Quantum Natural Proof

ANONYMOUS AUTHOR(S)

Q-Dafny.

1 INTRODUCTION

Quantum computers offer unique capabilities that can be used to program substantially faster algorithms compared to those written for classical computers. For example, Grover's search algorithm [Grover 1996, 1997] can query unstructured data in sub-linear time (compared to linear time on a classical computer), and Shor's algorithm [Shor 1994] can factorize a number in polynomial time (compared to the sub-exponential time for the best known classical algorithm).

It is well known that quantum computers provide quantum supremacy. Most quantum algorithms are not classically simulatable because of the property. Unfortunately, the current quantum computers are limited and noisy, so it is hard to test the algorithms in a quantum computer as well as a classical computer. However, an algorithm not being efficiently simulatable in a classical computer does not mean that it is not efficiently provable in the computer. An analogy is that for a lottery system, we can easily prove that someone can win a lottery in a certain probability, but it is extremely hard to find out who will win the lottery. For example, simulating Shor's algorithm [Burgholzer et al. 2021] is hard, but its property has been proved on paper and in Coq [Peng et al. 2022]. It is highly likely that we can discover an efficient and automatic proof framework to extract and certify the properties for quantum algorithms.

Unfortunately, previous quantum proof frameworks [Chareton et al. 2020; Hietala et al. 2021b; Le et al. 2022; Ying 2012] permit proofs with many human-interactions. It is unlikely that algorithms can be proved automatically in these frameworks. For example, the Shor's algorithm proof in Quantum Separation Logic [Le et al. 2022] was proved by assuming that the property of the oracle loop was given and the last part was omitted. The complete Shor's algorithm proof in VOQC [Hietala et al. 2021b] was done by intelligent researchers who spent two years. The reason is that these systems specify quantum programs with quantum states, such as density matrices and high denominational Hilbert spaces. These structures cannot be effectively captured in a classical computer. Although there is a mechanism [Yu and Palsberg 2021] to reduce the complexity of representing these quantum states, the key is that they lack the establishment of "computer understandable" axioms and theories to permit proof automation in verifying quantum algorithms. More sadly, the establishment is itself a hard problem.

On the other hand, there are many classical data state structures that have already had good proof automation theorems, such as first order array, linked list, and graph theories. If we can connect quantum states with these existing classical theories, many quantum algorithms can be reasoned by these existing classical proof theories. We propose Quantum Natural Proof (QNP), a system to map quantum algorithms to classical programs that run on the classical Hoare Logic style proof system, and efficiently and automatically certify quantum program properties. The key observation is that although quantum algorithms running on quantum computers have quantum supremacy, the structures of many algorithms are simple. In addition, the states appearing in these algorithms can be mapped to classical array structures.

Figure 1 provides the QNP development plan. In the first stage, we develop the Q-Dafny proof system including a quantum language (QWhile) that contains operations for writing oracles (©QASM/©QIMP), a type system to record the qubit state forms for easing property proofs, as well as a proof system built on top of the classical Hoare Logic array theory. In addition, Q-Dafny is compiled to Dafny, such that a quantum program with its user-defined properties is compiled to

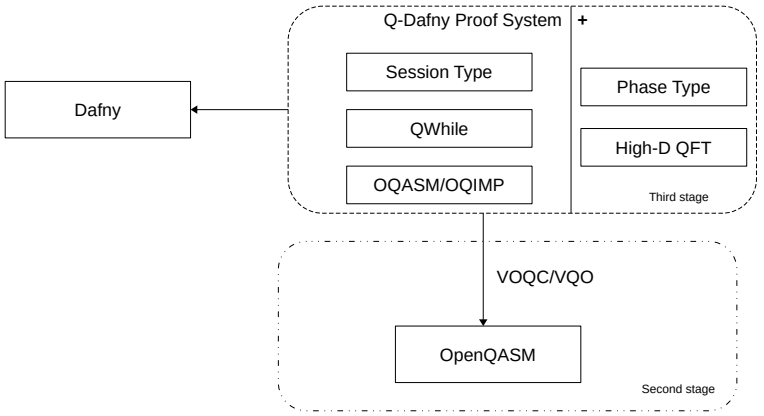


Fig. 1. QNP Development Stages and the Key Aspects

Dafny with additional auto-generated Q-Dafny axioms. The program properties are eventually automatically proved in Dafny with the auto-generated Q-Dafny axioms. The second stage is to compile programs in QWhile, as a quantum language, to ones in OpenQASM, such that a verified QWhile program can be run on a quantum computer. The third stage upgrades Q-Dafny's type system to track not only quantum state bases but also phases. Then, a multi-denominational quantum Fourier transformation (High-D QFT) theory can be built on top of the upgraded type system, so that the Q-Dafny+ proof system is capable of defining advanced quantum algorithms that rely on the High-D QFT theory. One example is quantum signal processing [Low and Chuang 2017].

In this document, we mainly focus on the explanation of the first stage. Here are three key aspects.

Based on Hoare Logic Array Theory. We first select the target mapping classical data structure – arrays, because of two reasons. First, quantum states can be represented by arrangement of quantum qubits which usually can be thought of as special arrays. Thus, quantum entanglement of some qubits can be thought as some properties defined on the qubits, such that once a qubit is measured, the other qubits consequentially perform some state changes. Second, classical array structures are the most commonly used data structure that has many proved theories and axioms, which does not rely on array sizes, for proof automation; while other data structure automated proof theories (axioms), such as linked lists, finish a property proof by an exclusive proof search on the list of elements in the data structure [Qiu et al. 2013]. To represent n qubits as an array in Q-Dafny and verify a property on them, sometimes, we create a 2^n array to capture the entanglement relations among the qubits and expect the array theory to prove the property symbolically regardless the array size.

Using a Session Type System to Classify State Forms. Consequentially, representing quantum states by arrays has its limitations. Conceptually, state representations in the Q-Dafny proof system implies the arrange of a set of axioms that facilitate program property proof automation. Nevertheless, quantum states are high dimensional while arrays are linear. This fact almost always indicates that the set of axioms might be huge and the way of applying the axioms for proof automation is not linear, so that the proof automation faces major obstacles.

```
method Shor ( a : int, N : int, n : int, m : int, x : Q[n], y : Q[n] )
 requires (n > 0)
 requires (1 < a < N)
 requires (N < 2^(n-1))
 requires (N^2 < 2^m ≤ 2 * N^2)
 requires (gcd(a, N) == 1)
 requires ( type(x) = Tensor n (Nor 0))
 requires ( type(y) = Tensor n (Nor 0))
 ensures (gcd(N, r) == 1)
 ensures (p.pos ≥ 4 / (PI ^ 2))
{
  x *= H ;
  y *= cl(y+1); //cl can be omitted.
  for (int i = 0; i < n; x[i]; i ++)
    invariant (0 ≤ i ≤ n)
    invariant (saturation(x[0..i]))
    invariant (type(y,x[0..i]) = Tensor n (ch (2^i) {k | j baseof x[0..i] && k = (a^j mod N,j)}))
    //psum(k=b,M,p(k),b(k)) = sum_{k=b}^M p(k)*b(k)
    invariant ((y,x[0..i]) == psum(k=0,2^i,1,(a^k mod N,k)))
  {
    y *= cl(a^(2^i) * y mod N);
  }

 M z := measure(y);//partial measurement, actually measure(y,r) r is the period
 x *= RQFT;
 M p := measure(x); //p.pos and p.base
 var r := post_period(m,p.base) // ∃ t. 2^m * t / r = p.base
}
```

Fig. 2. Shor's Algorithm in Q-Dafny

To overcome these obstacles, we identify three different quantum state representations (Figure 11) in Q-Dafny, which are associated with different axioms for proof automation. Then, the Q-Dafny session type system tracks the transformation of different state representations for different *sessions*, collections of qubit array segments that are possibly entangled. Conceptually, the different state representations guarantee the Q-Dafny proof system can be expressed in terms of the Hoare Logic array theory. In compiling Q-Dafny to Dafny, for proving a local property for a session, we generate and identify different axioms for different state representations, and we also generate axioms that handle the transformation between state representations.

