

A Verified Optimizer for Quantum Circuits



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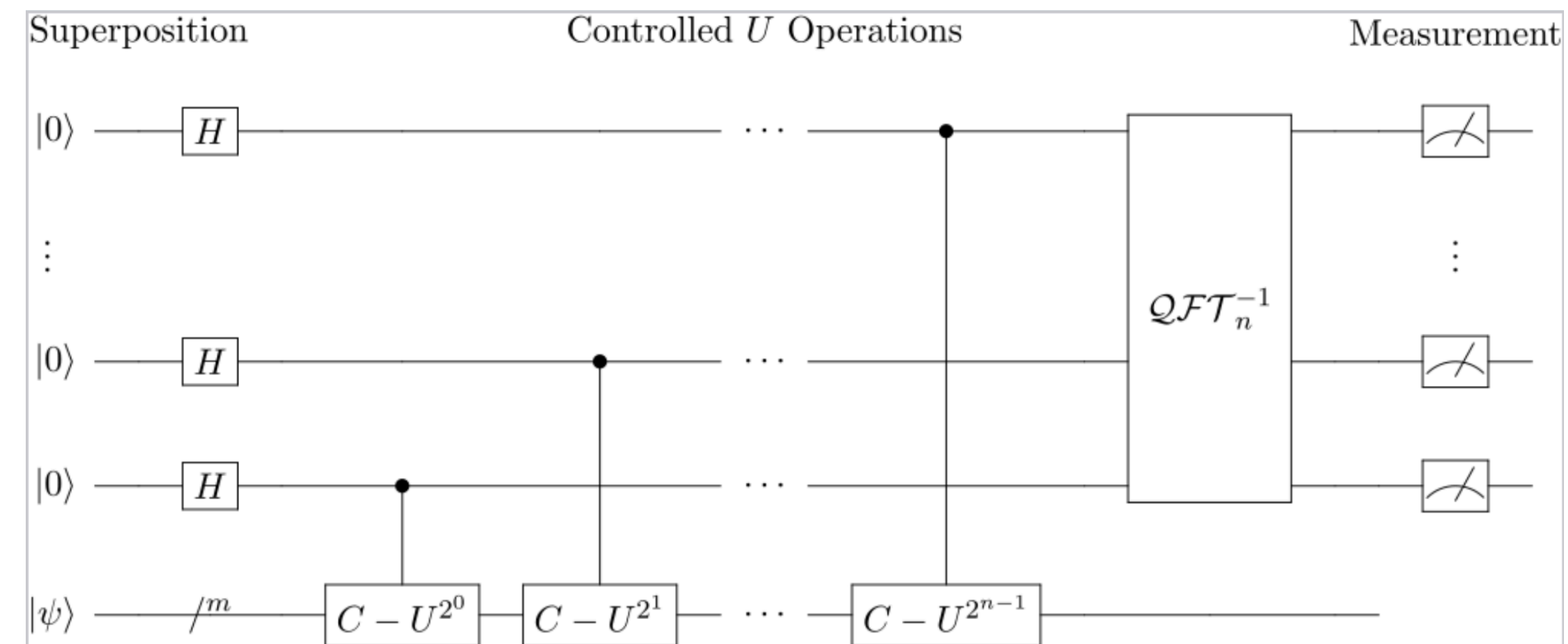
POPL 2021



Image from <https://www.ibm.com/quantum-computing/>

Writing Quantum Programs is Hard

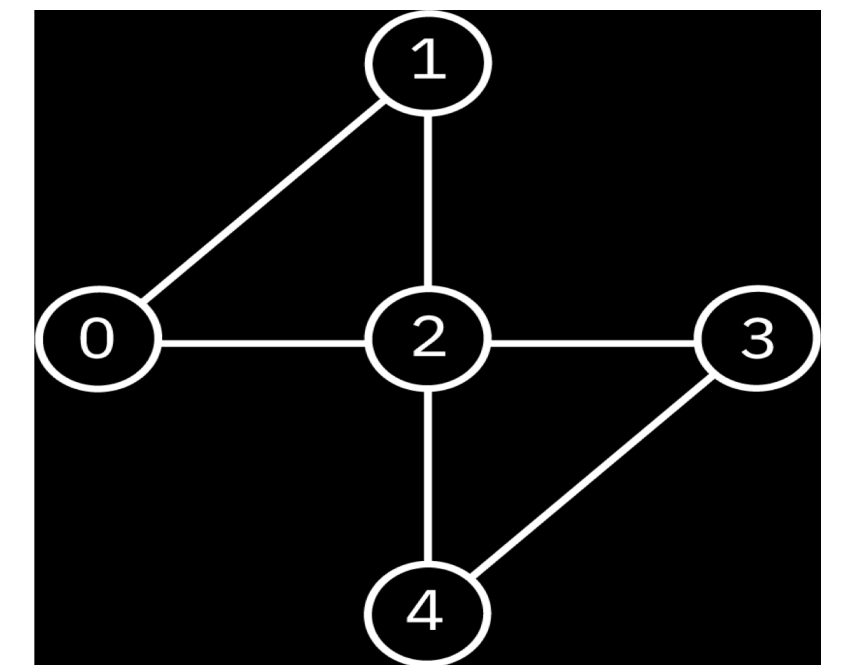
- Quantum indeterminacy \Rightarrow quantum programs are **probabilistic**
- Quantum programs are often written as **circuits**



- Quantum programs use **new primitives**
 - E.g. “prepare a uniform superposition”, “perform a Fourier transform”

Quantum Machines are Limited

- Machines today have a **few, unreliable qubits**
 - Typically 15-50 qubits in total
 - In the near future, we can expect machines with a few hundred qubits, able to run up to 1000 two-qubit gates
- They also have **hardware-specific constraints**
 - Limited set of available operations
 - Only allow two-qubit gates between certain pairs of qubits



Noisy, Intermediate Scale Quantum (NISQ) Computing -Preskill

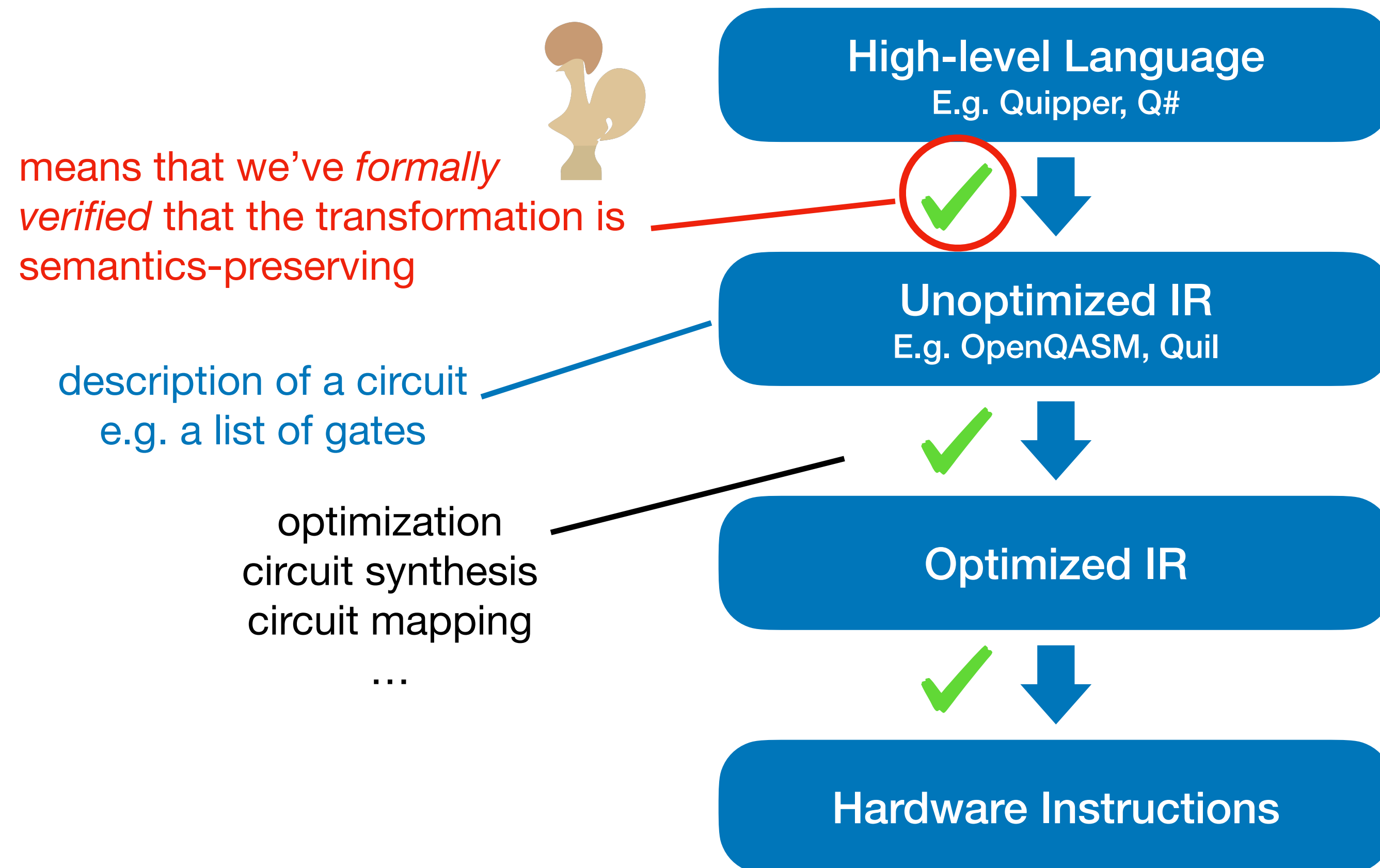
Quantum Compilers are Complicated

- Quantum compilers need to perform **sophisticated transformations** to account for limited resources, hardware constraints
- These transformations are hard to write... and harder to debug
 - Is an unexpected result due to a program bug? machine error? quantum indeterminacy?

