

Qubit Mapping and Routing tailored to Advanced Quantum ISAs: Not as Costly as You Think

Abstract

Qubit mapping/routing is a critical compilation stage for both near-term and fault-tolerant quantum computers, yet existing scalable methods typically impose several times the routing overhead in terms of circuit depth or duration. This performance gap stems from a fundamental disconnect: compilers relies on the simplified routing model (e.g., three-CX-unrolled SWAP insertion), which fails to exploit the intrinsic properties of hardware-native quantum gates.

Recent hardware breakthroughs have also enabled high-precision implementations of diverse instruction set architectures (ISAs) beyond standard CX-based gates. Advanced ISAs such as \sqrt{i} SWAP and ZZ(θ) offer superior circuit synthesis capabilities and inherent noise resilience. However, the absence of systematic compiler optimization strategies tailored to these advanced ISAs has prevented the community from leveraging their full capabilities.

To address this, we propose CANOPUS, a unified qubit mapping/routing framework across diverse quantum ISAs. Built upon the canonical representation of two-qubit gates, CANOPUS centers on qubit routing to perform deep co-optimization in an ISA-aware approach. CANOPUS leverages the two-qubit canonical representation and monodromy polytope theory to model the synthesis cost for more intelligent SWAP search during routing. Commutation relations between two-qubit gates can be formalized through the canonical form in our findings, providing a generalized approach to commutative optimizations. Experiments show that CANOPUS consistently reduces routing overhead by 30%-40% compared to state-of-the-art methods across versatile ISAs and topologies. Our work also presents a coherent method for co-exploration of program patterns, quantum ISAs, and hardware topologies. We have for the first time demonstrated that advanced quantum ISAs can be efficiently utilized within a unified routing framework, paving the way for more effective co-design of quantum software and hardware.

1 Introduction

Quantum computing is a revolutionary computational paradigm leveraging quantum mechanics principles like superposition and entanglement of qubit states [?]. It has been rapidly growing in recent decades due to its potential speedups in tasks such as integer factorization [?], solving linear equations [?], and microscale system simulation [?].

The holistic benchmarks of quantum computers such as quantum volume [?] are predicated on concurrent advancements in both hardware and software. Recently lots of systematic techniques regarding compiler optimizations and

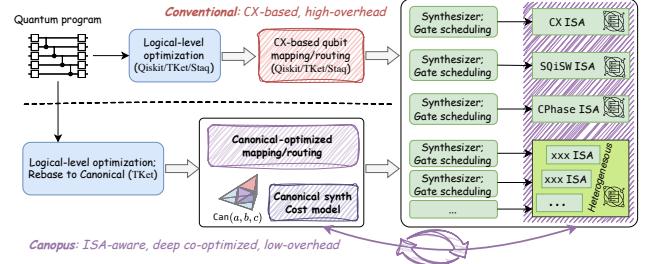


Figure 1. Compilation workflows by means of conventional approaches (top) and CANOPUS (bottom) targeting diverse quantum ISAs. CANOPUS integrates the synthesis cost model (monodromy polytopes within the Weyl chamber) by taking backend ISAs' synthesis properties into account. CANOPUS routing operates in the 2Q canonical representation while the specific synthesis is completed by backend synthesizer.

architectural supports have been presented to approach the ceiling of quantum hardware performance. Quantum compiler is essential in this process. It translates high-level programs into executable single-qubit (1Q) and two-qubit (2Q) gates on realistic quantum hardware. This involves several critical stages: (1) compiling programs into basic quantum gates, (2) perform hardware-agnostic (logical-level) circuit optimization, (3) resolve backend topology constraints via qubit placement and routing, and (4) converting circuits to native gates for final optimization and gate scheduling. The typical optimization goal of quantum compilers is to lower the 2Q gate count and circuit depth, given that 2Q gates exhibit much longer duration and higher error rate than 1Q gates. For mainstream quantum platforms like superconducting [?], 2Q gates can only operate between the near-neighbor physical qubit pairs. Thus ...

has prevented the community from leveraging their full capabilities and exploring cross-ISA hardware-software co-design

Consequently,

However, there are neither systematic compiler optimization strategies tailored to these advanced ISAs nor comprehensive cross-ISA evaluation to unlock their potential.

This gap severely limits compiler optimization potential and thus practical circuit execution performance.

Previous solutions to the qubit mapping/routing problem, ... CX-based routing model ...

$$\text{SWAP}_{q_0, q_1} = \text{CX}_{q_0, q_1} \text{CX}_{q_1, q_0} \text{CX}_{q_0, q_1}$$

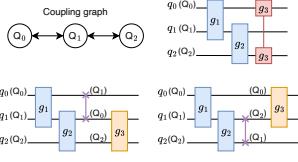


Figure 2. Mapping/routing to resolve physical-qubit topology constraints via SWAP insertion.

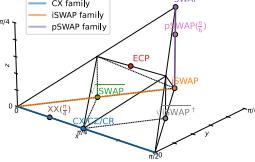


Figure 3. Geometric illustration of canonical gates confined to the Weyl chamber.

physical-qubit connectivity constraints, such as the 2D square topology on Google’s hardware [?] and the 2D heavy-hexagon topology on IBM’s hardware [?]

For instance, Google ... IBM ...

namely ...

only near-neighbor physical qubits can interact with each other to realize

connectivity ...

typical practice is to ...

dynamically remap ...

CANOPUS (**C**anonical-**O**ptimized **P**lacement **U**nity **S**uite) is a qubit mapping and routing framework that is tailored to advanced quantum ISAs, such as Can [?] and \sqrt{i} SWAP [?], which are adaptive to versatile hardware architectures. CANOPUS is designed to optimize the placement of qubits and the routing of quantum gates, taking into account the specific requirements of these advanced ISAs.

Our work addresses the “Babel Tower dilemma” in quantum compilation by establishing a canonical language for diverse two-qubit gates, enabling unified optimization across heterogeneous quantum ISAs. Our key contributions are summarized as follows:

- ...
- ...
- ...
- ...

LLVM-style optimization strategy

Our framework can be extended to integrate more fine-grain hardware information such as qubit-specific basis gate fidelities.

2 Background

¹

2.1 Qubit mapping/routing

Qubit placement and routing ... for connectivity-limited devices

2.2 Quantum gates realization in diverse ISAs

Definition 1 (Canonical gate). Any $2Q$ gate $U \in \text{SU}(4)$ can be expressed by the composition of its unique canonical form

$$\text{Can}(a, b, c) := e^{-i\frac{\pi}{2}(aXX + bYY + cZZ)}, \quad \frac{1}{2} \geq a \geq b \geq |c| \quad (1)$$

sandwiched by local $1Q$ gates such that we call U is locally equivalent to the canonical form $\text{Can}(a, b, c)$.

Canonical representation is ubiquitous as an effective ...

[ZY: It is ubiquitously used in many quantum computing task ...]

Although there are other conventions This definition aligns with the TK2 operation definition in TKET, ...