Enabling Complicated Oracle and Reflection Operations. The first stage session type system tracks only qubit bases. As a consequence, the set of quantum algorithms that are efficiently reasonable has the scheme $\mathtt{QFT}; U; \mathtt{QFT}^{-1}$, where $\mathtt{QFT}$ and $\mathtt{QFT}^{-1}$ are Hadamard or QFT gates that switch qubits array state forms between normal and superposition, U is an arbitrary combination of QWhile operations that use Hadamard or QFT gates in a manageable manner. For rich expressiveness, we permit two kinds of managed operations that might involve Hadamard or QFT gates: oracle assignments written in ⓠQASM/ⓠQIMP and quantum reflection operations (`amplify` and `diffuse` in Figure 3). The concept of "management" refers to the fact that there is a type system in ⓠQASM/ⓠQIMP to ensure the use of Hadamard or QFT gates do not cause entanglement, as well as the Hadamard or QFT gate usage in quantum reflections has a fixed implementation, such that its semantics is well-known and its property reasoning is captured by Q-Dafny.

Almost all near term quantum algorithms are definable in terms of the above scheme, such as GHZ, Grover's, Shor's, and Childs' Boolean equation algorithms. To prove properties about

Nat. Num	m, n	$\in$	$\mathbb{N}$
Real	r	$\in$	$\mathbb{R}$
Variable	x, y		
c-Mode Value	n		
q-Mode Value	(r, n)		
$\mathcal{O}$QASM Expr	μ		
Session	ζ	::=	$\overline{(x, n, m)}$
Type Predicate	T	::=	$x : \tau \mid x : \{\zeta : \tau\} \mid ...$
State Predicate	P, Q	::=	$x = n \mid x = (r, n) \mid \zeta = \rho \mid ...$
Mode	g	::=	$\mathtt{c} \mid \mathtt{q}$
Mode Check Result	q	::=	$g \mid \zeta$
Factor	l	::=	$x \mid x[a]$
Arith Expr	p, a	::=	$l \mid a + a \mid a * a \mid ...$
Bool Expr	b	::=	$x[a] \mid (a = a)@x[a] \mid (a < a)@x[a] \mid \neg b...$
Gate Expr	op	::=	$\mathtt{H} \mid \mathtt{QFT}^{[-1]}$
C/M Moded Expr	e	::=	$a \mid \mathtt{measure}(y)$
Statement	s	::=	$\{\} \mid \mathtt{let}\ x\ =\ e\ \mathtt{in}\ s \mid l \leftarrow op \mid \bar{l} \leftarrow a(\mu)$
		|	$s\ ;\ s \mid \mathtt{if}\ (b)\ \{s\} \mid \mathtt{for}\ (\mathtt{int}\ i\ =\ a_1\ ;\ i < a_2\ ;\ b(i)\ ;\ f(i))\ T(i)\ P(i)\ \{s\}$
		|	$\mathtt{amplify}\{x \leftarrow a\} \mid \mathtt{diffuse}(l)$

ρ: Quantum States see Figure 11

Fig. 3. Core QWhile Syntax, $\mathcal{O}$QASM Syntax is in Figure 12

advanced quantum algorithms, the session type system needs to track qubit phases, which will complicate its design, and it is the major task of stage 3 in the QNP development.

2 QWHILE: A HIGH-LEVEL QUANTUM LANGUAGE

We introduce the language syntax and type system for QWhile and introduce the Q-Dafny Proof system. As a running example, we specify Shor's algorithm and its proof in Q-Dafny in Figure 2. The Q-Dafny to Dafny compiler is under construction, but the compiled version of the Shor's algorithm proof has been finalized and can be found at https://github.com/inQWIRE/VQO/blob/naturalproof/Q-Dafny/examples/Shor-compiled.dfy.

2.1 Syntax

QWhile is a high-level language for describing quantum programs, which permits quantum control and for-loop statements. Figure 3 introduces the QWhile syntax.

A QWhile program consists of a sequence of C-like statements s. Values and variables (ranged by x and y) in a statement are classified as three different categories: compilation time classical values, classical values generated from quantum measurement, and quantum state registers. We use variable *modes* to classify the first two kinds as cand qmodes. We represent c-mode values as natural numbers, while M-mode values are represented as pairs of reals and natural numbers. The reals represent the conceptual occurrence probability of the result measurement, and the natural numbers are the measurement results. Any further arithmetic operations on M-mode values are applied on the measurement results, such as $(r, n_1) + n_2 = (r, n_1 + n_2)$.

Quantum registers refer to quantum qubit arrays in QWhile. They are always associated with disjoint sets of qubit array fragments, named *sessions*. We represent a qubit array fragment as (x, n, m), where x is a variable representing a qubit array, n is the start position in x for the array

Bit	d	::=	$0 \mid 1$
BitString	$\overline{d}$	::=	$\mathbb{N} \to d$
BitString Indexed Set	β	::=	$\{\overline{d}\} \mid \infty$
Phase Type	w	::=	$\bigcirc \mid \infty$
Type Element	t	::=	$\mathsf{Nor}\ \overline{d} \mid \mathsf{Had}\ w \mid \mathsf{CH}\ n\ \beta$
Type	τ	::=	$\bigotimes_n\ t$
Phase	$\alpha(n)$	:=	$e^{2\pi i \frac{1}{n}}$
Amplitude	θ	:=	r
Phi State	$\lvert\Phi(n)\rangle$	:=	$\frac{1}{\sqrt{2}}(\lvert 0\rangle + \alpha(n)\lvert 1\rangle)$
Quantum State	ρ	::=	$\alpha \lvert\overline{d}\rangle \mid \bigotimes_{k=0}^{m} \lvert\Phi(n_k)\rangle \mid \sum_{k=0}^{m} \theta_k \lvert\overline{d_k}\rangle$

Fig. 4. QWhile Sessions and Types and Quantum States

$$\frac{}{\Omega \vdash x : \Omega(x)} \qquad \frac{\Omega(x) = (x, 0, \Sigma(x))}{\Omega \vdash x[n] : [(x, n, n+1)]} \qquad \frac{\Omega \vdash a_1 : q_1 \qquad \Omega \vdash a_2 : q_2}{\Omega \vdash a_1 + a_2 : q_1 \sqcup q_2} \qquad \frac{\Omega \vdash a_1 : q_1 \qquad \Omega \vdash a_2 : q_2}{\Omega \vdash a_1 * a_2 : q_1 \sqcup q_2}$$

$$\frac{\Omega \vdash a_1 : q_1 \qquad \Omega \vdash a_2 : q_2 \Omega \vdash a_3 : q_3}{\Omega \vdash (a_1 = a_2)@x[n] : q_1 \sqcup q_2 \sqcup q_3} \qquad \frac{\Omega \vdash a_1 : q_1 \qquad \Omega \vdash a_2 : q_2 \Omega \vdash a_3 : q_3}{\Omega \vdash (a_1 < a_2)@x[n] : q_1 \sqcup q_2 \sqcup q_3} \qquad \frac{\Omega \vdash b : q}{\Omega \vdash \neg b : q} \qquad \frac{\Omega \vdash e : \zeta_2 \sqcup \zeta_1}{\Omega \vdash e : \zeta_1 \sqcup \zeta_2}$$

$$\zeta_1 \sqcup \zeta_2 = \zeta_1 \uplus \zeta_2 \zeta \sqcup g = \zeta \qquad g \sqcup \zeta = \zeta \qquad \mathsf{c} \sqcup \mathsf{c} = \mathsf{c} \qquad \mathsf{q} \sqcup \mathsf{c} = \mathsf{q} \qquad \mathsf{c} \sqcup \mathsf{q} = \mathsf{q} \qquad \mathsf{c} \le \mathsf{q} \le \zeta$$
$$\bot \uplus l = l \qquad l \uplus \bot = l \qquad [(x, v_1, v_2)] \uplus [(y, v_3, v_4)] = [(x, v_1, v_2), (y, v_3, v_4)]$$
$$[v_2, v_2] \cap [v_3, v_4] \neq \emptyset \Rightarrow [(x, v_1, v_2)] \uplus [(x, v_3, v_4)] = [(x, \mathtt{min}(v_1, v_3), \mathtt{max}(v_2, v_4))]$$

Fig. 5. Arith, Bool, Gate Mode Checking

fragment and m is the exclusive ending point. In Figure 2, an example array fragment for `x` is `x[0..i]`. `y` is an abbreviation of array fragment `y[0..n]` where `n` is the ending point of array `y`. `(y,x[0..i])` is a session containing two array fragments. It is worth noting that the ordering of fragments in a session only serves for recording the qubit positions in a quantum register. The swapping of fragment ordering does not affect the register state. In Q-Dafny, the fragment ordering might affect the property proof automation. In Figure 2, we fix fragment order as `(y,x[0..i])` to enhance the Shor's algorithm proof automation.