The image shows three overlapping GitHub issue tracker screenshots. The top-left screenshot is for **rigetti / pyquil**, showing 120 open issues. The middle-left screenshot is for **quantumlib / Cirq**, showing 296 open issues. The rightmost screenshot is for **Qiskit / qiskit**, showing 62 open issues. A specific issue in the qiskit tracker is highlighted: **Issue with circuit.draw('mpl') when used in Jupyter Notebook.** (bug), #1137, opened 4 days ago by Archit3115. The qiskit interface also shows 15 labels and 0 milestones.

Verified Compiler Stack

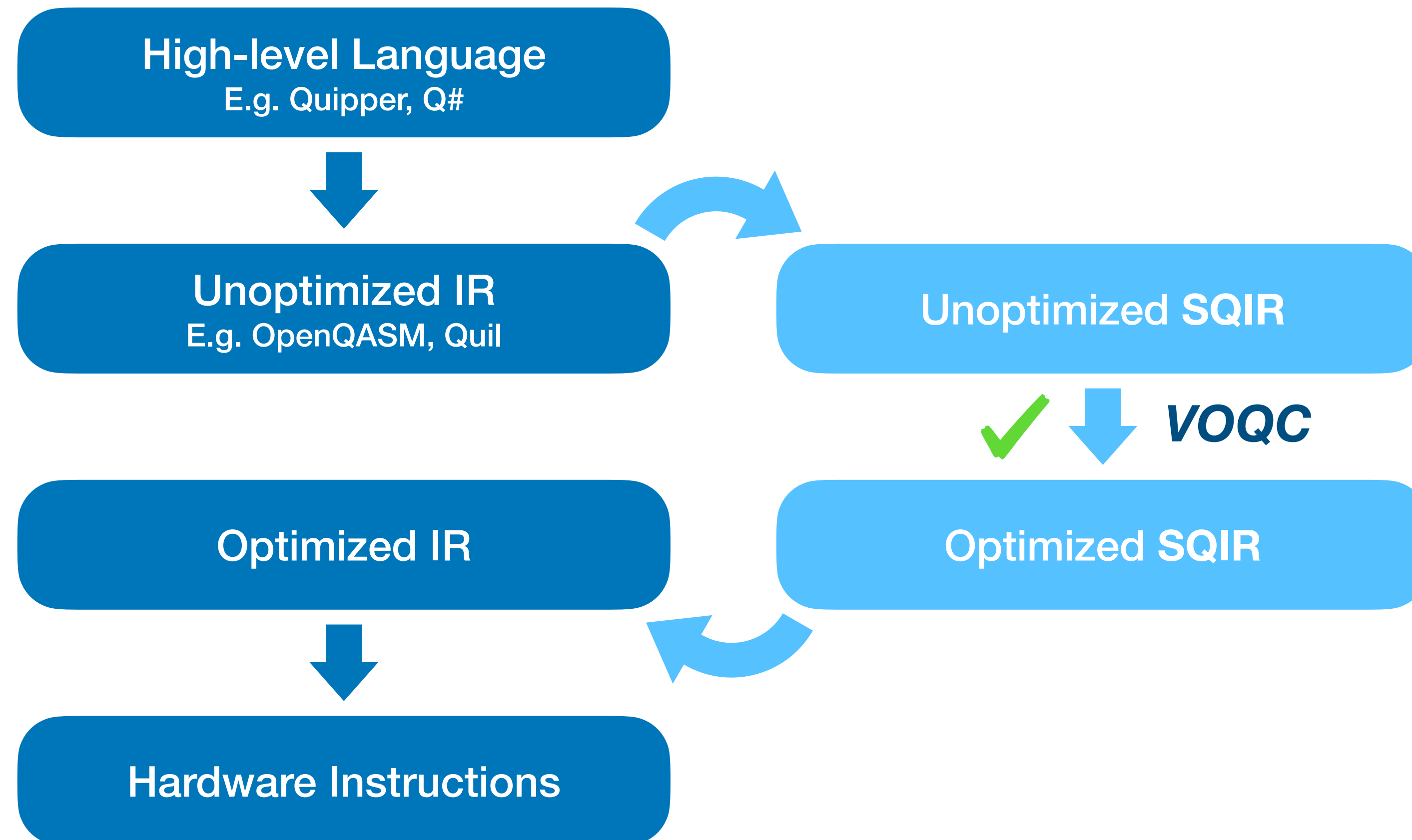
- End goal: *verified compiler stack* for quantum programs



- Challenge: The semantics of **quantum programs is very different** from classical programs
 - States represented as matrices of complex numbers
 - Programs involve probabilities, trigonometry
- Requires development of **new frameworks, libraries, and automation**

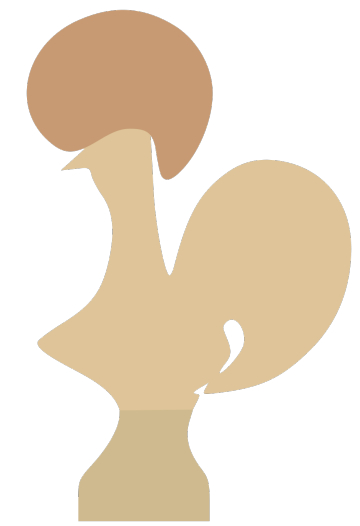
SQIR and VOQC

- Our paper: **VOQC**, a *Verified Optimizer for Quantum Circuits*, which is built on top of **SQIR**, a *Small Quantum Intermediate Representation* designed for proof



SQIR and VOQC

- SQIR and VOQC are implemented in around 11k lines of Coq code
 - 3.5k for core SQIR, source program proofs
 - 7.5k for VOQC libraries, optimizations, circuit mapper
 - We extend [QWIRE](#)'s matrix & complex number libraries by 3k lines
- Long version of the paper available at <https://arxiv.org/abs/1912.02250>
- Code available at <https://github.com/inQWIRE/SQIR>
- Artifact available at <https://zenodo.org/record/4268896>



Outline

- Intro to Quantum Programming
- SQIR
- VOQC
- Future Work

Qubits

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$|0\rangle$

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

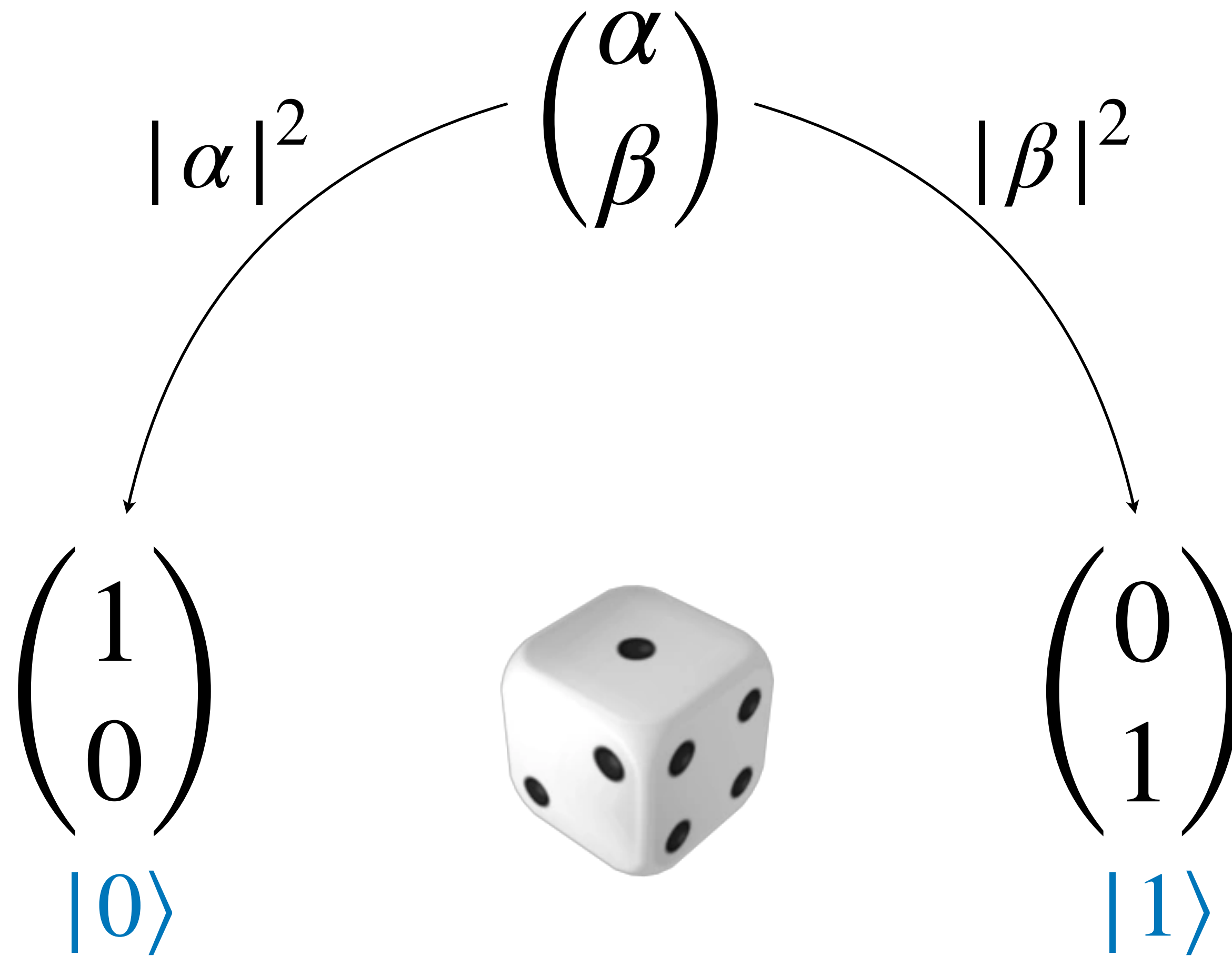
$$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$|1\rangle$