??

$$\text{pSWAP}(\theta) \sim \text{Can}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - \frac{\theta}{\pi}\right) \quad (2)$$

$$\text{XX}(\theta) = \text{Can}\left(\frac{\theta}{\pi}, 0, 0\right) \sim \text{YY}(\theta) \sim \text{ZZ}(\theta) \quad (3)$$

3 Motivation

Two-fold motivations:

1. The scalable qubit routing effects (2x-4x) is still a critical challenge in practical quantum computing systems
2. How to utilize the emerging advanced ISAs (hardware breakthroughs); across all phases of compilation, routing is the bottleneck and is the most easily handled for co-optimization

[ZY: Use a “optimal routing benchmark” to illustrate the OVERHEAD of existing methods]

[ZY: There should be many takeaways]

- Previous routing overhead is not precise for hardware execution
- Previous routing is costly and also not precise for hardware execution
- SWAP can be implemented in low overhead (gate duration) with the recent breakthrough gate schemes for advanced ISAs
- How to efficiently capture the rich commutation relations when performing co-optimization during qubit routing and gate scheduling

- ISA - gate duration - depth driven

Limitations of the conventional qubit routing models. Quisque facilisis auctor sapien. Pellentesque gravida hendrerit lectus. Mauris rutrum sodales sapien. Fusce hendrerit sem vel lorem. Integer pellentesque massa vel augue. Integer elit tortor, feugiat quis, sagittis et, ornare non, lacus. Vestibulum posuere pellentesque eros. Quisque venenatis ipsum dictum nulla. Aliquam quis quam non metus eleifend interdum. Nam eget sapien ac mauris malesuada adipiscing. Etiam eleifend neque sed quam. Nulla facilisi. Proin a ligula. Sed id dui eu nibh egestas tincidunt. Suspendisse arcu.

¹For convenient visualization

Co-optimization as the key to unlocking superiority of advanced ISAs. Vivamus vehicula leo a justo. Quisque nec augue. Morbi mauris wisi, aliquet vitae, dignissim eget, sollicitudin molestie, ligula. In dictum enim sit amet risus. Curabitur vitae velit eu diam rhoncus hendrerit. Vivamus ut elit. Praesent mattis ipsum quis turpis. Curabitur rhoncus neque eu dui. Etiam vitae magna. Nam ullamcorper. Praesent interdum bibendum magna. Quisque auctor aliquam dolor. Morbi eu lorem et est porttitor fermentum. Nunc egestas arcu at tortor varius viverra. Fusce eu nulla ut nulla interdum consectetur. Vestibulum gravida. Morbi mattis libero sed est.

Babel Tower dilemma for utilizing diverse ISAs. Vivamus vehicula leo a justo. Quisque nec augue. Morbi mauris wisi, aliquet vitae, dignissim eget, sollicitudin molestie, ligula. In dictum enim sit amet risus. Curabitur vitae velit eu diam rhoncus hendrerit. Vivamus ut elit. Praesent mattis ipsum quis turpis. Curabitur rhoncus neque eu dui. Etiam vitae magna. Nam ullamcorper. Praesent interdum bibendum magna. Quisque auctor aliquam dolor. Morbi eu lorem et est porttitor fermentum. Nunc egestas arcu at tortor varius viverra. Fusce eu nulla ut nulla interdum consectetur. Vestibulum gravida. Morbi mattis libero sed est.

- Formal description of 2Q gates to capture synthesis overhead / properties ?? - Formal description of synthesis cost model (monodromy polytopes)

(Coherent) Cross-ISA, topology, program pattern exploration. Vivamus vehicula leo a justo. Quisque nec augue. Morbi mauris wisi, aliquet vitae, dignissim eget, sollicitudin molestie, ligula. In dictum enim sit amet risus. Curabitur vitae velit eu diam rhoncus hendrerit. Vivamus ut elit. Praesent mattis ipsum quis turpis. Curabitur rhoncus neque eu dui. Etiam vitae magna. Nam ullamcorper. Praesent interdum bibendum magna. Quisque auctor aliquam dolor. Morbi eu lorem et est porttitor fermentum. Nunc egestas arcu at tortor varius viverra. Fusce eu nulla ut nulla interdum consectetur. Vestibulum gravida. Morbi mattis libero sed est.

[ZY: Routing overhead is not as costly as you think]

4 CANOPUS framework

4.1 Overview

4.2 2Q synthesis cost modeling

4.3 Routing in canonical form

In contrast to the regular heuristic cost function used in SABRE:

$$H = \frac{1}{|F|} \sum_{(i,j) \in F} \text{dist}[i, j] + \frac{k_E}{|E|} \sum_{(i,j) \in E} \text{dist}[i, j] \\ = \text{Avg}\{\text{dist}[i, j]\}_F + k_E \text{Avg}\{\text{dist}[i, j]\}_E \quad (4)$$

which involves the basic (left term) and lookahead (right term) components. In practice, there is a w_{decay} decay factor applied to H , which is not shown as it does not affect the composition of H .

Algorithm 1: Update L when adding a new 2Q gate

Input : G' (Routed DAG), π (current logic-to-physical mapping), L (last mapped layer), D (wire durations for each qubit), C (commutative pairs within L)
Output: Updated G' , L , D , C

```

/* g: resolved logical gate; g': routed gate */
1 g' ← G'.PUSHBACK(g, π[g.q₀], π[g.q₁]); // g'.qᵢ = π[g.qᵢ]
2 d ← MAX(D[g'.q₀], D[g'.q₁]) + SYNTHCOST(g);
3 D[g'.q₀] ← d; D[g'.q₁] ← d;
4 for pred ∈ G'.PREDECESSORS(g') do
5   if IS2QGATE(pred) then
6     if ISCOMMUTATIVECANONICALPAIR(g', pred) then
7       C[(pred.q₀, pred.q₁)] ← (g'.q₀, g'.q₁);
8     else
9       L.pop((pred.q₀, pred.q₁), None);
10      C.pop((pred.q₀, pred.q₁), None);
11    else
12      /* pred_pred must be None or a 2Q gate */
13      pred_pred ← NEXT(G'.PREDECESSORS(pred));
14      if pred_pred ≠ None then
15        L.pop((pred_pred.q₀, pred_pred.q₁), None);
16        C.pop((pred_pred.q₀, pred_pred.q₁), None);
16  L[(g'.q₀, g'.q₁)] ← g';

```

The heuristic cost function in CANOPUS is defined as:

$$H = c_g + w_d \Delta_{\text{depth}} \\ + c_{\text{swap}} (\Delta_{\text{Avg}\{\text{dist}[i,j]\}_F} + k_E \Delta_{\text{Avg}\{\text{dist}[i,j]\}_E}) \quad (5)$$

- Unified and highly-effective qubit routing approach in canonical form, with properties of quantum ISAs tailored to the routing process

4.4 Enhanced optimization via commutation

- Capture optimization opportunities exposed by gate commutation; while commutation relations can be uniformly described in canonical form

Theorem 1 (Canonical gate commutation). Let $\text{Can}(a, b, c)_{q₀, q₁}$ and $\text{Can}(a', b', c')_{q₁, q₂}$ denote canonical gates acting on qubits $(q₀, q₁)$ and $(q₁, q₂)$ respectively, with an overlapping qubit $q₁$. They are commutative if and only if

$$b = b' = c = c' = 0, \quad (6)$$

that is, when both consist solely of XX rotations.

[ZY: Proposition?? Theorem?]

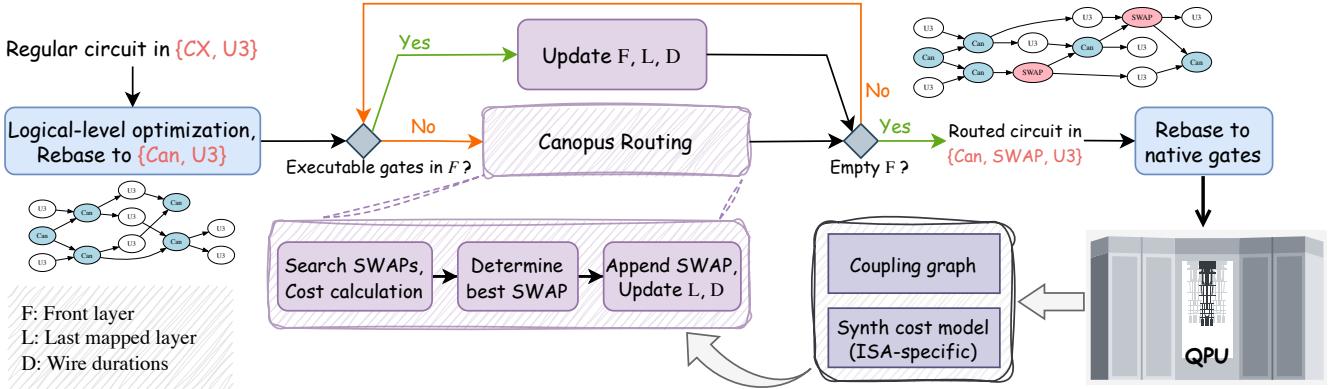


Figure 4. Overview of the CANOPUS framework. ...