We use $x[a]$ to represent the a-th position qubit in x. It is worth noting that the variable x in $x[a]$ must represent quantum registers. We name a variable x or an array index $x[a]$ as a factor. In a QWhile program, cand qmode variables act like stack variables and they must be bounded by variables introduced by `let` statements; while quantum registers represent arrays in a "quantum heap" and are bounded by Σ.

The statements s in the first row in Figure 3 are `{}`(SKIP) and assignment operations. Classic assignment (`let x = e in s`) evaluates e and assigns the value to `c`or qmode variable x that is used in s. Expressions e can be an arithmetic or a measurement operation. `let` x `= measure(`y`) in ...` assigns the measurement result of qubit array y to x. $l \leftarrow op$ and $\bar{l} \leftarrow a(\mu)$ are quantum assignments. The former applies a simple quantum gate (`H` or `QFT`) to a single qubit ($x[a]$) or a qubit array (x) [1]. $\bar{l} \leftarrow a(\mu)$ is a generalized quantum assignment that implements quantum oracle circuits a and applies an ©QASM/©QIMP operation on a list of qubit array $\bar{l}$. We assume all arithmetic (a) and Boolean (b) expressions are reversible. For example, the operation $(a_1 < a_2)@x[a]$ compares a_1

[1] `QFT` gate must apply to a variable x

and a_2 and stores the value in $x[a]$. μ is the circuit implementation of the expression a in ℚASM, whose syntax is given in Section 3. One can utilize ℚASM expressions (μ) to implement singleton X and $\mathtt{RZ}^{[-1]}\ n$ gates, thus, the QWhile syntax is universal with respect to quantum gates. In addition, ℚIMP is a C-like reversible arithmetic language built on ℚASM. The reversible expression a in Figure 3 is based on ℚIMP operations. For simplicity, we write $\overline{l} \leftarrow a$ in examples here to mean that it applies a ℚIMP circuit that computes a to $\overline{l}$.

The second row of statements in Figure 3 are control-flow operations. s_1 ; s_2 is a sequential operation. `if` (b) $\{s\}$ is a conditional and b might contain quantum factors. Every quantum factor l appearing in b must not appear in s. In QWhile, we define a `well_formed` predicate to check such property. `for` $(\mathtt{int}\ i\ =\ a_1\ ;\ i < a_2\ ;\ b(i)\ ;\ f(i))\ T(i)\ P(i)\ \{s\}$ is a possibly quantum for-loop depending on if the Boolean guard $b(i)$ ($b(i)$ is a Boolean expression that contains variable i) contains quantum factors (also needing to be `well_formed`). A classical variable i is introduced and it is initialized as the lower bound a_1, increments in each loop step by the monotonic increment function $f(i)$, and ends at the upper bound a_2. $T(i)$ is the type predicate (type predicate syntax in fig. 3) where for i-th loop step, $T(i)$ is true in the beginning and $T(f(i))$ is maintained after the execution. Similarly, $P(i)$ is the loop-invariant (state predicate in fig. 3) for the for-loop structure, where for i-th loop step, $P(i)$ is true in the beginning and $P(f(i))$ is maintained after the execution.

The last row contains quantum reflection operations, which are used to adjust the occurrence probability of some quantum states in a quantum qubit array. For example, in Grover's search algorithm [Grover 1996], the Grover's diffusion operation is a quantum reflection that increases the occurrence probability of a target quantum state in a qubit array being in superposition. We identify two kinds of quantum reflections that previous works tent to combine together. The first one is an amplifier ($\mathtt{amplify}\{x \leftarrow a\}$) that amplifies the occurrence probability of the target state, which is represented by a classical value a, in a quantum qubit array x. The second one is a diffusion operator ($\mathtt{diffuse}(x)$) that diffuses the state of a qubit array x to a superposition of all possible bases in x with possibly different amplitudes [2]. For example, applying the diffusion operator on a two-qubit array x having state $|00\rangle$ results in a superposition of $-\frac{1}{2}|00\rangle + \frac{1}{2}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{2}|11\rangle$. In general, if an n-qubit array x has the state $\sum_{j=0} \alpha_j |x_j\rangle$, the result of applying a diffusion operator is $\frac{1}{2^n}(2\sum_{i=0}^{2^n}(\sum_{j=0}\alpha_j)|i\rangle - \sum_{j=0}\alpha_j|x_j\rangle)$.

2.2 Type Checking: A Quantum Session Type System

The QWhile type system can be viewed as a mapping from lists of factors (x or $x[n]$) to QWhile types in Figure 11. Generally, factors represent a range of locations in a "quantum heap". Variable x can be viewed as a range $(x, 0, \Sigma(x))$, meaning the heap range starting at x and ending at $x + n$. Index $x[n]$ can be viewed as a range $(x, n, n + 1)$. Thus, a list of **quantum** factors is essentially a list of disjoint fragments, which it is called a *session*.

A type is written as $\bigotimes_n\ t$, where n refers to the total number of qubits in a session, and t describes the qubit state form. A session being type $\bigotimes_n\ \mathtt{Nor}\ \overline{d}$ means that every qubit is in normal basis (either $|0\rangle$ or $|1\rangle$), and $\overline{d}$ describes basis states for the qubits. The type corresponds to a single qubit basis state $\alpha(n)|\overline{d}\rangle$, where the global phase $\alpha(n)$ has the form $e^{2\pi i\frac{1}{n}}$ and $\overline{d}$ is a list of bit values. Global phases for `Nor` type are usually ignored in many semantic definitions. In QWhile, we record it because in quantum conditionals, such global phases might be turned to local phases.

$\bigotimes_n\ \mathtt{Had}\ w$ means that every qubit in the session has the state: $(\alpha_1|0\rangle + \alpha_2|1\rangle)$; the qubits are in superposition but they are not entangled. ◯ represents the state is a uniform superposition, while

[2]The possible bases do not depend on x's state, and it is only related to the qubit size of x; i.e., if x is a two qubit array, then the operation reflects the superposition of all possible two qubit states as: $\frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$.

∞ means the phase amplitude for each qubit is unknown. If a session has such type, it then has the value form $\bigotimes_{k=0}^{m} |\Phi(n_k)\rangle$, where $|\Phi(n_k)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + \alpha(n_k)\,|1\rangle)$.

All qubits in a session that has type $\bigotimes_n$ CH m β are supposedly entangled (eventual entanglement below). m refers to the number of possible different entangled states in the session, and the bitstring indexed set β describes each of these states, while every element in β is indexed by $i \in [0, m)$. β can also be ∞ meaning that the entanglement structure is unknown. For example, in quantum phase estimation, after applying the $\mathtt{QFT}^{-1}$ operation, the state has type $\bigotimes_n$ CH m ∞. In such case, the only quantum operation to apply is a measurement. If a session has type $\bigotimes_n$ CH m β and the entanglement is a uniform superposition, we can describe its state as $\sum_{i=0}^{m} \frac{1}{\sqrt{m}}\beta(i)$, and the length of bitstring $\beta(i)$ is n. For example, in a n-length GHZ application, the final state is: $|0\rangle^{\otimes n} + |1\rangle^{\otimes n}$. Thus, its type is $\bigotimes_n$ CH 2 $\{\overline{0}^n, \overline{1}^n\}$, where $\overline{d}^n$ is a n-bit string having bit d.