$$|\alpha|^2 + |\beta|^2 = 1$$

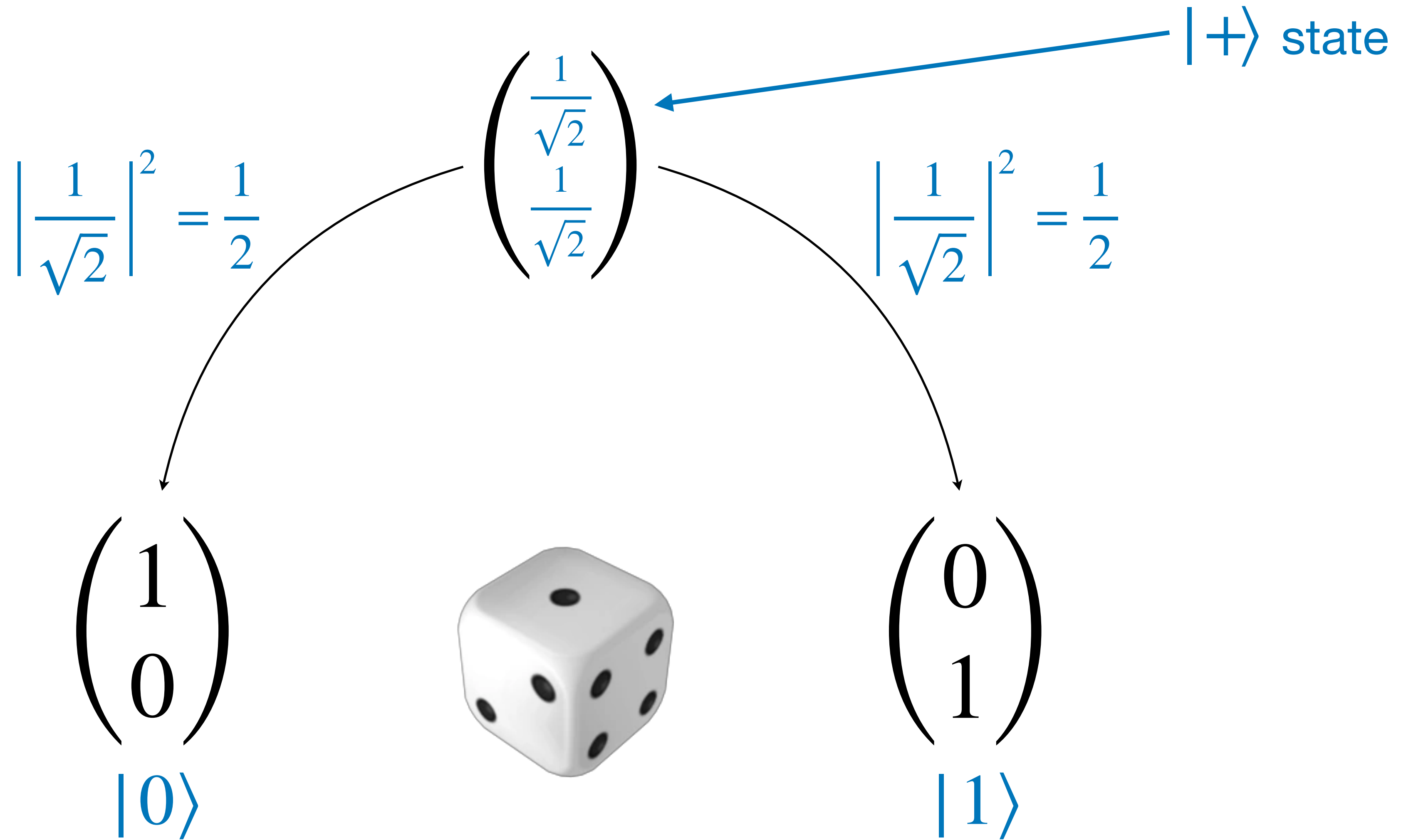
Superposition: Qubits can be in multiple states (0 or 1) at once

Measurement



Measurement: Looking at a qubit probabilistically turns it into a bit.

Measurement



Measurement: Looking at a qubit probabilistically turns it into a bit.

Operators

A unitary operator transforms, or *evolves*, a state

$$H |0\rangle = |+\rangle$$

$$H |+\rangle = |0\rangle$$

This is the *Hadamard* operator, H
(which is its own inverse)

Operators

Operators are represented as *unitary matrixes*

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

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

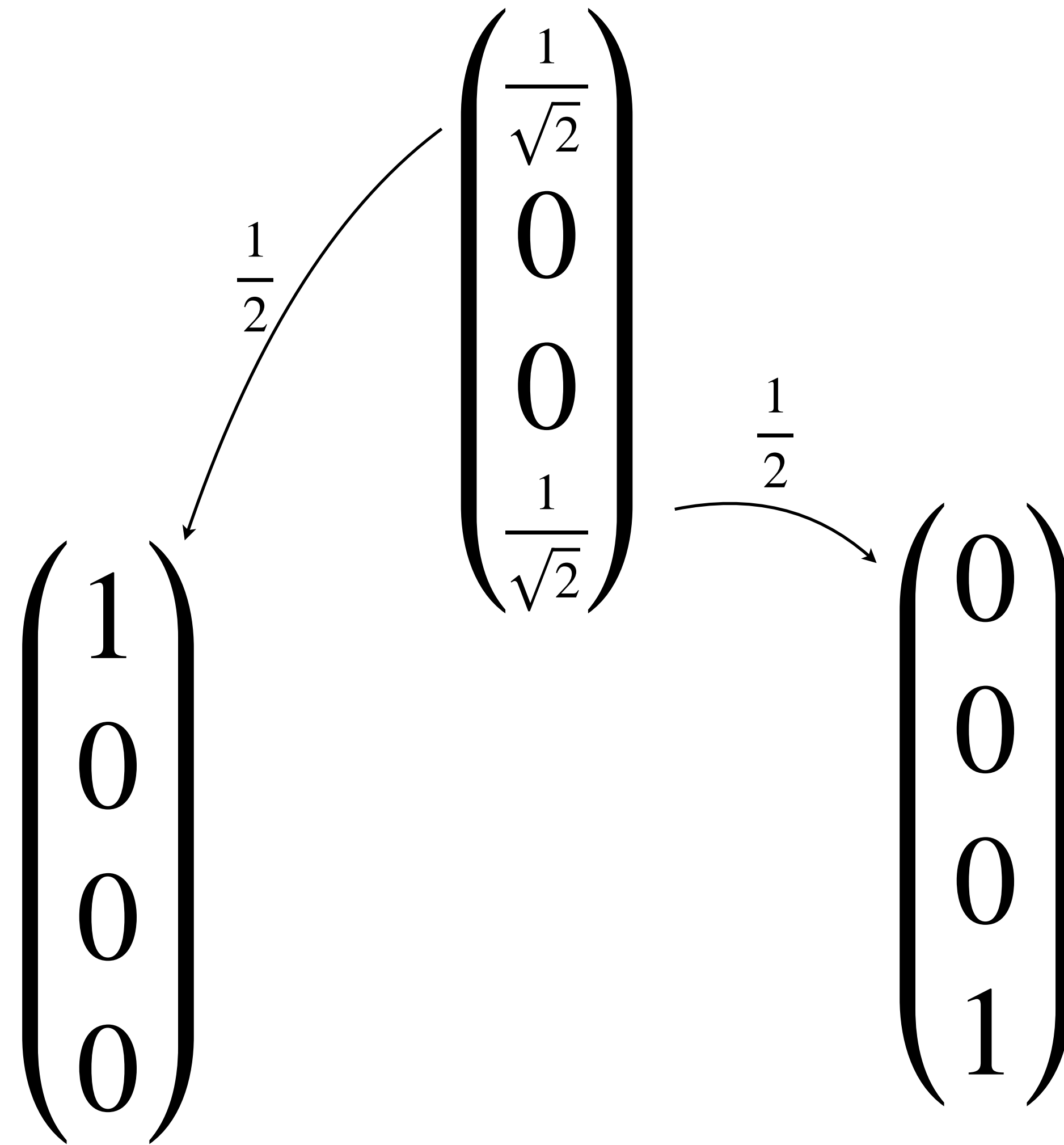
Multiple Qubits

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 1 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 1 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

$$|+\rangle \otimes |0\rangle = |+\rangle |0\rangle \quad \text{or} \quad |+0\rangle$$