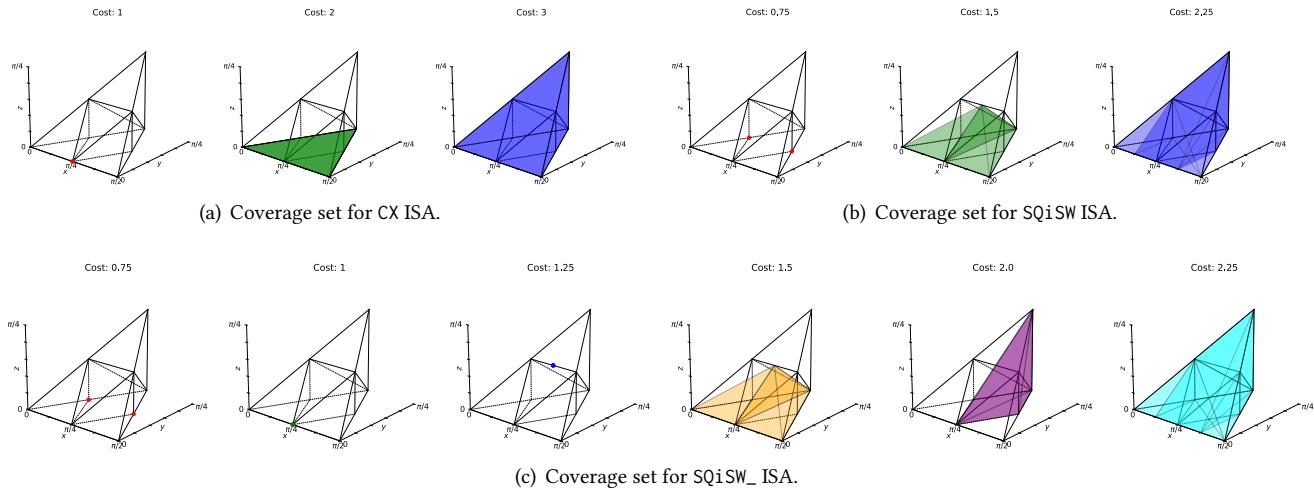


Figure 5. Coverage set examples. CX ISA: {CX, U3} gate set; SQiSW ISA: $\{\sqrt{iSWAP}, iSWAP, U3\}$ gate set; SQiSW_ISA: $\{\sqrt{iSWAP}, iSWAP, ECP, CX, U3\}$ gate set. Costs of Basis 2Q gates are set as CX ~ 1 , $\sqrt{iSWAP} \sim 0.75$, iSWAP ~ 1.5 , ECP ~ 1.25 .

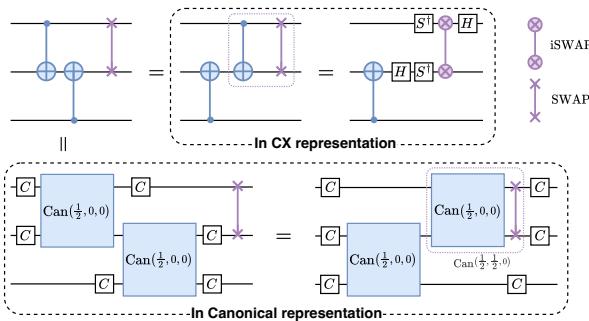


Figure 6. Canonical gate representation enables easily capturing commutative relations within real-world circuits.

Algorithm 2: Update D when adding a SWAP gate

Input : swap (encountered SWAP gate), can (canonical gate within L on the same qubits as swap), D, C
Output: Updated D

```

1 if (swap.q0, swap.q1) ∈ C then
2   q'0, q'1 ← C[(swap.q0, swap.q1)];
   /* Adjust D by finding matched qubits
      qi ∈ {swap.q0, swap.q1} and q'j ∈ {q'0, q'1} */
3   D[qi] ← D[q'j] + SYNTHCOST(can);
4   D[the other swap qubit] ← D[qi];
5   d ← MAX(D[swap.q0], D[swap.q1]) +
      SYNTHCOST(can.MIRROR()) - SYNTHCOST(can);
6   D[swap.q0] ← d; D[swap.q1] ← d;

```

5 Implementation

5.1 Core functionalities

5.2 Extensions

5.3 Scalability

6 Case Studies

6.1 QFT kernel

6.2 Co-exploration of routing and ISA selection

Table 1. Qubit routing comparison for the QFT kernel.

QFT kernel		qft_6		qft_12	
Topology	Method	#Can	Depth2Q	#Can	Depth2Q
1D Chain	Optimal	15	9	66	21
	TOQM	16	10	67	22
	CANOPUS	15	9	66	21
2D Square	TOQM	21	13	100	39
	CANOPUS	15	9	73 ($\pm 10\%$)	33 ($\pm 10\%$)

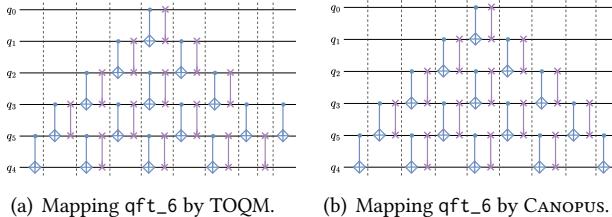


Figure 7. [ZY: Re-draw this figure] Mapping/routing comparison for the QFT kernel. For convenient visualization, only CPhase and SWAP gates are shown. (a) TOQM generates a sub-optimal mapping scheme, with 2Q depth of 10. (b) CANOPUS generates the optimal scheme in a perfect butterfly structure, with 2Q depth of 9.

provides cross-compiler but also cross-ISA comparisons under the coherent basis gate cost and routing overhead settings.

7.1 Experimental settings

7.1.1 ISAs and basis gate costs. We consider six different ISAs (including the conventional CX ISA) listed in ???. These mainly cover a wide range of powerful basis gates from CX-family and iSWAP-family gates. Particularly, SQiSW [?] proves to a more powerful ISA option and has been adopted by recent software projects [??]. ZZPhase ISA containing three fractional $ZZ(\theta)$ rotation gates is adopted by QISKit’s latest synthesis functionalities [??]. Mirorr [ZY: TODO: find the initial paper about mirror gate]

[?]

We also involve the Het ISA that is the composition of ZZPhase and SQiSW.

The unit costs for the involved basis gates are set as:

$$\left\{ \begin{array}{l} CX : 1, ZZ(\pi/t) : 2/t, \sqrt{iSWAP} : 0.75, \\ iSWAP : 1.5, ECP : 1.25, pSWAP(\pi/t) : 2 - 1/t \end{array} \right\} \quad (7)$$

[ZY: Plot a weyl chamber to illustrate the cost settings]

7.1.2 Benchmarks. We select a set of medium-size benchmarks from QASMBench [?] and MQTBench [?] spanning various categories of quantum programs. These benchmarks first go through logical-level optimization by TKET [?] and

Table 2. Selected quantum ISAs.