The type $\bigotimes_n$ CH m β corresponds to the value form $\sum_{k=0}^{m} \theta_k\, |\overline{d_k}\rangle$. θ_k is an amplitude real number, and $\overline{d_k}$ is the basis. Basically, $\sum_{k=0}^{m} \theta_k\, |\overline{d_k}\rangle$ represents a size m array of basis states that are pairs of θ_k and $\overline{d_k}$. For a session ζ of type CH, one can use $\zeta[i]$ to access the i-th basis state in the above summation, and the length is m. In the Q-Dafny implementation section, we show how we can represent θ_k for effective automatic theorem proving.

The QWhile type system has the type judgment: $\Omega, \mathcal{T} \vdash_g s : \zeta \triangleright \tau$, where g is the context mode, mode environment Ω maps variables to modes or sessions (q in Figure 3), type environment $\mathcal{T}$ maps a session to its type, s is the statement being typed, ζ is the session of s, and τ is ζ's type. The QWhile type system in Figure 8 has several tasks. First, it enforces context mode restrictions. Context mode g is either cor q. Q represents the current expression lives inside a quantum conditional or loop, while crefers to other cases. In a Q context, one cannot perform M-mode operations, i.e., no measurement is allowed. There are other well-formedness enforcement. For example, the session of the Boolean guard b in a conditional/loop is disjoint with the session in the conditional/loop body, i.e., qubits used in a Boolean guard cannot appear in its conditional/loop body.

Second, the type system enforces mode checking for variables and expressions in Figure 14. In QWhile, c-mode variables are evaluated to values during type checking. In a `let` statement (Figure 8), c-mode expression is evaluated to a value n, and the variable x is replaced by n in s. The expression mode checking (Figure 14) has the judgment: $\Omega \vdash (a \mid b) : q$. It takes a mode environment Ω, and an expression (a, b), and judges if the expression has the mode g if it contains only classical values, or a quantum session ζ if it contains some quantum values. All the supposedly c-mode locations in an expression are assumed to be evaluated to values in the type checking step, such as the index value $x[n]$ in difference expressions in Figure 14. It is worth noting that the session computation ($\uplus$) is also commutative as the last rule in Figure 14.

Third, by generating the session of an expression, the QWhile type system assigns a type τ for the session indicating its state format, which will be discussed shortly below. Recall that a session is a list of quantum qubit fragments. In quantum computation, qubits can entangled with each other. We utilize type τ (Figure 11) to state entanglement properties appearing in a group of qubits. It is worth noting that the entanglement property refers to *eventual entanglement*, .i.e. a group of qubits that are eventually entangled. Entanglement classification is tough and might not be necessary. In most near term quantum algorithms, such as Shor's algorithm [Shor 1994] and Childs' Boolean equation algorithm (BEA) [Childs et al. 2007], programmers care about if qubits eventually become entangled during a quantum loop execution. This is why the normal basis type ($\bigotimes_n$ Nor $\overline{d}$) can also be a subtype of a entanglement type ($\bigotimes_n$ CH 1 $\{\overline{d}\}$) in our system (Figure 7).

Entanglement Types. We first investigate the relationship between the types and entanglement states. It is well-known that every single quantum gate application does not create entanglement

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9
$x[i]$	Nor	Had	Had	Had	Had	Had	Had	CH	CH
y	any	Nor	Nor	Had	Had	CH	CH	CH	CH
y's operation type	any	$\mathcal{X}$	$\mathcal{R}$	$\mathcal{X}$	$\mathcal{R}$	$\mathcal{X}$	$\mathcal{R}$	$\mathcal{X}$	$\mathcal{R}$
Output Type Entangled?	N	Y	N	N	Y	Y	Y	Y	Y

Fig. 6. Control Gate Entanglement Situation

$$\otimes_n \ \mathsf{Nor}\ \overline{d} \sqsubseteq \otimes_n \ \mathsf{CH}\ 1\ \{\overline{d}\} \qquad \otimes_n \ \mathsf{CH}\ 2^n\ \beta \sqsubseteq \otimes_n \ \mathsf{CH}\ 2^n\ \infty \qquad \otimes_n \ \mathsf{Had}\ \bigcirc \sqsubseteq \otimes_n \ \mathsf{CH}\ 2^n\ \mathcal{P}(n)$$

Fig. 7. Session Type Subtyping

(X, H, and RZ). It is enough to classify entanglement effects through a control gate application, i.e., `if` $(x[i])$ $\{e(y)\}$, where the control node is $x[i]$ and e is an operation applying on y.

A qubit can be described as $\alpha_1 |b_1\rangle + \alpha_2 |b_2\rangle$, where α_1/α_2 are phase amplitudes, and b_1/b_2 are bases. For simplicity, we assume that when we applying a quantum operation on a qubit array y, we either solely change the qubit amplitudes or bases. We identify the former one as $\mathcal{R}$ kind, referring to its similarity of applying an RZ gate; and the latter as $\mathcal{X}$ kind, referring to its similarity of applying an X gate. The entanglement situation between $x[i]$ and y after applying a control statement `if` $(x[i])$ $\{e(y)\}$ is described in Figure 6.

If $x[i]$ has input type Nor, the control operation acts as a classical conditional, i.e., no entanglement is possible. In most quantum algorithms, $x[i]$ will be in superposition (type Had) to enable entanglement creation. When y has type Nor, if y's operation is of $\mathcal{X}$ kind, an entanglement between $x[i]$ and y is created, such as the GHZ algorithm; if the operation is of $\mathcal{R}$ kind, there is not entanglement after the control application, such as the Quantum Phase Estimation (QPE) algorithm.

When $x[i]$ and y are both of type Had, if we apply an $\mathcal{X}$ kind operation on y, it does not create entanglement. An example application is the phase kickback pattern. If we apply a $\mathcal{R}$ operation on y, this does create entanglement. This kind of operations appears in state preparations, such as preparing a register x to have state $\sum_{t=0}^{N} i^{-t} |t\rangle$ in Childs' Boolean equation algorithm [Childs et al. 2007]. The main goal for preparing such state is not to entanglement qubits, but to prepare a state with phases related to its bases.

The case when $x[i]$ and y has type Had and CH, respectively, happens in the middle of executing a quantum loop, such as in the Shor's algorithm and BEA. Applying both $\mathcal{X}$ and $\mathcal{R}$ kind operations result in entanglement. In this narrative, algorithm designers intend to merge an additional qubit $x[i]$ into an existing entanglement session y. $x[i]$ is commonly in uniform superposition, but there can be some additional local phases attached with some bases, which we named this situation as saturation, i.e., In an entanglement session written as $\sum_{i=0}^{n} |x_l, y, x_r\rangle$, for any fixing x_l and x_r bases, if y covers all possible bases, we then say that the part y in the entanglement is in saturation. This concept is important for generating auto-proof, which will be discussed in Section 2.3.

When $x[i]$ and y are both of type CH, there are two situations. When the two parties belong to the same entanglement session, it is possible that an $\mathcal{X}$ or $\mathcal{R}$ operation de-entangles the session. Since QWhile tracks eventual entanglement. In many cases, HAD type can be viewed as a kind of entanglement. In addition, the QWhile type system make sure that most de-entanglements happen at the end of the algorithm by turning the qubit type to CH m ∞, so that after the possible de-entanglement, the only possible application is a measurement.