Multi-qubit states are constructed via the tensor product

Measurement 2.0



Measurement 2.0

$$\begin{array}{ccc} & \begin{array}{c} \frac{1}{2} \\ \curvearrowright \\ \left(\begin{array}{c} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \end{array} \right) \\ \curvearrowleft \\ \frac{1}{2} \end{array} & \\ \left(\begin{array}{c} 1 \\ 0 \end{array} \right) \otimes \left(\begin{array}{c} 1 \\ 0 \end{array} \right) & & \left(\begin{array}{c} 0 \\ 1 \end{array} \right) \otimes \left(\begin{array}{c} 0 \\ 1 \end{array} \right) \\ |00\rangle & & |11\rangle \end{array}$$

Entanglement

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 1 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$? \otimes ?$$

Entangled qubits are not probabilistically independent — they cannot be decomposed. Connection at a distance!

Multi-Qubit Unitaries

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\text{CNOT } |+\rangle |0\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$$

More Unitaries

A *universal* sets of unitaries can be used to approximate any unitary operator using a finite sequence of gates

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{bit flip}$$

$|0\rangle \mapsto |1\rangle$
 $|1\rangle \mapsto |0\rangle$

$$R_z(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix} \quad \text{phase shift}$$

$|0\rangle \mapsto |0\rangle$
 $|1\rangle \mapsto e^{i\theta} |1\rangle$

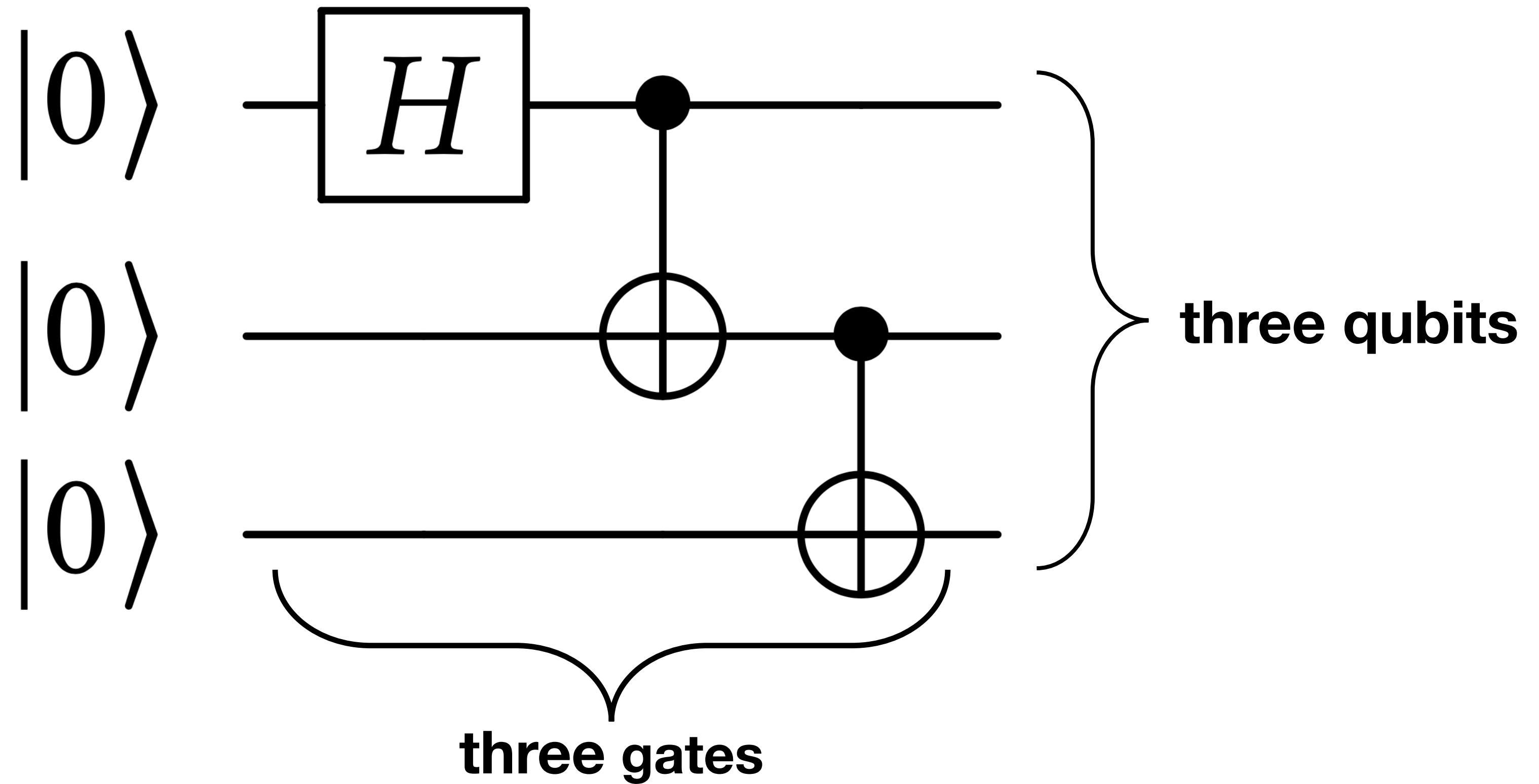
General Quantum States

- So far we have seen *pure states*
 - E.g. $|0\rangle, |1\rangle, |+\rangle$
- A *mixed state* is a (classical) probability distribution over pure states
 - E.g. $\begin{cases} |0\rangle \text{ with probability } 1/2 \\ |1\rangle \text{ with probability } 1/2 \end{cases}$
- Density matrices allow us to describe both pure and mixed states