ISA	2Q basis gates	Description
CX	{CX}	Conventional CX gate
ZZPhase	$\{ZZ_{\frac{\pi}{6}}, ZZ_{\frac{\pi}{4}}, ZZ_{\frac{\pi}{2}}\}$	Discrete CX-family gates, i.e., $\{\sqrt[3]{CX}, \sqrt{CX}, CX\}$ [?]
SQiSW	$\{\sqrt{iSWAP}, iSWAP\}$	Half evolution of iSWAP and iSWAP [?]
ZZPhase_	ZZPhase + $\{pSWAP_{\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{2}}\}$	ZZPhase ISA with the mirror gates
SQiSW_	SQiSW + {ECP, CX}	SQiSW ISA with the mirror gates [?]
Het	ZZPhase + SQiSW	Heterogeneous CX-family and iSWAP-family gates

Table 3. Benchmarks information. These metrics are collected from the circuits after logical-level optimization by TKET, thus including only Can and U3 gates. Circuit cost (C_{count} and C_{depth}) is calculated in CX ISA.

Program	#Qubit	#Can	Depth2Q	C_{count}	C_{depth}
bigadder [?]	18	114	79	130.0	88.0
bv [?]	19	18	18	18.0	18.0
gem [?]	13	377	376	511.0	510.0
ising [?]	26	25	2	50.0	4.0
knn [?]	25	72	50	84.0	62.0
multiplier [?]	15	198	122	222.0	133.0
qec9xz [?]	17	32	12	32.0	12.0
qft [?]	18	153	33	306.0	66.0
qpeexact [?]	16	127	43	260.0	86.0
qram [?]	20	110	70	130.0	78.0
sat [?]	11	210	182	252.0	204.0
swap_test [?]	25	72	50	84.0	62.0
wstate [?]	27	52	28	52.0	28.0

are rebased to {Can, U3} as the input of qubit routing compilers. Information of benchmarks after logical-level optimization are summarized in ??, where “Circuit cost” denotes the circuit duration assuming each canonical gate will be finally rebased to CX ISA and the duration (cost) of each CX is set to 1.

7.1.3 Baselines.

7.2 Circuit duration reduction

7.3 Co-exploration of routing and ISA selection

7.4 Breakdown analysis

7.4.1 Commutative optimization. In this section, we analyze individual factors in the improvement brought by CANOPUS, mainly about the commutative optimization mechanism and the heuristic depth-cost weight factor.

7.4.2 Depth weight factor. Note that the ...

[ZY: about comm_opt effect]

7.5 Real-system experiments

[ZY: Fractional gate IBM]

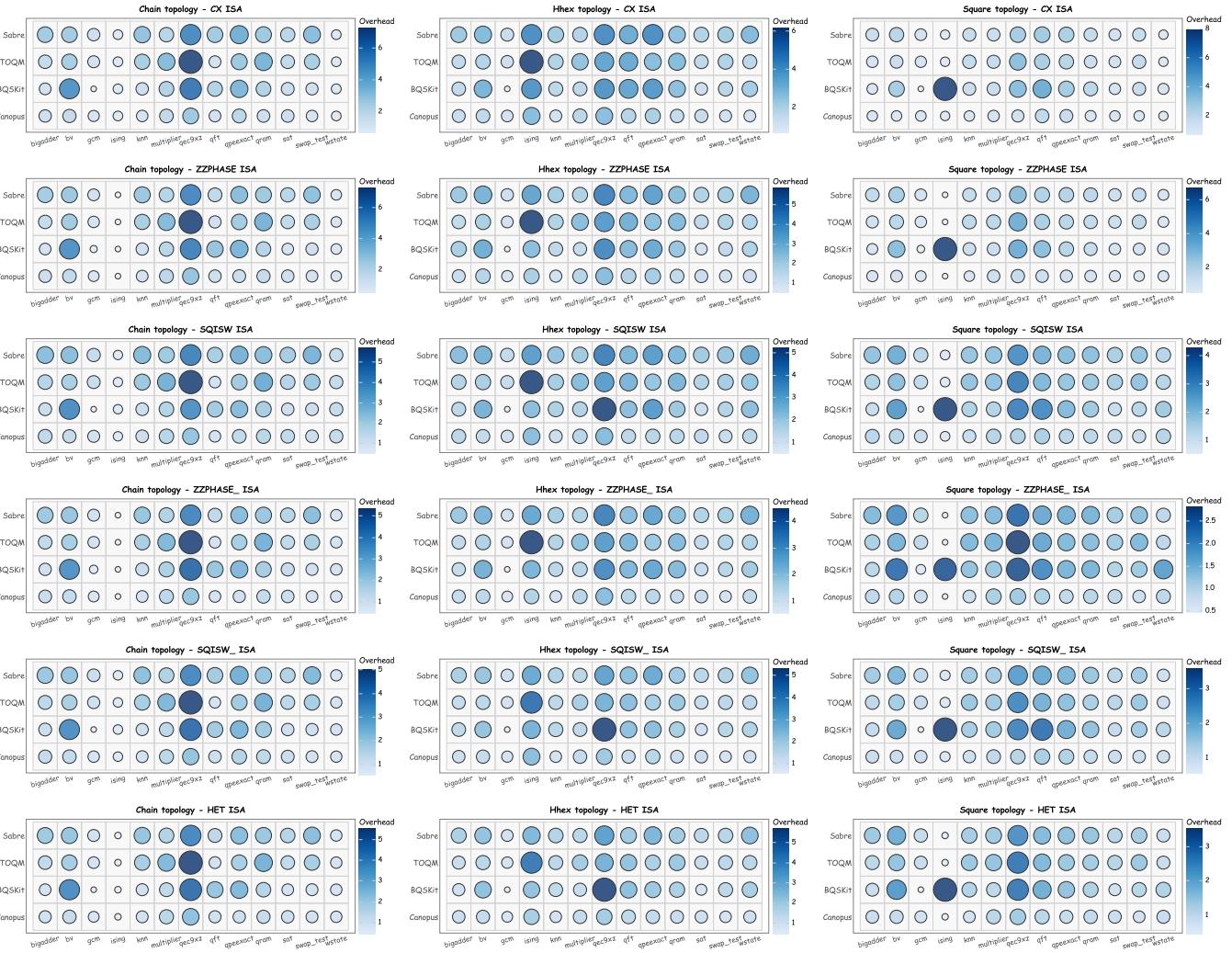


Figure 8. Detailed benchmarking results for different compilers (SABRE, TOQM, BQSKit, CANOPUS) across diverse topologies (columns from left to right: 1D Chain, 2D HHex, 2D Square) and quantum ISAs (rows from top to bottom: CX, ZZPhase, SQiSW, ZZPhase_{_}, SQiSW_{_}, Het). Sizes and colors of the bubbles represent the values for routing overhead (multiples of the routed and rebased circuits compared to that of prior-routing ones).

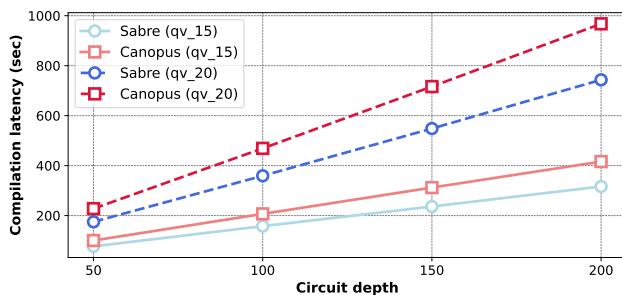


Figure 9. Compilation latency comparison.

8 Related Works

Qubit mapping/routing is one of the most well-explored topics of quantum compiler research, as it shares the similar methodologies with instruction scheduling [??] and register allocation [??] in classical computing. Conventional methods focus on the simplified routing model, that is, #SWAP-minimal insertion, three-CX-unrolled SWAP gate, and CX-based latency metric. That brings a gap between quantum hardware performance and its ceiling, which is particularly evident with the progress of underlying instruction models for modern quantum hardware.