If $x[i]$ and y are in different entanglement sessions, the situation is similar to when $x[i]$ having Had and y having CH type. It merges the two sessions together through the saturation $x[i]$. For example, in BEA, The quantum Boolean guard computes the following operation $(z < i)@x[i]$

TA-NOR

$$\frac{\Omega \vdash \overline{l} : \zeta \qquad [\![a]\!]\,|\overline{d}\rangle = \alpha\,|\overline{d'}\rangle}{\Omega, \mathcal{T}\,[\zeta \mapsto \bigotimes_n \mathsf{Nor}\ \overline{d}] \vdash_g \overline{l} \leftarrow a : \zeta \triangleright_g \bigotimes_n \mathsf{Nor}\ \overline{d'}}$$

TA-HAD

$$\frac{\Omega \vdash \overline{l} : \zeta \qquad \zeta \subseteq \zeta' \qquad (\forall \overline{d}\ .\ [\![a]\!]\,|\overline{d}\rangle = |\overline{d'}\rangle)}{\Omega, \mathcal{T}\,[\zeta' \mapsto \bigotimes_n \mathsf{Had}\ \bigcirc] \vdash_g \overline{l} \leftarrow a : \zeta' \triangleright \bigotimes_n \mathsf{Had}\ \bigcirc}$$

TEXP

$$\frac{\Omega[x \mapsto \mathsf{c}], \mathcal{T} \vdash_g s[v/x] : \zeta \triangleright \tau}{\Omega, \mathcal{T} \vdash_g \mathtt{let}\ x\ =\ v\ \mathtt{in}\ s : \zeta \triangleright \tau}$$

TMEA

$$\frac{\begin{array}{c}\Omega \vdash y : \zeta \qquad n' = \mathtt{size}(\zeta') \qquad m' = \mathtt{size}(\{\overline{c'} | \overline{c} \cdot \overline{c'} \in \beta \cdot \beta' \wedge \overline{c} = \mathtt{val}(x)\}) \\ \Omega[x \mapsto \mathsf{q}], \mathcal{T}\,[\zeta' \mapsto \bigotimes_{n'} \mathsf{CH}\ m'\ \{\overline{c'} | \overline{c} \cdot \overline{c'} \in \beta \cdot \beta' \wedge \overline{c} = \mathtt{val}(x)\}] \vdash_{\mathsf{c}} s : \zeta'' \triangleright \tau\end{array}}{\Omega, \mathcal{T}\,[\zeta \uplus \zeta' \mapsto \bigotimes_n \mathsf{CH}\ m\ (\beta \cdot \beta')] \vdash_{\mathsf{c}} \mathtt{let}\ x\ =\ \mathtt{measure}(y)\ \mathtt{in}\ s : \zeta'' \triangleright \tau}$$

TA-CH

$$\frac{\Omega \vdash \overline{l} : \zeta \qquad \zeta' = \zeta \uplus \zeta_r}{\Omega, \mathcal{T}\,[\zeta' \mapsto \bigotimes_n \mathsf{CH}\ k\ \beta] \vdash_g \overline{l} \leftarrow a : \zeta' \triangleright \bigotimes_n \mathsf{CH}\ k\ \{\overline{d'} \cdot \overline{d_r} \mid \overline{d} \cdot \overline{d_r} \in \beta(\downarrow \zeta) \cdot \beta(\downarrow \zeta_r) \wedge [\![a]\!]\,|\overline{d}\rangle = \alpha\,|\overline{d'}\rangle\}}$$

TA-Mu

$$\frac{\Omega, \mathcal{T}\,[\zeta_1 \uplus \zeta_3 \uplus \zeta_2 \uplus \zeta_4 \mapsto \bigotimes_n \mathsf{CH}\ k\ \beta_1 \cdot \beta_3 \cdot \beta_2 \cdot \beta_4] \vdash_g s : \zeta_1 \uplus \zeta_3 \uplus \zeta_2 \uplus \zeta_4 \triangleright \bigotimes_n \mathsf{CH}\ k\ \beta_1 \cdot \beta_3' \cdot \beta_2' \cdot \beta_4}{\Omega, \mathcal{T}\,[\zeta_1 \uplus \zeta_2 \uplus \zeta_3 \uplus \zeta_4 \mapsto \bigotimes_n \mathsf{CH}\ k\ \beta_1 \cdot \beta_2 \cdot \beta_3 \cdot \beta_4] \vdash_g s : \zeta_1 \uplus \zeta_2 \uplus \zeta_3 \uplus \zeta_4 \triangleright \bigotimes_n \mathsf{CH}\ k\ \beta_1 \cdot \beta_2' \cdot \beta_3' \cdot \beta_4}$$

TSEQ-1

$$\frac{\Omega, \mathcal{T} \vdash_g s_1 : \zeta \triangleright \bigotimes_n \mathsf{Nor}\ \overline{d} \qquad \zeta \cup \zeta' \qquad \Omega, \mathcal{T}\,[\zeta \mapsto \bigotimes_n \mathsf{Nor}\ \overline{d}] \vdash_g s_2 : \zeta' \triangleright \bigotimes_{n'} \mathsf{Nor}\ \overline{d'}}{\Omega, \mathcal{T} \vdash_g s_1\ ;\ s_2 : \zeta \uplus \zeta' \triangleright \bigotimes_{n+n'} \mathsf{Nor}\ \overline{d} \cdot \overline{d'}}$$

TSEQ-2

$$\frac{\Omega, \mathcal{T} \vdash_g s_1 : \zeta \triangleright \bigotimes_n \mathsf{CH}\ k\ \beta \qquad \Omega, \mathcal{T}\,[\zeta \mapsto \bigotimes_n \mathsf{CH}\ k\ \beta] \vdash_g s_2 : \zeta' \triangleright \tau}{\Omega, \mathcal{T} \vdash_g s_1\ ;\ s_2 : \zeta' \triangleright \tau}$$

TIF

$$\frac{\begin{array}{c}\Omega \vdash b(@x[v]) : \zeta \qquad \mathcal{T}(\zeta) = \bigotimes_n \mathsf{CH}\ k\ (\beta_1 \cdot 0 \cup \beta_2 \cdot 1) \\ \zeta \cup \zeta' \qquad \mathtt{last}(\zeta) = (x, v, v+1) \qquad \Omega, \mathcal{T} \vdash_{\mathsf{q}} s : \zeta' \triangleright \bigotimes_{n'} \mathsf{CH}\ k'\ \beta'\end{array}}{\Omega, \mathcal{T}\,[\zeta \mapsto \bigotimes_n \mathsf{CH}\ k\ \beta] \vdash_g \mathtt{if}\ (x[v])\ \{s\} : \zeta \uplus \zeta' \triangleright \bigotimes_{n+n'} \mathsf{CH}\ (k \times k')\ (\beta_1 \cdot 0 \cdot \beta' \cup \beta_2 \cdot 1 \cdot \beta')}$$

TLOOP

$$\frac{\begin{array}{c}v_1 \le v < v_2 \qquad \Omega \vdash f(v) : \mathsf{c} \qquad \Omega \vdash b(@x[v]) : \zeta(v) \\ \zeta(v) \cup \zeta'(v) \qquad \mathtt{last}(\zeta) = (x, v, v+1) \qquad \Omega, \mathcal{T} \vdash_g \mathtt{if}\ (b(@x[v]))\ \{s\} : \zeta(v) \uplus \zeta'(v) \triangleright \tau(v)\end{array}}{\Omega, \mathcal{T} \vdash_g \mathtt{for}\ (\mathtt{int}\ i\ =\ v_1\ ;\ i < v_2\ ;\ b(@x[i])\ ;\ f(i))\ T(i)\ P(i)\ \{s\} : \zeta(v_2) \uplus \zeta'(v_2) \triangleright \tau(v_2)}$$

TDIS

$$\frac{\Omega \vdash x : \zeta \qquad \zeta' = \zeta \uplus \zeta_r \qquad n' = \mathtt{size}(\zeta) \qquad m' = \mathtt{size}(\{\mathcal{P}(n') \cdot \overline{d_r} \mid \overline{d} \cdot \overline{d_r} \in \beta(\downarrow \zeta) \cdot \beta(\downarrow \zeta_r)\})}{\Omega, \mathcal{T}\,[\zeta' \mapsto \bigotimes_n \mathsf{CH}\ m\ \beta] \vdash_g \mathtt{diffuse}(x) : \zeta' \triangleright \bigotimes_n \mathsf{CH}\ m'\ \{\mathcal{P}(n') \cdot \overline{d_r} \mid \overline{d} \cdot \overline{d_r} \in \beta(\downarrow \zeta) \cdot \beta(\downarrow \zeta_r)\}}$$

$\overline{d} \cdot \overline{d'}$: list concatenation. $\zeta \cup \zeta'$: The two sessions are disjoint.
$\beta(\downarrow \zeta)$: Get the position range of ζ in the session and form a new set of bitstrings containing only the positions in the range.
$[\![a]\!]\,|\overline{d}\rangle$: $\mathcal{O}_{\text{QASM}}$ semantics of interpreting reversible expression a in Figure 16.