$$\rho = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

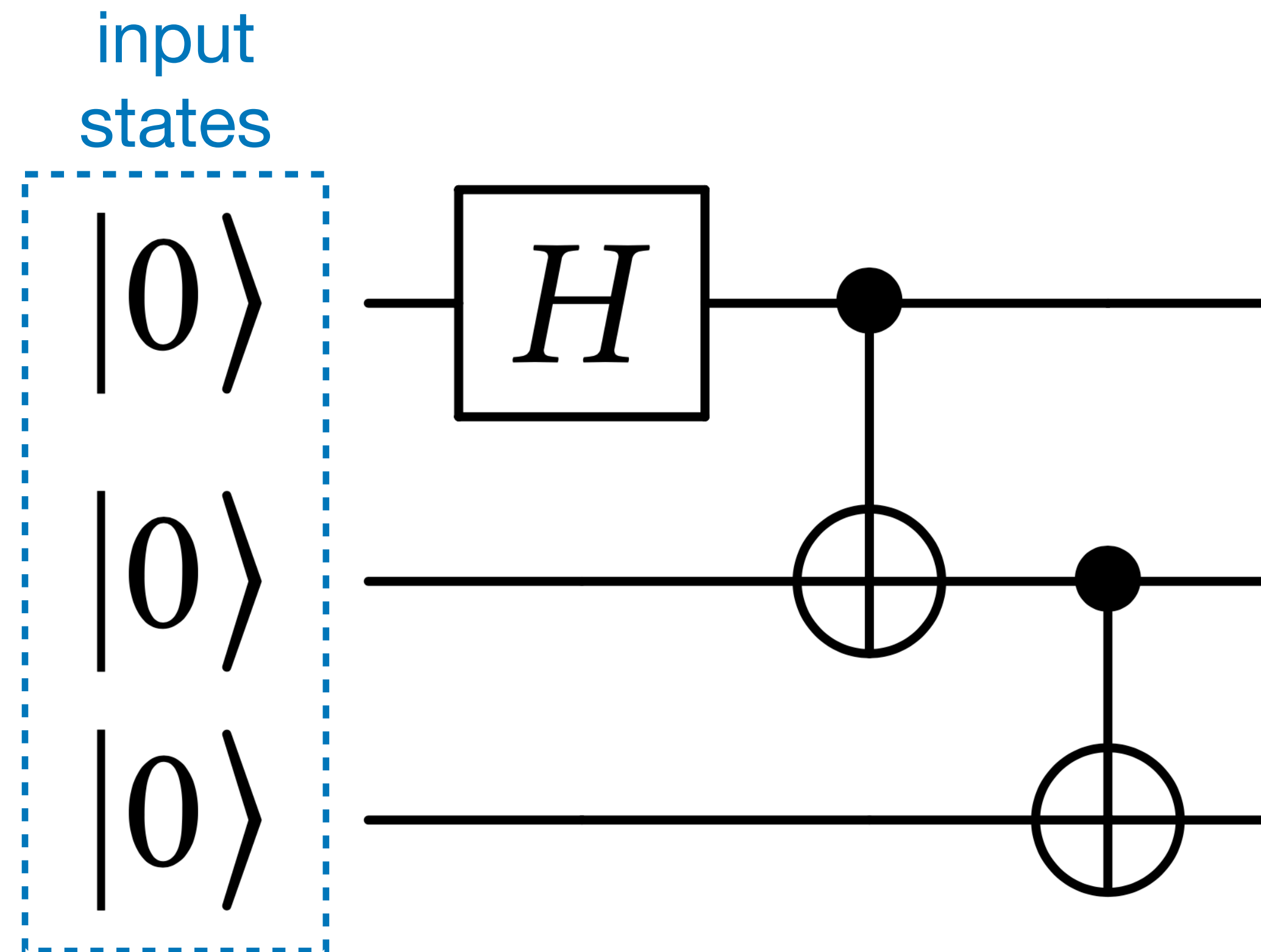
Circuits

Quantum programs are often written as circuits



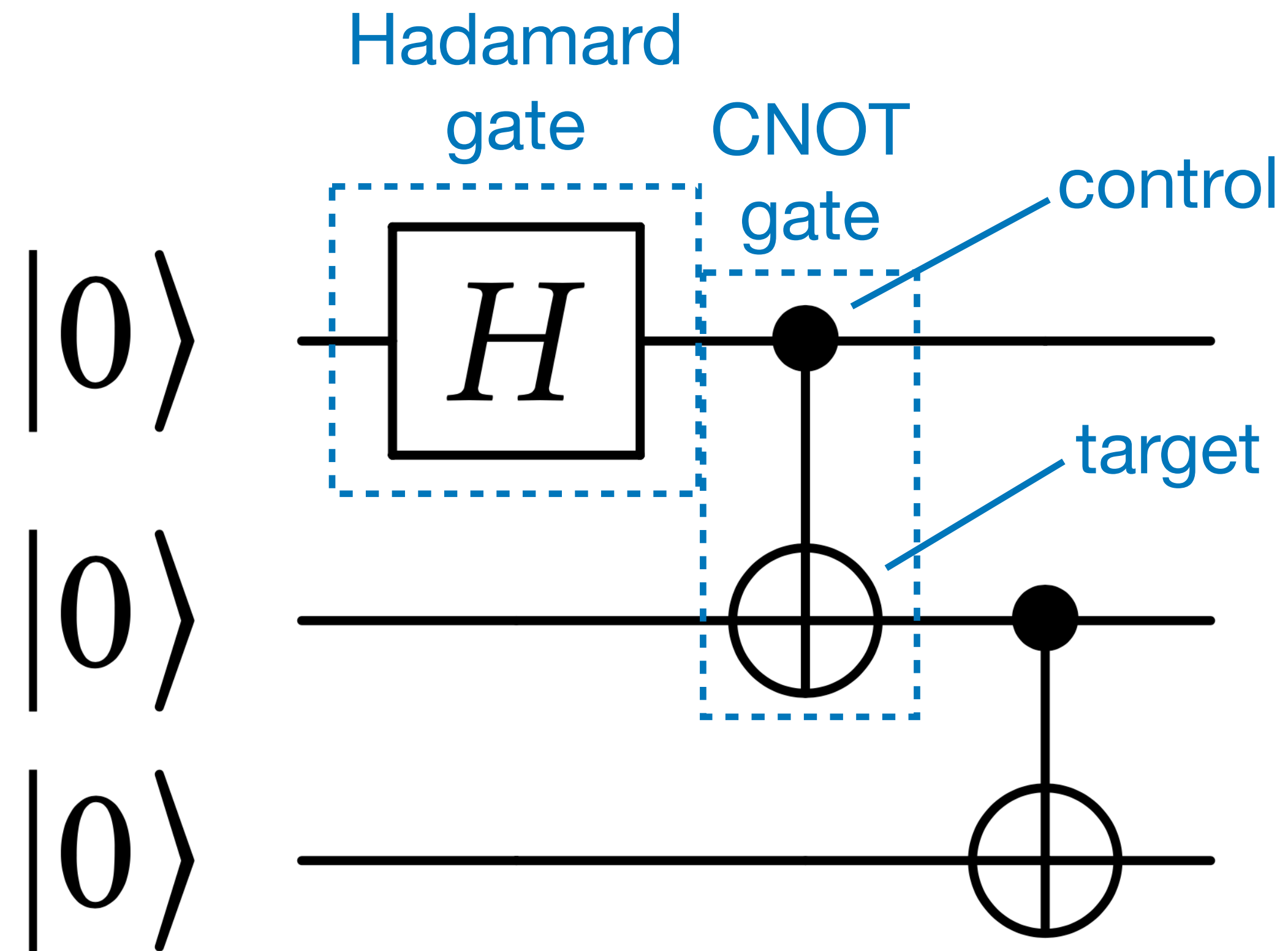
Circuits

Quantum programs are often written as circuits

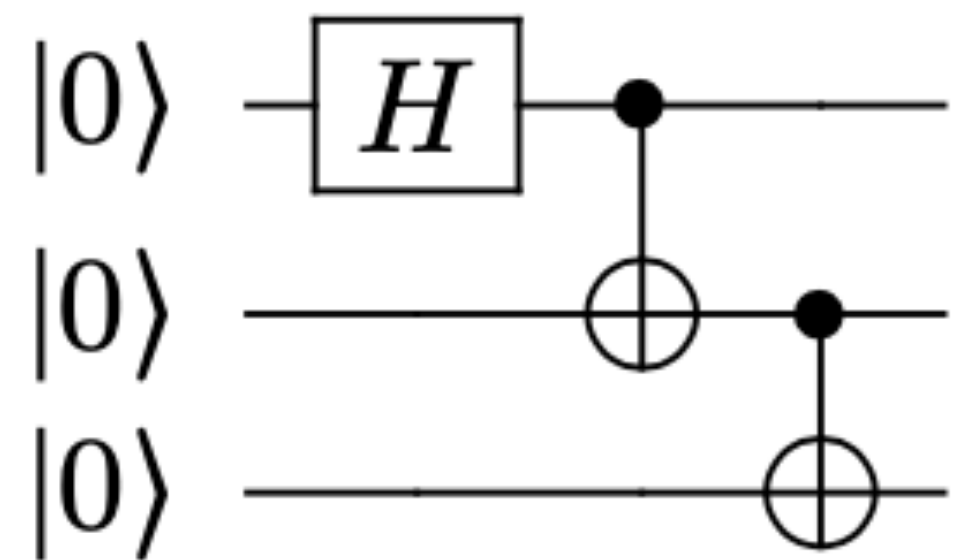


Circuits

Quantum programs are often written as circuits



Quantum Programming



Circuit

```
H 0
CNOT 0 1
CNOT 1 2
```

Quil (Rigetti)