?] introduces an A*-based algorithm to minimize SWAP gate overhead for concurrent CNOT gate layers. The approach partitions the circuit into layers and solves the mapping problem subsequently. ?] also utilizes the circuit DAG layering thought to tackle the qubit mapping problem and proposes the bidirectional routing procedure to acquire a better initial mapping desired to result in #SWAP inserted minimization as expected. It also briefly discusses the trade-off between the inserted SWAP count and the circuit depth but does not prioritize optimizing circuit depth. Some other works leverage algorithmic procedures similar to SABRE to improve parallelism among inserted SWAPs and other 2Q gates [? ? ?], or attempt to minimize circuit depth via graph matching [?]. ?] systematically investigates the time (circuit depth) optimality of qubit mapping and proposed an A*-based method TOQM that results in better results than the SOTA solver-based depth-driven algorithm [?]. However, the optimality of qubit routing is a complex task. There are rarely theoretical studies that claims the holistic optimality of some SWAP insertion schemes provided the quantum ISAs, device topologies, and synthesis cost models. In our field tests, TOQM does not lead to time-optimal results compared to our heuristic CANOPUS, and the optimal mapping scheme for specific patterns such as QFT kernel analyzed in [?] are not indeed optimal, according to our case study in ??.

With the recent development of advanced quantum ISAs such as superconducting fractional gates [?], ion-trapped partial entangling gates [? ?], and the AshN scheme [?], some works began exploring how to efficiently utilize these ISAs to make compiler optimizations closer to hardware characteristics. ?] investigates the practical performance of SQiSW ISA proposed by ?] and the synthesis capability when incorporating the basis gates' mirrors into the ISA. The modified SABRE algorithm in [?] provides an attempt of the collaborative gate decomposition and qubit routing approach, while the optimization opportunities considered therein are limited and the algorithmic techniques are not sophisticated. BQSKit [?] and the series of works behind [? ? ? ?] provides a toolkit to rebase arbitrary 2Q unitaries to specific ISAs through approximate synthesis (structural search and numerical optimization) that is not computational efficient. Approximate synthesis by BQSKit does not ensure an optimal schemes for two-qubit and multi-qubit synthesis cases. In addition, due to the lack of native compilation strategies and rational synthesis cost model, ?] claims that alternative ISAs are hard to be comparable to CX when evaluating quantum hardware roofline by BQSKit. As for applicability of expanded ISAs to QEC, Google's latest theoretical [?] and experimental [?] works demonstrate the CX-iSWAP combination ISA could benefits suppressing fault-tolerant threshold. ?] proposes a routing-based method enhanced by CX-iSWAP for overcoming ancilla defects among surface code blocks while preserving encoded logical information.

9 Conclusion

It is promising to explore novel Clifford circuit optimization techniques drawing on the canonical gate representation.

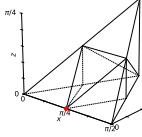
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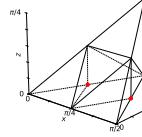
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Cost: 1

**Figure 10.** Coverage set for CX ISA.

Cost: 0,75

**Figure 11.** Coverage set for SQiSW ISA.

A Canonical gate and 2Q circuit synthesis

In this section we show the basic mathematical properties the its canonical form of 2Q unitary and then discuss the synthesis capability of some 2Q basis gates.

A.1 Canonical decomposition

$SU(N)$ is a real manifold with dimension $N^2 - 1$, within which any element is a *special unitary* matrix with determinant equal to 1. Since the global phase does not affect quantum computation processes, it is sufficient to focus on the mathematical properties of special unitaries in the area of circuit synthesis. A generic 2Q gate, despite having 15 real parameters, can have its nonlocal behavior fully characterized by only 3 real parameters. This method, known as *Canonical decomposition* or *KAK decomposition* from Lie algebra theory, is widely adopted in quantum computing [? ? ? ?]. Specifically, for any $U \in SU(4)$, there exists a unique $\vec{\eta} = (x, y, z) \in W \subseteq \mathbb{R}^3$, along with $V_1, V_2, V_3, V_4 \in SU(2)$ and a global phase, such that

$$U = g \cdot (V_1 \otimes V_2) e^{-i\vec{\eta} \cdot \vec{\Sigma}} (V_3 \otimes V_4), \quad g \in \{1, i\} \quad (8)$$

where $\vec{\Sigma} \equiv (XX, YY, ZZ)$ [?]. The set

$$W := \left\{ (x, y, z) \in \mathbb{R}^3 \mid \frac{\pi}{4} \geq x \geq y \geq |z|, z \geq 0 \text{ if } x = \frac{\pi}{4} \right\} \quad (9)$$

is known as the *Weyl chamber* [?], and $\vec{\eta} \in W$ is known as the *Weyl coordinate* of U . We also refer to a gate of the form

$$\text{Can}(a, b, c) := e^{-i\frac{\pi}{2}(aXX + bYY + cZZ)} = \begin{pmatrix} e^{-i\frac{c\pi}{2}} \cos \frac{(a-b)\pi}{2} & 0 & 0 & -ie^{-i\frac{c\pi}{2}} \sin \frac{(a-b)\pi}{2} \\ 0 & e^{i\frac{c\pi}{2}} \cos \frac{(a+b)\pi}{2} & -ie^{i\frac{c\pi}{2}} \sin \frac{(a+b)\pi}{2} & 0 \\ 0 & -ie^{i\frac{c\pi}{2}} \sin \frac{(a+b)\pi}{2} & e^{i\frac{c\pi}{2}} \cos \frac{(a+b)\pi}{2} & 0 \\ -ie^{-i\frac{c\pi}{2}} \sin \frac{(a-b)\pi}{2} & 0 & 0 & e^{-i\frac{c\pi}{2}} \cos \frac{(a-b)\pi}{2} \end{pmatrix} \quad (10)$$

as a *canonical* gate. Two 2Q gates U and V are considered *locally equivalent* if they differ only by 1Q gates, meaning their canonical coefficients can be transformed into one another via the equivalence rules [?]:

1. $(a, b, c) \sim (b, a, c)$ or $(a, b, c) \sim (c, b, a)$, i.e., any permutation of the coefficients;
2. $(a, b, c) \sim (-a, -b, c)$;
3. $(a, b, c) \sim (a - 1, b, c)$;
4. $(1/2, b, c) \sim (1/2, b, -c)$.

Note that we align the conventional that canonical coefficient (a, b, c) differs from Weyl coordinate (x, y, z) by a $\frac{\pi}{2}$ factor. Unless otherwise specified, the canonical coefficients of gates in quantum ISAs and circuits are confined to $\frac{1}{2} \geq a \geq b \geq |c|$. While for the Weyl chamber visualization by means of `weylchamber` [?], we assume the Weyl coordinates are confined to $\{\frac{\pi}{4} \geq x \geq y \geq z \geq 0\} \cup \{\frac{\pi}{4} \geq \frac{\pi}{2} - x \geq y \geq z \geq 0\}$, as illustrated by ???. Conversion of Weyl coordinates for different conventions is not simple according to the equivalence rules above.

A.2 Quantum ISA and the synthesis capability

A quantum ISA typically includes qubit initialization, a universal gate set, and measurement. It serves as an interface between software and hardware by mapping high-level semantics of quantum programs to low-level native quantum operations or pulse sequences on hardware. The universal gate set, especially specified by its 2Q basis gates, is the key component of a quantum ISA that dominates its hardware-implementation accuracy and cost, as well as software-expressivity sufficiency.

