 3. This argument can be similarly applied to \( C \). Therefore, \( C-D \) was an useful edge in the original graph.

2. **Bound of edge numbers in a good graph**

We first consider the case where \( G \) doesn’t have any parallel edges and deal with the parallel edge case in the proof of Proposition 5.

**Lemma 5.** Consider a good graph without any parallel edges and with at least 3 vertices. Then, there can be at most one vertex with degree 1.

**Proof.** Suppose there are at least 2 vertices with degree 1, and let \( X \) and \( Y \) be two of them. Let \( e_X \) and \( e_Y \) be the edges incident to \( X \) and \( Y \) respectively, and without loss of generality suppose \( w(e_X) < w(e_Y) \). (\( e_X \) and \( e_Y \) cannot be the same edge, because otherwise \( X \) and \( Y \) will be disconnected from other vertices.) Then \( e_Y \) cannot be a useful edge with respect to \( X \) and \( Y \), as the direction starting from \( Y \) has to end on \( X \) (it cannot end on \( Y \) because there is no parallel edge) and have to go through \( e_X \), but \( e_X \) has a smaller weight. Then there cannot be any path of useful edges that connects \( X \) and \( Y \).

We now prove the core result which with Lemma 4 leads directly to Theorem 2.
Proposition 3. Any good graph with \( n \geq 3 \) vertices should have at least \( \frac{15n-3}{14} \) edges.

Proof. No parallel edges: We first consider graphs without any parallel edges.

Given a connected graph \( G \) without any parallel edges, we can consider the subgraph generated by its set of vertices with degree 2. Each connected component in this subgraph consists of vertices connected one after another. We call each component a chain. We now consider two cases:

1. In the degenerate case where a chain is a cycle, we can directly argue:
   - Suppose one component is a cycle and there are other connected components, then the cycle must be disconnected from other vertices in the original graph, and the graph cannot be good.
   - Otherwise suppose the cycle is the only connected component, then the original graph itself must be a cycle. This could be further divided into two cases based on the total number of vertices.
     - A cycle with 3 vertices is a good graph and obeys \( m \geq \frac{15n-3}{14} \).
     - A cycle with at least 4 vertices cannot be a good graph. Consider any 2 vertices that are not neighbors in the cycle. There are 2 paths connecting this pair of vertices, and each path contains at least 2 edges. The edge with largest weight in each path each cannot be useful with respect to this pair, so these 2 vertices are not connected by useful edges.

2. No chains are cycles. Then, we first establish the following lemma:

Lemma 6. For a good graph without any parallel edges or any cycle chains, each chain can have at most 4 vertices.

Proof. Suppose a chain has at least 5 vertices. Denote the first 5 vertices starting from one end by \( P_1, P_2, \ldots, P_5 \). Let \( M \neq P_2 \) and \( N \neq P_4 \) be the vertices connected to \( P_1 \) and \( P_3 \) respectively. Then we define \( e_k \) as the edge connecting \( P_k \) and \( P_{k+1} \), \( 1 \leq k \leq 4 \). The edges \( (M, P_1) \) and \( (P_5, N) \) are denoted by \( e_0 \) and \( e_5 \) respectively. Now we consider the useful edges with respect to \( M \) and \( P_2 \). \( e_0 \) and \( e_1 \) cannot be both useful, so the path of useful edges between \( M \) and \( P_2 \) should go through the edges \( e_2, e_3, \ldots \), which implies

\[
w(e_2) < w(e_3).
\]

Similar analysis could be done to \( P_2 \) and \( N \) and yield \( w(e_2) > w(e_3) \), which leads to a contradiction.

Now, suppose that every vertex has degree at least 2. We can replace each chain by a single edge between the pair of vertices that the chain connects and remove all the disconnected vertices. In this new graph each vertex has degree at least 3, so we have

\[
n' \leq \frac{2}{3} m',
\]

where \( n' \) and \( m' \) are the number of vertices and edges respectively of the new graph. Letting \( n_2 \) be the number of vertices of degree 2, by Lemma[6]

\[
n_2 \leq 4m'.
\]

The numbers of vertices and edges in the original graph are \( n' + n_2 \) and \( m' + n_2 \), so we have

\[
\frac{n' + n_2}{m' + n_2} \geq \frac{m' + 4m'}{n' + 4m'} \geq \frac{m' + 4m'}{\frac{2}{3} m' + 4m'} = \frac{15}{14}.
\]

Hence, \( m \geq \frac{15}{14} n \).

By Lemma[6] there can only be at most 1 vertex with degree 1. In that case we can remove that vertex and apply the calculation above, which shows that \( m \geq \frac{15}{14} (n - 1) + 1 = \frac{15n-1}{14} \).

In summary, if there are no parallel edges, we must have \( m \geq \min\{\frac{15}{14} n, \frac{15n-1}{14}, \frac{15n-3}{14}\} = \frac{15n-3}{14} \). Note that we have this bound purely for the \( n = 3 \) cycle case. For \( n > 3 \), we can improve this to \( \frac{15n-3}{14} \).

Allowing parallel edges: we prove the theorem by induction. As we have already known, the statement is true for \( n = 3 \). For \( n > 3 \), if there is no parallel edges, the theorem is proved true above. Otherwise, we can contract a pair of vertices connected by parallel edges and the resulting graph with \( n - 1 \) vertices is still a good graph, thus by the inductive hypothesis should have at least \( \frac{15(n-1)-3}{14} \) edges. Then the number of edges in the original graph is at least \( \frac{15(n-1)-3}{14} + 2 > \frac{15n-3}{14} \).
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Note that there are many ways one can choose the canonicalization. Our convention follows the one in [45] and [39].

Note that the convention in [38] for the Weyl coordinates is 2 times that of ours.
[61] Note that this is possible for a numerical simulation, but in a real experimental settings a sampling approach is necessary.
[62] Note that the approach of [8] assumes a parametric gate implementation, while we mostly consider the standard flux tuning implementa-
tion, which does not allow the additional phase shift.
[63] This error is denoted as $\phi$ in [19].