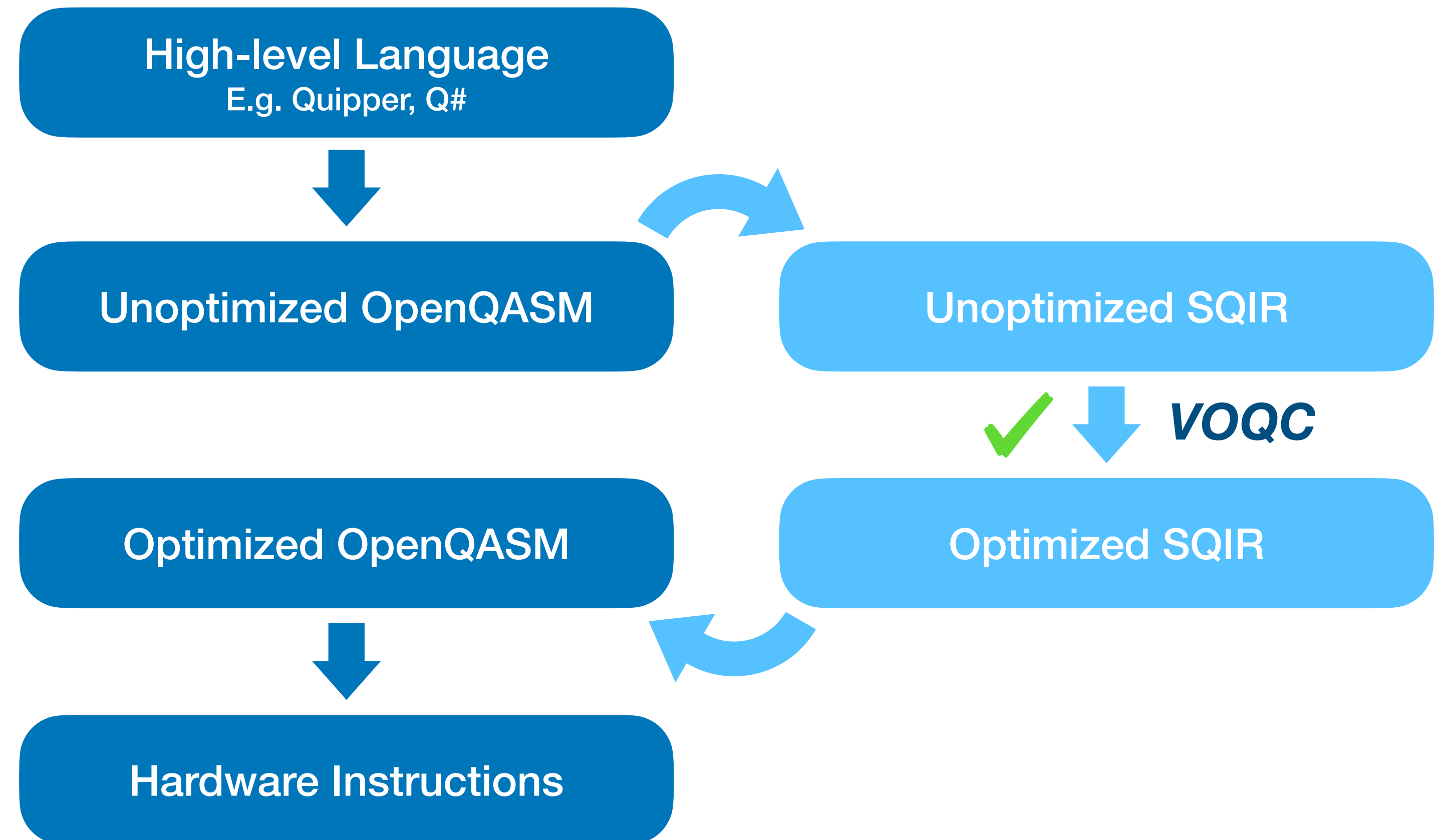
```
def ghz_state(qubits):
    program = Program()
    program += H(qubits[0])
    for q1,q2 in zip(qubits, qubits[1:]):
        program += CNOT(q1, q2)
    return program
```

PyQuil (Rigetti)

Many “high-level” quantum programming languages (e.g. [PyQuil](#), [Cirq](#), [Qiskit](#), [Quipper](#), [QWIRE](#)) are libraries for constructing circuits

SQIR: Small Quantum Intermediate Representation

- SQIR programs, embedded in Coq, are assigned a *denotational semantics* of matrices
- Two variations of SQIR
 - *Unitary SQIR*: No measurement
 - *Full SQIR*: Adds branching measurement operator



Unitary SQIR

- Semantics parameterized by *gate set G* and *dimension d* of a *global register*

$$U ::= U_1; U_2 \mid G \ q \mid G \ q_1 \ q_2$$

E.g. $apply_1(X, q, d) = I_{2^q} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes I_{2^{(d-q-1)}}$

- The denotation (semantics) of U is a $2^d \times 2^d$ unitary matrix

$$\begin{aligned} \llbracket U_1; U_2 \rrbracket_d &= \llbracket U_2 \rrbracket_d \times \llbracket U_1 \rrbracket_d \\ \llbracket G_1 \ q \rrbracket_d &= \begin{cases} apply_1(G_1, q, d) & \text{well-typed} \\ 0_{2^d} & \text{otherwise} \end{cases} \\ \llbracket G_2 \ q_1 \ q_2 \rrbracket_d &= \begin{cases} apply_2(G_2, q_1, q_2, d) & \text{well-typed} \\ 0_{2^d} & \text{otherwise} \end{cases} \end{aligned}$$

$q < d$

$q_1 < d \wedge q_2 < d \wedge q_1 \neq q_2$

Non-Unitary SQIR

- Semantics parameterized by *gate set* G and *dimension* d of a *global register*

$$P ::= \text{skip} \mid P_1; P_2 \mid U \mid \text{meas } q \mid P_1 \mid P_2$$

- The denotation of P is a function over $2^d \times 2^d$ density matrices

$$\begin{aligned} \{\text{skip}\}_d(\rho) &= \rho \\ \{P_1; P_2\}_d(\rho) &= (\{P_2\}_d \circ \{P_1\}_d)(\rho) \\ \{U\}_d(\rho) &= \llbracket U \rrbracket_d \times \rho \times \llbracket U \rrbracket_d^\dagger \\ \{\text{meas } q \mid P_1 \mid P_2\}_d(\rho) &= \{P_2\}_d(|0\rangle_q \langle 0| \times \rho \times |0\rangle_q \langle 0|) \\ &\quad + \{P_1\}_d(|1\rangle_q \langle 1| \times \rho \times |1\rangle_q \langle 1|) \end{aligned}$$

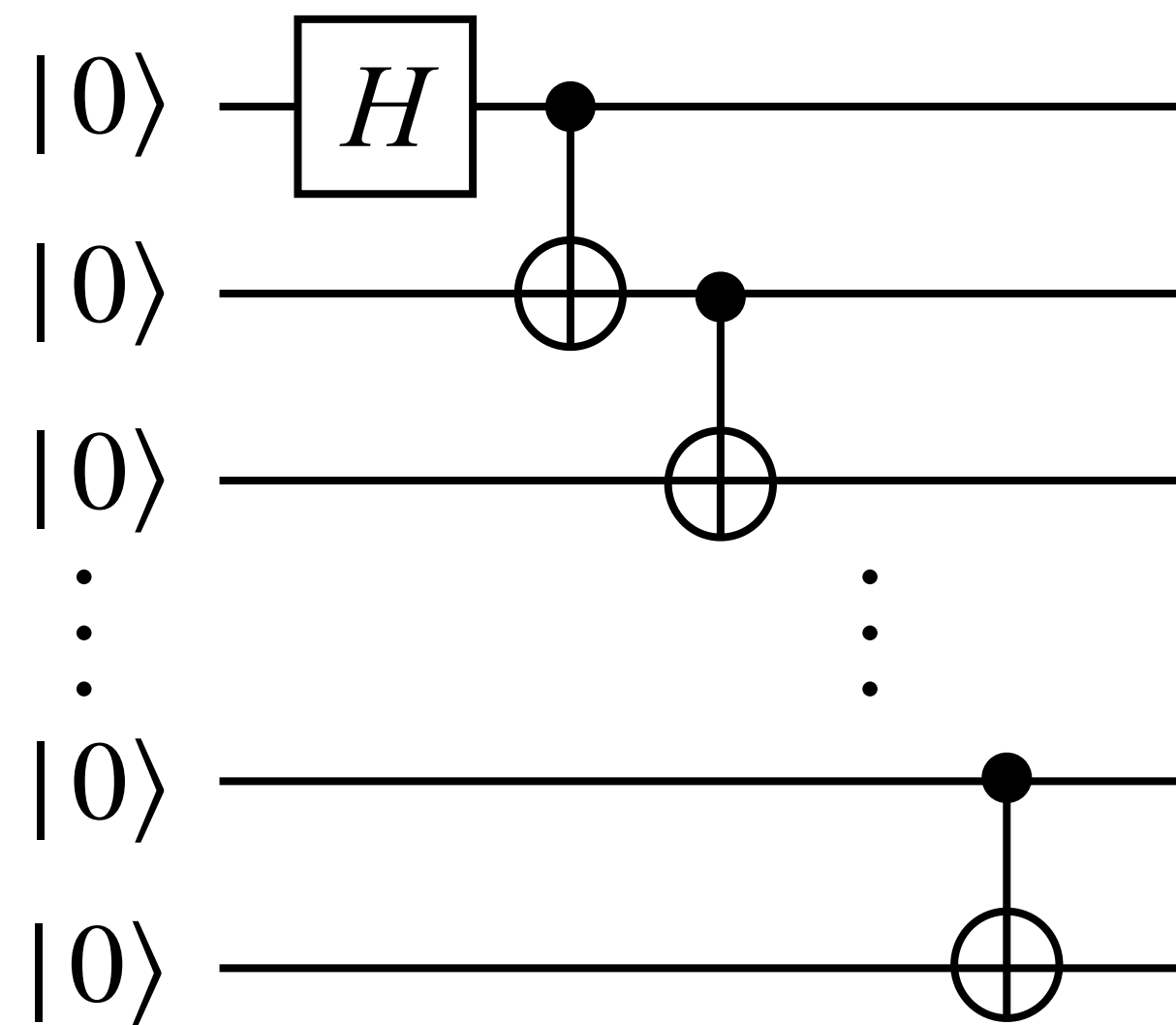
Standard semantics;
also used in QHL¹
and QWIRE²

¹ Ying. *Floyd-Hoare logic for quantum programs*. TOPLAS 2012.