Fig. 8. Session Type System

on a Had type variable z (state: $\sum_{k=0}^{2^n} |k\rangle$) and a Nor type factor $x[i]$ (state: $|0\rangle$). The result is an entanglement $\sum_{k=0}^{2^n} |k, k < i\rangle$, where the $x[i]$ position stores the Boolean bit result $k < i$. [3] The

[3] When $k < i$, $x[i] = 1$ while $\neg(k < i)$, $x[i] = 0$.

algorithm further merges the $|z, x[i]\rangle$ session with a loop body entanglement session y. In this cases, both $|z, x[i]\rangle$ and y are of CH type.

Session Type System. Selected type rules are given in Figure 8. As we have mentioned above, the type system tracks possible eventual entanglement for a group of qubits, which we named a session. The type judgment is given as $\Omega, \mathcal{T} \vdash_g s : \zeta \triangleright \tau$.

Rule TEXP is the type rule for c-mode expressions. The expression a is evaluated and variable x is substituted with the value v in s. TMEA is a similar rule as TEXP, but for M-mode variable. We allow partial measurements in QWhile. Thus, we need to find out a possible entanglement session $\zeta \uplus \zeta'$ that contains y's session (ζ), that is going to disappear because of measurement. Then, we re-calculate the entanglement type information for ζ'.

TA-NOR, TA-HAD and TA-CH are rules for quantum assignments with different input types. $[\![a]\!]$ appearing in these rules is a semantic function for interpreting the expressions a. The semantic function takes an expression in Nor type and output a Nor value, i.e., inputting classical values and output classical results. The semantics of ⓠQASM (Figure 16) and the arithmetic language ⓠQIMP is the role model of such semantic function. In TA-HAD, when $\overline{l}$ is in uniform superposition (Had ◯), for every bit in $\overline{l}$, if the semantic function judges that its global phase keeps in uniformity, .i.e, 1, the output type is still a uniform superposition without entanglement. In TA-CH, the factor $\overline{l}$ that is assigning might be a sub-session ζ of the whole entanglement session ζ', such that $\zeta' = \zeta \cdot \zeta_r$. Here, for every element $\overline{d} \cdot \overline{d_r} \in \beta$, we find out the corresponding part $\overline{d}$ belonging to the session ζ ($\overline{d} \cdot \overline{d_r} \in \beta(\downarrow \zeta) \cdot \beta(\downarrow \zeta_r)$), and updates the $\overline{d}$ in the result type.

Rules TSeq-1 and TSeq-2 describe the type for a sequence operation. If s_1 and s_2 are of type Nor or Had (rule TSeq-1), the output session order can be mutated as long as the two sessions are disjoint. If the two sessions are not disjoint, we only need to keep the type for ζ', since it is obvious that $\zeta \subseteq \zeta'$. If s_1 and s_2 are of type CH (rule TSeq-2), we only permit the case when $\zeta \subseteq \zeta'$ for simplicity. It has no technical difficulty to allow τ to be a list and two entanglement sessions to bind together, but it makes the type system a lot messier, and there is no current algorithms that require the modification of two distinct entanglement sessions inside a conditional block. On the other hand, if two distinct entanglement sessions live in a conditional block, the block can always be split into two different conditionals with the same Boolean guard.

Rule TIF describes the type for conditionals when the Boolean guard $b(@x[v])$ having type CH, and $x[v]$ is the result bit storing the Boolean evaluation result. The result type of such conditionals is an CH type by merging the session of $b(@x[v])$ into the entanglement session. Assume that the CH bases for $b(@x[v])$ are $\beta_1 \cdot 0$ and $\beta_2 \cdot 1$, meaning that we can split nicely for all possible bases of a quantum state to two different sets where the last bit, which represents the $x[v]$ position, is 0 and 1. For the 0 set, we extend $\beta_1 \cdot 0$ to $\beta_1 \cdot 0 \cdot \beta$ by doing a cross product of the elements in set $\beta_1 \cdot 0$ and set β. For the 1 set, the cross product is applied on set $\beta_1 \cdot 0$ and set β', where β' is the result type bases of the body statement s. It is worth noting that by the subtyping relation in Figure 7, any type can be turned to a CH type. When the Boolean guard has type Nor, it is no more than a classical conditional. When the Boolean guard has type Had, its behavior is similar to the CH case.

Rule TLOOP describes the type for a for-loop. It is a generalization of the conditional case when the Boolean guard $b(@x[i])$ having type CH. In the type rule, we pick a number v to represent variable i, and check if a single loop step `if` $(b(@x[v]))$ $\{s\}$ is well typed. If so, we can conclude that when we replace v by v_2, the for-loop is type checked.

Rule TDIS types a diffusion operator. The rule finds the right part of x in the session ζ'. For every right session bitstring $\overline{d}$ in $\overline{d_l} \cdot \overline{d} \cdot \overline{d_r}$, it generates a set of new type sequence by replacing $\overline{d}$ with elements in the power set $\mathcal{P}(n')$, where n' is the bit length of $\overline{d}$. Here, we need to compute the size

$$\text{PA-NOR}\quad \frac{(\mathcal{T},\mathcal{T}') \models_g (T, \bar{l} \leftarrow a, T') : \zeta \triangleright \bigotimes_n \texttt{Nor}\ \bar{d}}{\Omega \vdash_g \{T\}\ \{P[[\![a]\!]\zeta/\zeta]\}\ \bar{l} \leftarrow a\ \{T'\}\ \{P\}}$$

$$\text{PA-CH}\quad \frac{(\mathcal{T},\mathcal{T}') \models_g (T, \bar{l} \leftarrow a, T') : \zeta \uplus \zeta' \triangleright \bigotimes_n \texttt{CH}\ m\ \beta \qquad \mathcal{T}(\bar{l}) = \zeta}{\Omega \vdash_g \{T\}\ \{P[\forall k < m.\ [\![a]\!](\zeta[k])/\zeta[k]]\}\ \bar{l} \leftarrow a\ \{T'\}\ \{P\}}$$

$$\text{P-MEA}\quad \frac{(\mathcal{T}[\forall \zeta' .\ \zeta \uplus \zeta' \mapsto \bigotimes_{n+n'} \texttt{CH}\ (m \times m')\ (\beta \cdot \beta')], \mathcal{T}'[\forall \zeta' .\ \zeta' \mapsto \bigotimes_{n'} \texttt{CH}\ m'\ \beta']) \models_{\mathsf{c}} (T, y, T'') : \zeta \triangleright \bigotimes_n \texttt{CH}\ m\ \beta \qquad v < m \qquad \Omega[x \mapsto M, y \mapsto \bot] \vdash_{\mathsf{c}} \{T''\}\ \{P[(\mathsf{as}^2(\zeta[v]), \mathsf{bs}(\zeta[v]))/x, \bot/\zeta]\}\ s\ \{T'\}\ \{Q\}}{\Omega \vdash_{\mathsf{c}} \{T\}\ \{P\}\ \texttt{let}\ x\ =\ \texttt{measure}(y)\ \texttt{in}\ s\ \{T'\}\ \{Q\}}$$

$$\text{P-IF}\quad \frac{(\mathcal{T},\mathcal{T}') \models_{\mathsf{q}} (T, s, T') : \zeta' \triangleright \bigotimes_{n'} \texttt{CH}\ m'\ \beta' \qquad \Omega \vdash b(@x[v]) : \zeta \uplus [(x, v, v+1)] \qquad \mathcal{T}(\zeta \uplus [(x, v, v+1)]) = \bigotimes_n \texttt{CH}\ 2m\ (\beta_1 \cdot 0 \cup \beta_2 \cdot 1)}{\Omega \vdash_g \{T\}\ \{P[(\zeta \uplus 0 \uplus \zeta')\texttt{++}(\zeta \uplus 1 \uplus [\![s]\!]\zeta')/\zeta \uplus [(x, v, v+1)] \uplus \zeta']\}\ \texttt{if}\ (b(@x[v]))\ \{s\}\ \{T'\}\ \{P\}}$$