CX or CNOT is the most popular basis gate provides by hardware vendors and considered by various quantum compiler optimization methods. The superconducting Cross-Resonance gate [?] and ion-trapped Mølmer-Sørensen gate [?] are both CX-equivalent gates with the same canonical form $\text{Can}(\frac{1}{2}, 0, 0)$. In the superconducting platforms with XY-coupled Hamiltonian like Google's Sycamore [?], iSWAP $\sim \text{Can}(\frac{1}{2}, \frac{1}{2}, 0)$ is another representative native 2Q basis gate and could be

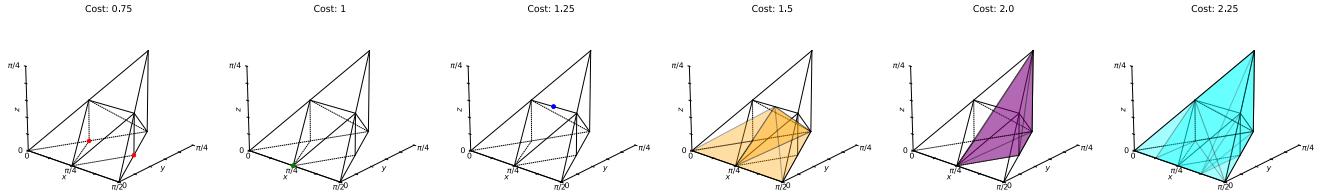


Figure 12. Coverage set for SQiSW_ISA.

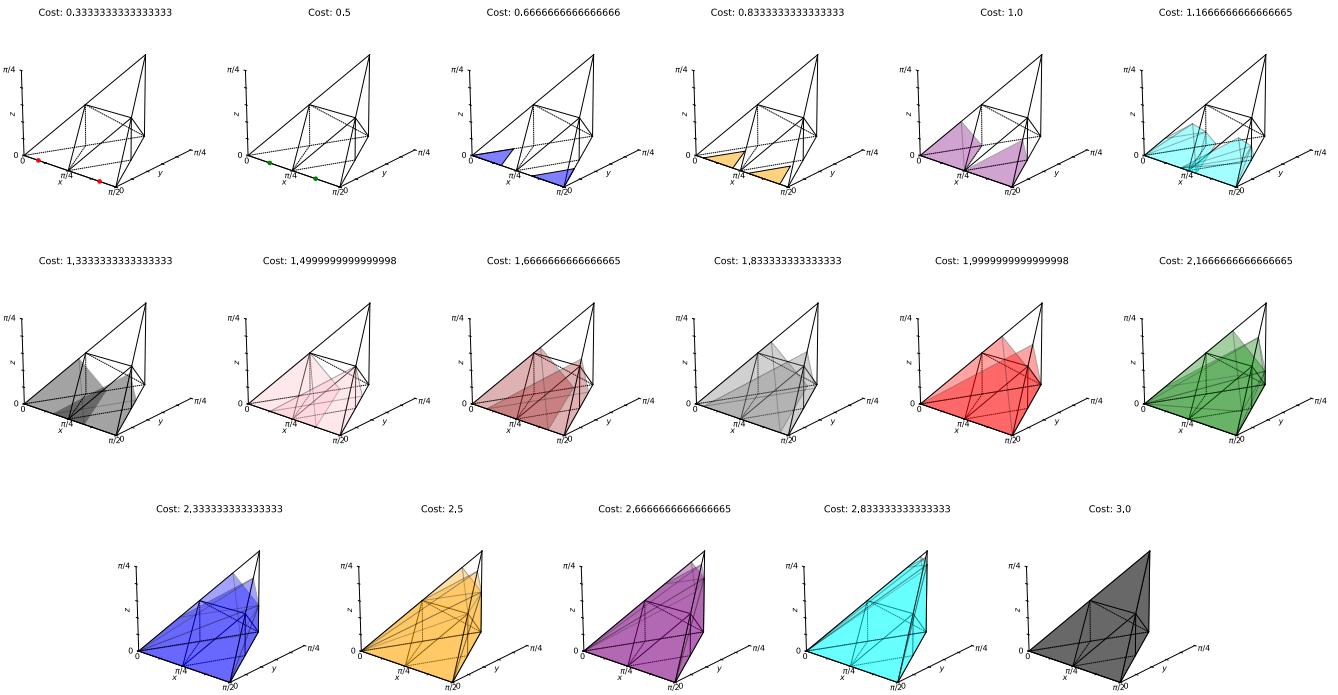


Figure 13. Coverage set for ZZPhase ISA.

less sensitive to leakage error than the native CZ gate. Recent experimental advances demonstrate that more basis gates could be implemented natively and calibrated in high precision [???]. Particularly, some basis gates like $\sqrt{i\text{SWAP}} \sim \text{Can}(\frac{1}{4}, \frac{1}{4}, 0)$ and fractional ZZ(θ) $\sim \text{Can}(a, 0, 0)$ gates offers more promising ISA selections as they exhibit shorter gate duration, higher gate accuracy, and stronger synthesis capability.

The synthesis capability or computational power of basis gates can be geometrically illustrated by monodrome polytopes within the Weyl chamber. The coverage set for CX depicted in ?? implies that

1. One CX gate is required to synthesize 2Q gates $\sim \text{Can}(\frac{1}{2}, 0, 0)$, i.e., CX-equivalent gates $(V_1 \otimes V_2)\text{CX}(V_3 \otimes V_4)$;
2. Two CX gates are required to synthesize 2Q gates $\sim \text{Can}(a, b, 0)$, i.e., $(V_1 \otimes V_2)\text{CX}(V_3 \otimes V_4)\text{CX}(V_5 \otimes V_6)$;
3. Three CX gates are required to synthesize 2Q gates $\sim \text{Can}(a, b, c)$, i.e., $(V_1 \otimes V_2)\text{CX}(V_3 \otimes V_4)\text{CX}(V_5 \otimes V_6)\text{CX}(V_7 \otimes V_8)$.

We assume the cost of one CX gate is 1.0, polytopes in different colors denotes the minimal circuit cost (duration) for the coverage set if synthesized by CX and arbitrary 1Q gates. That is, on average, the number of CX gates required to synthesize arbitrary 2Q gates is 3. In contrast, the number for SQiSW ISA is 2.21 [?].

Monodromy polytope theory [?] provides a framework for determining the synthesis coverage set and circuit cost (in 2Q depth) for any set of basis gates with specified costs, while the specific gate decomposition process is left to the synthesizer to complete. For the selected ISAs in ?? with the basis gate costs assumed in ??, ????????????? describes their coverage sets, respectively. With the enrichment of quantum ISA (e.g., combining gate families, involving mirror gates) and heterogeneous basis gate cost settings, the coverage set reveals a richer variety of convex polyhedra. That implies more optimization effects for the ISA-aware routing mechanism in CANOPUS.