² Paykin et al. *QWIRE: A core language for quantum circuits*. POPL 2017.

SQIR Metaprogramming

- SQIR programs just express circuits. We can express parameterized circuit families using Coq as a meta programming language



```
Fixpoint ghz (n : ℕ) : ucom base n :=  
  match n with  
  | 0 => SKIP  
  | 1 => H 0  
  | S n' => ghz n'; CNOT (n'-1) n'  
end.
```

- The ghz Coq function returns a SQIR program (of type ucom base n) whose semantics is the n-qubit GHZ state

Proofs of Correctness in Coq

- We might like to prove that evaluating `ghz n` on $|0\rangle^{\otimes n}$ produces $|GHZ^n\rangle$
 - where $|GHZ^n\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})$

```
Definition GHZ (n : N) : Vector (2 ^ n) :=
  match n with
  | 0      => I 1
  | S n' => 1/sqrt 2 * |0>^n + 1/sqrt 2 * |1>^n
  end.
```

```
Lemma ghz_correct : forall n : N,
  n > 0 -> [[ghz n]]_n x |0>^n = GHZ n.
```

Proof.

...

Qed.

Designed for Proof

- SQR was conceived as a simplified version of QWIRE¹; we use QWIRE's libraries for matrices and complex numbers
- SQR proofs are simpler than QWIRE's because we:
 1. Reference **qubits using concrete indices** (`CNOT 2 1` vs. `CNOT x y`)
 - ▶ Easy to map gate arguments to the right column/row in the matrix
 - ▶ Disjointness is *syntactic*; important for proving equivalences
 2. **Separate the unitary core from the full language** with measurement
 - ▶ Unitary matrix semantics simpler than *density matrix* formulation
 3. Assign a **denotation of the zero-matrix to ill-typed programs**
 - ▶ E.g., `CNOT 1 1`, which violates no-cloning

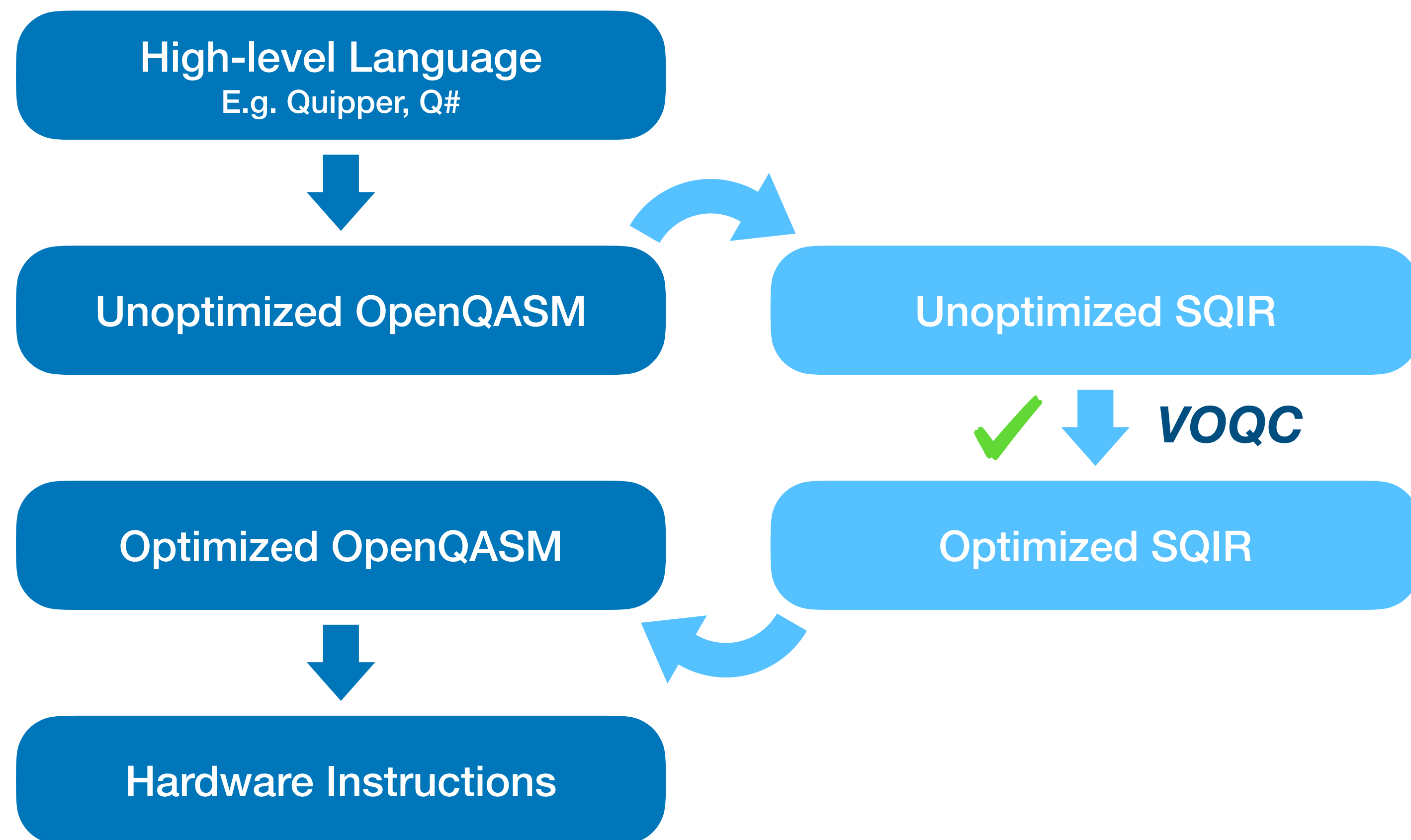
¹Paykin, Rand and Zdancwic. *QWIRE: A core language for quantum circuits*. POPL 2017.

Proofs so Far

- We have formally verified several source programs correct
 - Quantum teleportation / superdense coding
 - GHZ state preparation
 - Deutsch-Jozsa algorithm
 - Simon's algorithm
 - Grover's search algorithm
 - Quantum phase estimation (key part of Shor's algorithm)
- These proofs as well as the basic support of SQIR (lemmas, tactics, etc.) constitute about 3500 lines of Coq code
- For more details see <https://arxiv.org/abs/2010.01240>

VOQC: A Verified Optimizer for Quantum Circuits

- Transformations are represented as Coq functions over SQIR circuits
 - Extracted to executable OCaml code
- We prove (verify) that transformations are *semantics-preserving*
 - Can also prove that the output program respects machine constraints

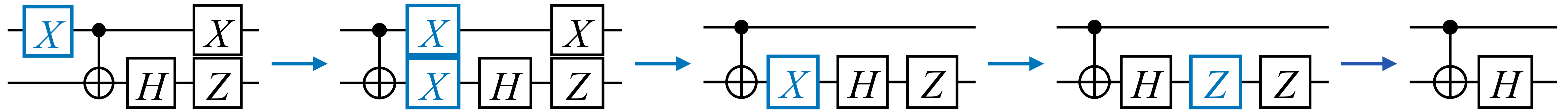


VOQC in Sum

- Most of VOQC (2200 LOC) consists of verified implementations of optimizations developed by Nam et al.¹
 - Replacement (peephole optimizations)
 - Propagation (commutation) and cancellation
 - Rotation merging (non-local coalescing)
- Some optimizations for non-unitary programs, inspired by Qiskit (800 LOC)
 - Remove z-rotations before measurement
 - Classical state propagation
- Another 2100 LOC for program manipulation; 2100 more for circuit mapping

¹Nam, Ross, Su, Childs and Maslov. *Automated Optimization of Large Quantum Circuits with Continuous Parameters*. npj 2018.

Example: X Propagation



- Based on Nam et al¹ “not propagation”
- We verify **semantics-preservation**
 - At each step, the denotation of the program (i.e. unitary matrix) does not change
- We prove this via induction on the structure of the input program
 - ~30 lines to implement optimization
 - ~270 lines to prove semantics-preservation

¹Nam, Ross, Su, Childs and Maslov. *Automated Optimization of Large Quantum Circuits with Continuous Parameters*. npj 2018.