$$\text{P-LOOP}\quad \frac{(\mathcal{T},\mathcal{T}') \models_g (T(i), \texttt{if}\ (b(@x[i]))\ \{s\}, T(f(i))) : \zeta \triangleright \tau \qquad \Omega \vdash_g \{T(i)\}\ \{P(i)\}\ \texttt{if}\ (x[i])\ \{s\}\ \{T(f(i))\}\ \{P(f(i))\}}{\Omega \vdash_g \{T(a_1)\}\ \{P(a_1)\}\ \texttt{for}\ (\texttt{int}\ i\ =\ a_1\ ;\ i < a_2\ ;\ x[i]\ ;\ f(i))\ T(i)\ P(i)\ \{s\}\ \{T(a_2)\}\ \{P(a_2)\}}$$

$$\text{P-DIS}\quad \frac{(\mathcal{T},\mathcal{T}') \models_g (T, \texttt{diffuse}(x), T') : \zeta \triangleright \bigotimes_{n'} \texttt{CH}\ m'\ \beta' \qquad \mathcal{T}(x) = \{\zeta : \bigotimes_{n'} \texttt{CH}\ m\ \beta\} \qquad \zeta = \zeta' \uplus (x, 0, \Sigma(x)) \qquad \beta_1 \cdot \beta_2 = \beta(\downarrow (x, 0, \Sigma(x))) \cdot \beta(\downarrow \zeta')}{\Omega \vdash_g \{T\}\ \{P[\texttt{dis}(n', \zeta, \beta, \beta_1, \beta_2)/\zeta]\}\ \texttt{diffuse}(x)\ \{T'\}\ \{P\}}$$

$\texttt{ln}(\zeta)$: length of ζ $\quad \mathsf{as}(\zeta[v])$: the amplitude of $\zeta[v]$ $\quad \mathsf{bs}(\zeta[v])$: the base of $\zeta[v]$ $\quad$ ++: array concatenation.

$$\texttt{dis}(n, \zeta, \beta, \beta_1, \beta_2) \equiv \{\tfrac{1}{2^{n-1}}(\textstyle\sum_k \mathsf{as}(\zeta[k]) - \mathsf{as}(\zeta[j]))\beta_1[j] \mid \beta_1[j] \in \mathcal{P}(n)\} \cup \bigcup_{j \in \beta_2} \{\tfrac{1}{2^n} \textstyle\sum_k \mathsf{as}(\zeta[k])z \mid z \in \mathcal{P}(n) \wedge (\forall k.\ z \cdot \beta_2[j] \neq \beta[k])\}$$

Fig. 9. Selected Proof System Rules

of the new bitstring set as m'. Sometimes, this computation can be hard, but for most quantum algorithms, depending on the session data structures, the `size` can be computed effectively.

2.3 Logic Proof System

The reason of having the session type system in Figure 8 is to enable the proof system given in Figure 9. Every proof rule is a structure as $\Omega \vdash_g \{T\}\ \{P\}\ s\ \{T'\}\ \{Q\}$, where g and Ω are the type entities mentioned in Section 2.2. T and T' are the pre- and post- type predicates for the statement s, meaning that there is type environments $\mathcal{T}$ and $\mathcal{T}'$, such that $\mathcal{T} \models T, \mathcal{T}' \models T', g, \Omega, \mathcal{T} \vdash s : \zeta \triangleright \tau$, and $(\zeta \mapsto \tau) \in \mathcal{T}'$. We denote $(\mathcal{T},\mathcal{T}') \models (T, s, T') : \zeta \triangleright \tau$ as the property described above. P and Q are the pre- and post- Hoare conditions for statement s.

The proof system is an imitation of the classical Hoare Logic array theory. We view the three different quantum state forms in Figure 11 as arrays with elements in different forms, and use the session types to guide the occurrence of a specific form at a time. Sessions, like the array variables in the classical Hoare Logic theory, represent the stores of quantum states. The state changes are implemented by the substitutions of sessions with expressions containing operation's semantic transitions. The substitutions can happen for a single index session element or the whole session.

Rule PA-NOR and PA-CH specify the assignment rules. If a session ζ has type `Nor`, it is a singleton array, so the substitution $[\![a]\!]\zeta/\zeta$ means that we substitute the singleton array by a term with the a's application. When ζ has type `CH`, term $\zeta[k]$ refers to each basis state in the entanglement. The

assignment is an array map operation that applies a to every element in the array. For example, in Figure 2 line 12, we apply a series of H gates to array x. Its post-condition is $[(x,0,n)] = \bigotimes_{k=0}^{n} |\Phi(0)\rangle$, where $[(x,0,n)]$ is the session representing register variable x. Thus, replacing the session $[(x,0,n)]$ with the H application results in a pre-condition as $\mathtt{H}[(x,0,n)] = \bigotimes_{k=0}^{n} |\Phi(0)\rangle$, which means that $[(x,0,n)]$ has the state $|0\rangle^n$.

Rule P-MEA is the rule for partial/complete measurement. y's session is ζ, but it might be a part of an entangled session $\zeta \uplus \zeta'$. After the measurement, M-mode x has the measurement result $(\mathtt{as}(\zeta[v])^2, \mathtt{bs}(\zeta[v]))$ coming from one possible basis state of y (picking a random index v in ζ), $\mathtt{as}(\zeta[v])$ is the amplitude and $\mathtt{bs}(\zeta[v])$ is the base. We also remove y and its session ζ ($\perp/\zeta$) in the new pre-condition because it is measured away. The removal means that the entangled session $\zeta \uplus \zeta'$ is replaced by ζ' with the re-computation of the amplitudes and bases for each term.

Rule P-IF deals with a quantum conditional where the Boolean guard $b(@x[v])$ is of type $\bigotimes_n$ CH $2m$ $(\beta_1 \cdot 0 \cup \beta_2 \cdot 1)$. The bases are split into two sets $\beta_1 \cdot 0$ and $\beta_2 \cdot 1$, where the last bit represents the base state for the $x[v]$ position. In quantum computing, a conditional is more similar to an assignment, where we create a new array to substitute the current state represented by the session $\zeta \uplus [(x,v,v+1)] \uplus \zeta'$. Here, the new array is given as $(\zeta \uplus 0 \uplus \zeta')$++$(\zeta \uplus 1 \uplus [\![s]\!]\zeta')$, where we double the array: if the $x[v]$ position is 0, we concatenate the current session ζ' for the conditional body, if $x[v] = 1$, we apply $[\![s]\!]$ on the array ζ' and concatenate it to $(\zeta \uplus 1)$.

For each element in array ζ, we add a bit 0 or 1 on top of the base depending on if the index lives in $[0,m)$ or $[m,2m)$. Rule P-Loop is an initiation of the classical while rule in Hoare Logic but the loop guard can be quantum. In QWhile, we only has `for-loop` structure and we believe it is enough to specify any current quantum algorithms. For any i, if we can maintain the loop invariant $P(i)$ and $T(i)$ with the post-state $P(f(i))$ and $T(f(i))$ for a single conditional `if` $(x[i])$ $\{s\}$, the invariant is maintained for multiple steps for i from the lower-bound a_1 to the upper bound a_2.

Rule P-DIS proves a distributor `diffuse`(x). The quantum semantics for `diffuse`(x) is $\frac{1}{2^n}(2\sum_{i=0}^{2^n}(\sum_{j=0}\alpha_j)|i\rangle - \sum_{j=0}\alpha_j|x_j\rangle)$. As an array operation, `diffuse`(x) with the session ζ is an array operation as follows: assume that $\zeta = (x,0,\Sigma(x)) \uplus \zeta_1$, for every k, if $\zeta[k]$'s value is $\theta_k(\overline{d_x} \cdot \overline{d_1})$, for any bitstring z in $\mathcal{P}(\Sigma(x))$, if $z \cdot \overline{d_1}$ is not a base for $\zeta[j]$ for any j, then the state is $\frac{1}{2^{n-1}}\sum_{k=0}\theta_k(z \cdot \overline{d_1})$; if the base of $\zeta[j]$ is $z \cdot \overline{d_1}$, then the state for $\zeta[j]$ is $\frac{1}{2^{n-1}}(\sum_{k=0}\theta_k) - \theta_j(z \cdot \overline{d_1})$.

REFERENCES

Stephane Beauregard. 2003. Circuit for Shor's Algorithm Using 2n+3 Qubits. *Quantum Info. Comput.* 3, 2 (March 2003), 175–185.