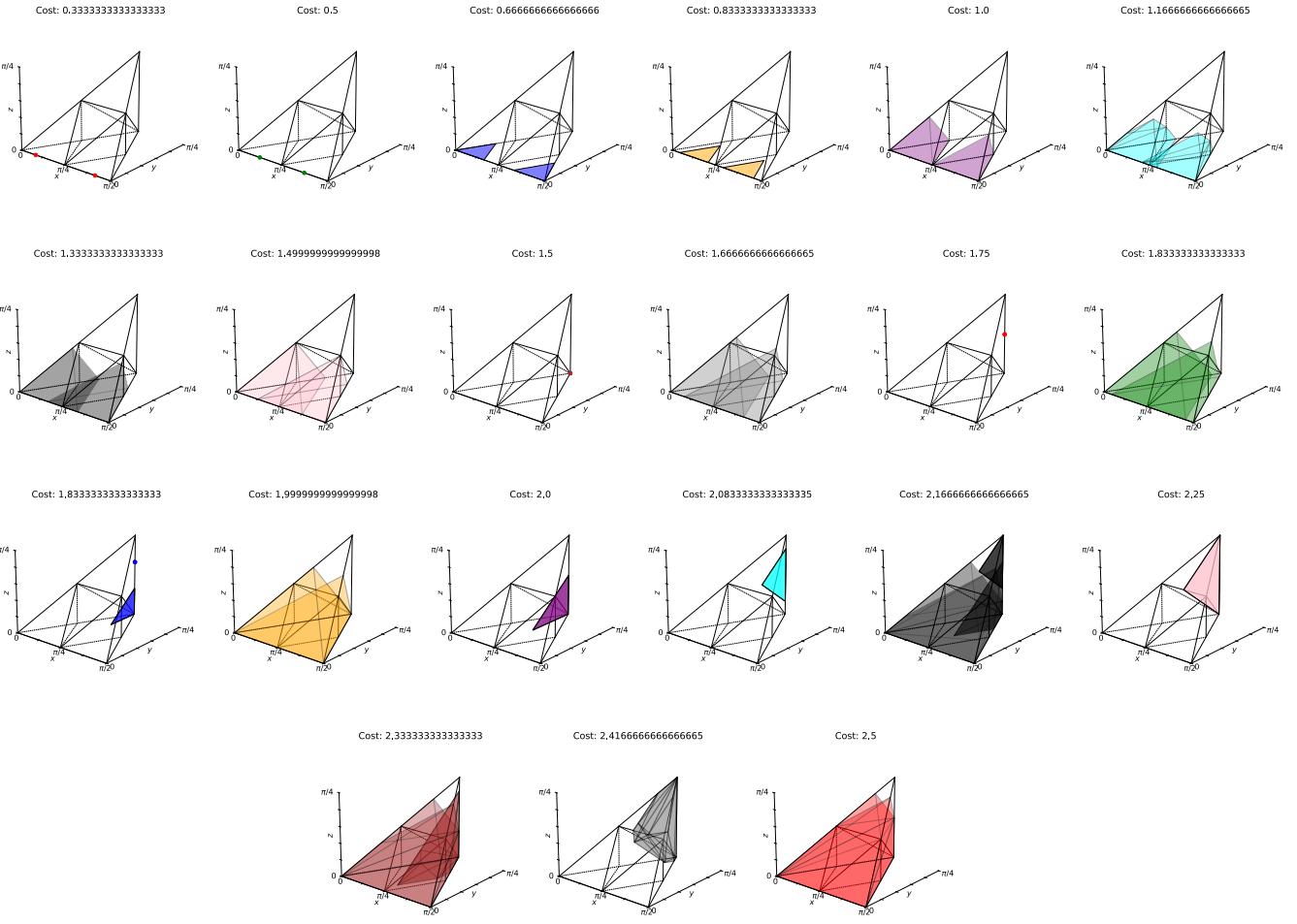
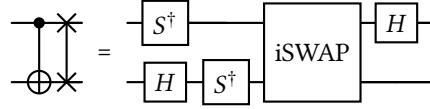


Figure 14. Coverage set for ZZPhase_ISA.

A.3 2Q gate mirroring

The mirror symmetry of a 2Q gate U is defined as the composition of the original gate and a SWAP gate [?], i.e., $\text{SWAP} \cdot U$. For example, CX and iSWAP is a typical pair of mirror gates as shown below.



In general, the mirroring rule for Canonical coefficients is described as

$$\text{SWAP} \cdot \text{Can}(a, b, c) \sim \left(a + \frac{1}{2}, b + \frac{1}{2}, c + \frac{1}{2} \right) \sim \left(a + \frac{1}{2} - 1, b + \frac{1}{2} - 1, c + \frac{1}{2} - 1 \right) \sim \begin{cases} \left(\frac{1}{2} - c, \frac{1}{2} - b, a - \frac{1}{2} \right), & \text{if } c \geq 0 \\ \left(\frac{1}{2} + c, \frac{1}{2} - b, \frac{1}{2} - a \right), & \text{if } c < 0 \end{cases}. \quad (11)$$

The mirror pair of CX and iSWAP is a special case implying that a CX-iSWAP combination ISA could result in lower overhead in routing-synthesis collaborative optimization. [?] once considers inserting SWAP gates to get mirrored gates with lower synthesis overhead compared to the original gates, given the all-to-all topology and continuous ZZ(θ) gate set on ion-trapped hardware. [?] discusses that integrating $\sqrt{\text{iSWAP}}$'s mirror gate, i.e, ECP $\sim \text{Can}\left(\frac{1}{4}, \frac{1}{4}, 0\right)$ gate, into the powerful SQiSW ISA, could further improve the ISA's synthesis capability and end-to-end routing-synthesis co-optimization on limited topologies.

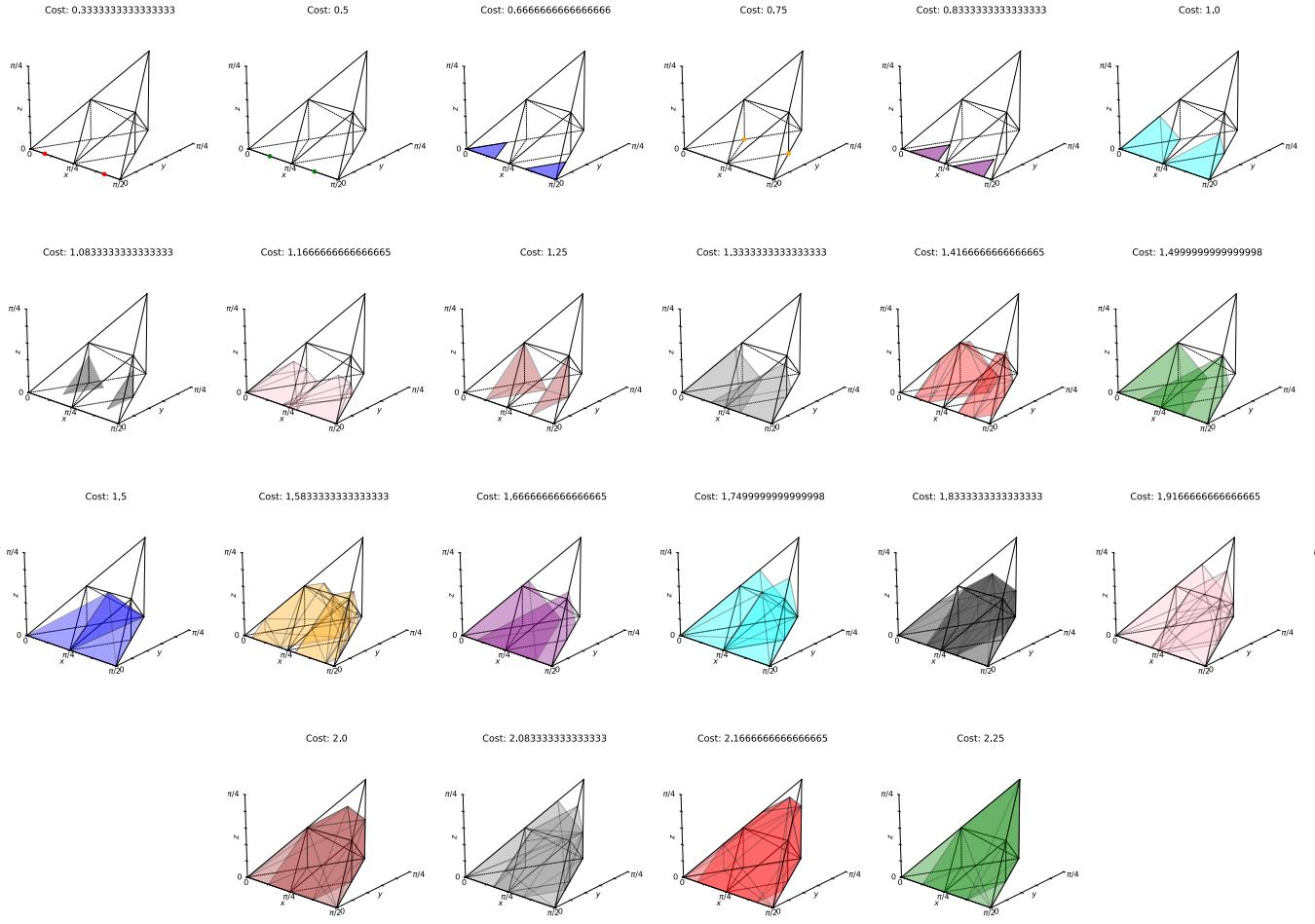


Figure 15. Coverage set for Het ISA.