Verifying Matrix Equivalences

- Many proofs use unitary equivalences; e.g., X propagation's proof uses:
 - ▶ X gates cancel: $X\ m; X\ m \equiv I\ m$
 - ▶ X commutes with CNOT control: $X\ m; CNOT\ m\ n \equiv CNOT\ m\ n; X\ m; X\ n$
 - ▶ X commutes with CNOT target: $X\ n; CNOT\ m\ n \equiv CNOT\ m\ n; X\ n$
 - ▶ H transforms X to Z: $X\ m; H\ m \equiv H\ m; Z\ m$
- We prove these as lemmas
 - ▶ Doing so is tedious, so we developed Coq tactics to convert matrix expressions into a *grid normal form* to facilitate automation

Grid Normal Form

- Consider the equivalence $X\ n; CNOT\ m\ n \equiv CNOT\ m\ n; X\ n$
- Per our semantics, this requires proving

$$apply_1(X, n, d) \times apply_2(CNOT, m, n, d) = apply_2(CNOT, m, n, d) \times apply_1(X, n, d)$$

- ▶ where

$$apply_1(X, n, d) = I_{2^n} \otimes \sigma_x \otimes I_{2^q}$$

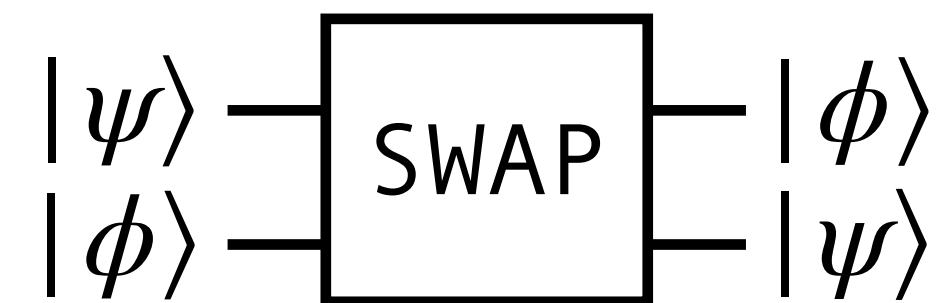
$$apply_2(CNOT, m, n, d) = I_{2^m} \otimes |1\rangle\langle 1| \otimes I_{2^p} \otimes \sigma_x \otimes I_{2^q} + I_{2^m} \otimes |0\rangle\langle 0| \otimes I_{2^p} \otimes I_2 \otimes I_{2^q}$$

- Our automation reduces both sides of the equality to *grid normal form*

$$I_{2^m} \otimes |1\rangle\langle 1| \otimes I_{2^p} \otimes I_2 \otimes I_{2^q} + I_{2^m} \otimes |0\rangle\langle 0| \otimes I_{2^p} \otimes \sigma_x \otimes I_{2^q}$$

Also: Circuit Mapping

- Given an input program & description of machine connectivity, *circuit mapping* produces a program that satisfies connectivity constraints
 - Usually uses SWAP gates to “move” qubits by exchanging their values



- E.g. $\text{CNOT } 0 \ 2$, $\boxed{0} \leftrightarrow \boxed{1} \leftrightarrow \boxed{2} \rightarrow \text{SWAP } 0 \ 1; \text{CNOT } 1 \ 2$
- We prove that the output program is equivalent to the original, up to permutation of indices
 - Above, $[[\text{CNOT } 0 \ 2]]_3 = P \times [[\text{SWAP } 0 \ 1; \text{CNOT } 1 \ 2]]_3$ where P implements the permutation $\{0 \rightarrow 1, 1 \rightarrow 0, 2 \rightarrow 2\}$

Evaluation

- 1 <https://qiskit.org/>
- 2 <https://cqcl.github.io/pytket/build/html/index.html>
- 3 <https://arxiv.org/pdf/1710.07345.pdf>
- 4 <https://arxiv.org/pdf/1303.2042.pdf>
- 5 <https://github.com/Quantomatic/pyzx>

- Is VOQC any good? Maybe we just verified simple optimizations
- So: Compared our *verified* optimizer against existing *unverified* optimizers
 - ▶ IBM Qiskit Terra v0.15.12¹
 - ▶ Cambridge CQC tket v0.6.0²
 - ▶ Nam et al,³ both L and H levels (used by IonQ)
 - ▶ Amy et al⁴
 - ▶ PyZX v0.6.0⁵

Benchmark

- Used **benchmark suite of Amy et al**¹
 - 28 programs: Arithmetic circuits, implementations of multiple-control Toffoli gates, and Galois field multiplier circuits
 - Ranging from 45 to 13,593 gates and 5 to 96 qubits
 - Uses the Clifford+T gate set (CNOT, H, S and T)
- We measured **effectiveness in terms of gate reductions**
 - Both T gate and total
- Measured optimization time (not parsing or printing)

¹Amy, Maslov and Mosca. *Polynomial-Time T-Depth Optimization of Clifford+T Circuits Via Matroid Partitioning*. TCAD 2013.

Results

- 1 <https://qiskit.org/>
- 2 <https://cqcl.github.io/pytket/build/html/index.html>
- 3 <https://arxiv.org/pdf/1710.07345.pdf>
- 4 <https://arxiv.org/pdf/1303.2042.pdf>
- 5 <https://github.com/Quantomatic/pyzx>

Geo. mean compilation times						
Qiskit ¹	tket ²	Nam ³ (L)	Nam (H)	Amy ⁴	PyZX ⁵	VOQC ✓
0.812s	0.129s	0.002s	0.018s	0.007s	0.384s	0.013s

VOQC is the same ballpark

Geo. mean reduction in gate count			
Qiskit	tket	Nam (H)	VOQC ✓
10.1%	10.6%	24.8%	17.8%

VOQC only outperformed by Nam

Geo mean. reduction in T gate count			
Amy	PyZX	Nam (H)	VOQC ✓
39.7%	42.6%	41.4%	41.4%

VOQC only outperformed by PyZX

No Bugs!

Bugs found in prior work^{1,2} via translation validation

Name	Total Gate Count						Name	T-Gate Count					
	Original	Qiskit	t ket)	Nam (L)	Nam (H)	VOQC		Original	Amy	PyZX	Nam (L)	Nam (H)	VOQC
adder_8	900	805	775	646	606	682	adder_8	399	215	173	215	215	215
barenco_tof_3	58	51	51	42	40	50	barenco_tof_3	28	16	16	16	16	16
barenco_tof_4	114	100	100	78	72	95	barenco_tof_4	56	28	28	28	28	28
barenco_tof_5	170	149	149	114	104	140	barenco_tof_5	84	40	40	40	40	40
barenco_tof_10	450	394	394	294	264	365	barenco_tof_10	224	100	100	100	100	100
csla_mux_3	170	156	155	161	155	158	csla_mux_3	70	62	62	64	64	64
csum_mux_9	420	382	361	294	266	308	csum_mux_9	196	112	84	84	84	84
gf2^4_mult	225	206	206	187	187	192	gf2^4_mult	112	68	68	68	68	68
gf2^5_mult	347	318	319	296	296	291	gf2^5_mult	175	111	115	115	115	115
gf2^6_mult	495	454	454	403	403	410	gf2^6_mult	252	150	150	150	150	150
gf2^7_mult	669	614	614	555	555	549	gf2^7_mult	343	217	217	217	217	217
gf2^8_mult	883	804	806	712	712	705	gf2^8_mult	448	264	264	264	264	264
gf2^9_mult	1095	1006	1009	891	891	885	gf2^9_mult	567	351	351	351	351	351
gf2^10_mult	1347	1238	1240	1070	1070	1084	gf2^10_mult	700	410	410	410	410	410
gf2^16_mult	3435	3148	3150	2707	2707	2695	gf2^16_mult	1792	1040	1040	1040	1040	1040
gf2^32_mult	13593	12506	12507	10601	10601	10577	gf2^32_mult	7168	4128	4128	4128	4128	4128
mod5_4	63	58	58	51	51	56	mod5_4	28	16	8	16	16	16
mod_mult_55	119	106	102	91	91	90	mod_mult_55	49	37	35	35	35	35
mod_red_21	278	227	224	184	180	214	mod_red_21	119	73	73	73	73	73
qcla_adder_10	521	469	460	411	399	438	qcla_adder_10	238	162	162	162	162	164
qcla_com_7	443	398	392	284	284	314	qcla_com_7	203	95	95	95	95	95
qcla_mod_7	884	793	780	636	624	723	qcla_mod_7	413	249	237	237	235	249
rc_adder_6	200	170	172	142	140	157	rc_adder_6	77	63	47	47	47	47
tof_3	45	40	40	35	35	40	tof_3	21	15	15	15	15	15
tof_4	75	66	66	55	55	65	tof_4	35	23	23	23	23	23
tof_5	105	92	92	75	75	90	tof_5	49	31	31	31	31	31
tof_10	255	222	222	175	175	215	tof_10	119	71	71	71	71	71
vbe_adder_3	150	138	139	89	89	101	vbe_adder_3	70	24	24	24	24	24
Geo. Mean Reduction	-	10.1%	10.6%	23.3%	24.8%	17.8%	Geo. Mean Reduction	-	39.7%	42.6%	41.4%	41.4%	41.4%

¹ Nam, Ross, Su, Childs and Maslov. *Automated Optimization of Large Quantum Circuits with Continuous Parameters*. npj 2018.

² Kissinger and van de Wetering. *PyZX: Large scale automated diagrammatic reasoning*. QPL 2019.

Summary and Future Work

- **SQIR** and **VOQC**: Two building blocks of a verified quantum software stack
 - Powerful enough to verify **state-of-the-art optimizations**, and prove source programs **correct** (QPE; Grover's)
 - Resulted in **novel frameworks, libraries, automation** for quantum program proofs