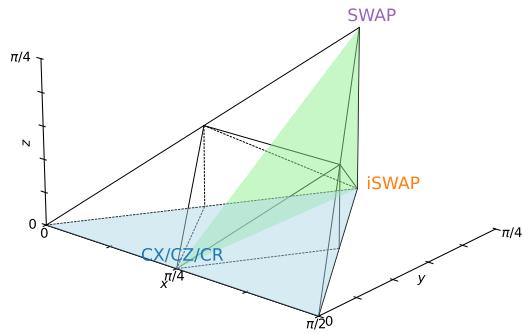


Figure 16. Morir symmetry for $\text{Can}(a, b, 0)$ and $\text{Can}(\frac{1}{2}, b', c')$ gate families.

B Commutative relation of canonical gates

Herein we present detailed proof for ???. The *if* direction is trivial, and hence we justify the *only if* direction, relying on the following two lemmas.

Lemma 1. Let A, B be two Hermitian matrices with eigenvalues in the range $[-2, 2]$. If $[e^{-i\frac{\pi}{2}A}, e^{-i\frac{\pi}{2}B}] = 0$ then $[A, B] = 0$.

Proof. This follows from the fact that compatible observables (commuting operators) can be simultaneously diagonalized. In this case, the respective unitary matrix $e^{-i\frac{\pi}{2}A}$ commutes with $e^{-i\frac{\pi}{2}B}$. Denote by A_λ the eigenspace corresponding to the eigenvalue λ of $e^{-i\frac{\pi}{2}A}$, i.e. $e^{-i\frac{\pi}{2}A} = \bigoplus_\lambda \lambda A_\lambda$. Then we have

$$\forall \vec{v} \in A_\lambda, e^{-i\frac{\pi}{2}B} e^{-i\frac{\pi}{2}A} \vec{v} = e^{-i\frac{\pi}{2}B} \lambda \vec{v} = \lambda e^{-i\frac{\pi}{2}B} \vec{v} = e^{-i\frac{\pi}{2}A} e^{-i\frac{\pi}{2}B} \vec{v}, \quad (12)$$

and thus $e^{-i\frac{\pi}{2}B} \vec{v} \in A_\lambda$. Thus A_λ is $e^{-i\frac{\pi}{2}B}$ -invariant and the restriction $e^{-i\frac{\pi}{2}B}|_{A_\lambda}$ of $e^{-i\frac{\pi}{2}B}$ to A_λ is still unitary since it preserves inner products. Hence it is diagonalizable and we can find an orthonormal basis $w_{\lambda_1}, w_{\lambda_2}, \dots, w_{\lambda_k}$ consisting of eigenvectors of $e^{-i\frac{\pi}{2}B}|_{A_\lambda}$. Note that these are also eigenvectors of $e^{-i\frac{\pi}{2}A}$ (with eigenvalue λ). Following the same token as above, for each eigenspace E_{λ_i} of $e^{-i\frac{\pi}{2}A}$, we can construct an orthonormal basis β_i for it consisting of eigenvectors of $e^{-i\frac{\pi}{2}B}$. Finally since the eigenspaces of different eigenvalues of $e^{-i\frac{\pi}{2}A}$ are orthogonal to each other, $\beta = \cup_i \beta_i$ forms an orthonormal basis of the entire Hilbert space \mathcal{H}_n consisting of the coeigenvectors of both $e^{-i\frac{\pi}{2}A}$ and $e^{-i\frac{\pi}{2}B}$.

Now let U be a unitary matrix with the vectors in β being its columns, then

$$\begin{aligned} U^\dagger e^{-i\frac{\pi}{2}A} U &= D_A \\ U^\dagger e^{-i\frac{\pi}{2}B} U &= D_B \end{aligned} \quad (13)$$

In general, an eigenvector of $e^{-i\frac{\pi}{2}A}$ need *not* be that of A . However, since A has its eigenvalues in the range $[-2, 2]$, the map

$$f : [-2, 2] \rightarrow U(1), a \rightarrow e^{-i\frac{\pi}{2}a} \quad (14)$$

is injective. Consequently different eigenvalues of A correspond to different eigenvalues of $e^{-i\frac{\pi}{2}A}$, and hence the eigenspaces of $e^{-i\frac{\pi}{2}A}$ and A coincide. Therefore, we have that

$$\begin{aligned} U^\dagger A U &= \Sigma_A \\ U^\dagger B U &= \Sigma_B \end{aligned} \quad (15)$$

and since $[\Sigma_A, \Sigma_B] = 0$ as they are diagonal, $[A, B] = 0$. We obtain the desired result. \square

Lemma 2. Let $P_1 = (a_1 X_1 X_2 + b_1 Y_1 Y_2 + c_1 Z_1 Z_2) I_3$, $P_2 = I_1 (a_2 X_2 X_3 + b_2 Y_2 Y_3 + c_2 Z_2 Z_3)$ with $|c_1| \leq b_1 \leq a_1 \leq \frac{1}{2}$, $|c_2| \leq b_2 \leq a_2 \leq \frac{1}{2}$. If $[P_1, P_2] = 0$ and $P_1, P_2 \neq 0$, then $b_1 = b_2 = c_1 = c_2 = 0$.

Proof. Consider the product $P_1 P_2$. We assume for the sake of contradiction that $b_1 \neq 0$. Using $[X, Y] = 2iZ$, $[Y, Z] = 2iX$, $[Z, X] = 2iY$, we expand

$$[P_1, P_2] = 2i(a_1 b_2 X_1 Z_2 Y_3 - b_1 a_2 Y_1 Z_2 X_3 + b_1 c_2 Y_1 X_2 Z_3) - 2i(a_1 c_2 X_1 Y_2 Z_3 + c_1 a_2 Z_1 Y_2 X_3 + c_1 b_2 Z_1 X_2 Y_3).$$

Since the each Pauli string is linearly independent in the 8×8 operator basis, e.g. term $Y_1 Z_2 X_3$ cannot be canceled out by any other terms, contradictory to the fact that $[P_1, P_2] = 0$. Hence, vanishing of $[P_1, P_2]$ requires

$$a_1 b_2 = a_1 c_2 = b_1 c_2 = b_1 a_2 = c_1 a_2 = c_1 b_2 = 0.$$

Since $P_1, P_2 \neq 0$, at least a_1, a_2 is nonzero, leading to $b_1 = b_2 = c_1 = c_2 = 0$. \square

Using ?? and ?? above, it is straightforward to prove ?. We see that $\|P_1\| \leq \|a_1 X_1 X_2 I_3\| + \|b_1 Y_1 Y_2 I_3\| + \|c_1 Z_1 Z_2 I_3\| \leq |a_1| + |b_1| + |c_1| \leq \frac{3}{2}$, where $\|\cdot\|$ is the operator norm. Hence, eigenvalues of P_1 are in range of $[-2, 2]$. Same as the eigenvalues of P_2 . Now if $[e^{-i\frac{\pi}{2}P_1}, e^{-i\frac{\pi}{2}P_2}] = 0$, then we have that $[P_1, P_2] = 0$ according to ??, and thus $b_1 = b_2 = c_1 = c_2 = 0$ according to ??, which proves the *only if* direction.

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