Lukas Burgholzer, Hartwig Bauer, and Robert Wille. 2021. Hybrid Schrödinger-Feynman Simulation of Quantum Circuits With Decision Diagrams. arXiv:2105.07045 [quant-ph]

Christophe Chareton, Sébastien Bardin, François Bobot, Valentin Perrelle, and Benoit Valiron. 2020. Toward Certified Quantum Programming. *arXiv e-prints* (2020). arXiv:2003.05841 [cs.PL]

Andrew Childs, Ben Reichardt, Robert Spalek, and Shengyu Zhang. 2007. Every NAND formula of size N can be evaluated in time $N^{1/2+o(1)}$ on a Quantum Computer. (03 2007).

Lov K. Grover. 1996. A Fast Quantum Mechanical Algorithm for Database Search. In *Proceedings of the Twenty-Eighth Annual ACM Symposium on Theory of Computing* (Philadelphia, Pennsylvania, USA) *(STOC '96)*. Association for Computing Machinery, New York, NY, USA, 212–219. https://doi.org/10.1145/237814.237866 arXiv:quant-ph/9605043

Lov K. Grover. 1997. Quantum Mechanics Helps in Searching for a Needle in a Haystack. *Phys. Rev. Lett.* 79 (July 1997), 325–328. Issue 2. https://doi.org/10.1103/PhysRevLett.79.325 arXiv:quant-ph/9706033

Kesha Hietala, Robert Rand, Shih-Han Hung, Liyi Li, and Michael Hicks. 2021a. Proving Quantum Programs Correct. In *Proceedings of the Conference on Interative Theorem Proving (ITP)*.

Kesha Hietala, Robert Rand, Shih-Han Hung, Xiaodi Wu, and Michael Hicks. 2021b. A Verified Optimizer for Quantum Circuits. In *Proceedings of the ACM Conference on Principles of Programming Languages (POPL)*.

Xuan-Bach Le, Shang-Wei Lin, Jun Sun, and David Sanan. 2022. A Quantum Interpretation of Separating Conjunction for Local Reasoning of Quantum Programs Based on Separation Logic. *Proc. ACM Program. Lang.* 6, POPL, Article 36 (jan 2022), 27 pages. https://doi.org/10.1145/3498697

Guang Hao Low and Isaac L. Chuang. 2017. Optimal Hamiltonian Simulation by Quantum Signal Processing. *Physical Review Letters* 118, 1 (Jan 2017).

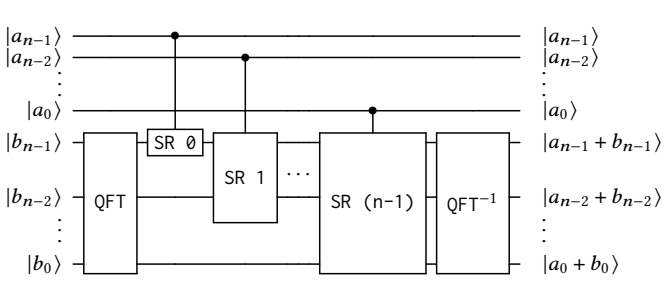
Yuxiang Peng, Kesha Hietala, Runzhou Tao, Liyi Li, Robert Rand, Michael Hicks, and Xiaodi Wu. 2022. A Formally Certified End-to-End Implementation of Shor's Factorization Algorithm. https://doi.org/10.48550/ARXIV.2204.07112

Xiaokang Qiu, Pranav Garg, Andrei Stefanescu, and Parthasarathy Madhusudan. 2013. Natural proofs for structure, data, and separation. In *ACM SIGPLAN Conference on Programming Language Design and Implementation, PLDI '13, Seattle, WA, USA, June 16-19, 2013*, Hans-Juergen Boehm and Cormac Flanagan (Eds.). ACM, 231–242. https://doi.org/10.1145/2491956.2462169

P.W. Shor. 1994. Algorithms for quantum computation: discrete logarithms and factoring. In *Proceedings 35th Annual Symposium on Foundations of Computer Science*. 124–134. https://doi.org/10.1109/SFCS.1994.365700

Mingsheng Ying. 2012. Floyd–Hoare Logic for Quantum Programs. *ACM Trans. Program. Lang. Syst.* 33, 6, Article 19 (Jan. 2012), 49 pages. https://doi.org/10.1145/2049706.2049708

Nengkun Yu and Jens Palsberg. 2021. Quantum Abstract Interpretation. In *Proceedings of the 42nd ACM SIGPLAN International Conference on Programming Language Design and Implementation* (Virtual, Canada) *(PLDI 2021)*. Association for Computing Machinery, New York, NY, USA, 542–558. https://doi.org/10.1145/3453483.3454061



(a) Quantum circuit

```
Fixpoint rz_adder' (a b:var) (n:ℕ)
  := match n with
     | 0 ⇒ ID (a,0)
     | S m ⇒ CU (a,m) (SR m b);
              rz_adder' a b m
     end.
Definition rz_adder (a b:var) (n:ℕ)
  := Rev a ; Rev b ; QFT b ;
     rz_adder' a b n;
     QFT⁻¹ b; Rev b ; Rev a.
```

(b) 𝒪QASM metaprogram (in Coq)

Fig. 10. Example 𝒪QASM program: QFT-based adder

Bit	b	::=	$0 \mid 1$
Natural number	n	$\in$	$\mathbb{N}$
Real	r	$\in$	$\mathbb{R}$
Phase	$\alpha(r)$	::=	$e^{2\pi i r}$
Basis	τ	::=	`Nor` $\mid$ `Phi` n
Unphased qubit	$\overline{q}$	::=	$\lvert b\rangle \mid \lvert\Phi(r)\rangle$
Qubit	q	::=	$\alpha(r)\overline{q}$
State (length d)	φ	::=	$q_1 \otimes q_2 \otimes \cdots \otimes q_d$

Fig. 11. 𝒪QASM state syntax

3 𝒪QASM: AN ASSEMBLY LANGUAGE FOR QUANTUM ORACLES

We designed 𝒪QASM to be able to express efficient quantum oracles that can be easily tested and, if desired, proved correct. 𝒪QASM operations leverage both the standard computational basis and an alternative basis connected by the quantum Fourier transform (QFT). 𝒪QASM's type system tracks the bases of variables in 𝒪QASM programs, forbidding operations that would introduce entanglement. 𝒪QASM states are therefore efficiently represented, so programs can be effectively tested and are simpler to verify and analyze. In addition, 𝒪QASM uses *virtual qubits* to support *position shifting operations*, which support arithmetic operations without introducing extra gates during translation. All of these features are novel to quantum assembly languages.

This section presents 𝒪QASM states and the language's syntax, semantics, typing, and soundness results. As a running example, we use the QFT adder [Beauregard 2003] shown in Figure 10. The Coq function `rz_adder` generates an 𝒪QASM program that adds two natural numbers `a` and `b`, each of length `n` qubits.

3.1 𝒪QASM States

An 𝒪QASM program state is represented according to the grammar in Figure 11. A state φ of d qubits is a length-d tuple of qubit values q; the state models the tensor product of those values. This means that the size of φ is $O(d)$ where d is the number of qubits. A d-qubit state in a language like SQIR is represented as a length 2^d vector of complex numbers, which is $O(2^d)$ in the number of qubits. Our linear state representation is possible because applying any well-typed 𝒪QASM program on any well-formed 𝒪QASM state never causes qubits to be entangled.

A qubit value q has one of two forms $\overline{q}$, scaled by a global phase $\alpha(r)$. The two forms depend on the *basis* τ that the qubit is in—it could be either `Nor` or `Phi`. A `Nor` qubit has form $|b\rangle$ (where

Position	p	::=	(x, n)	Nat. Num n	Variable x
Instruction	ι	::=	$\texttt{ID}\ p \mid \texttt{X}\ p \mid \texttt{RZ}^{[-1]}\ n\ p \mid \iota\ ;\ \iota$		
		|	$\texttt{SR}^{[-1]}\ n\ x \mid \texttt{QFT}^{[-1]}\ n\ x \mid \texttt{CU}\ p\ \iota$		
		|	$\texttt{Lshift}\ x \mid \texttt{Rshift}\ x \mid \texttt{Rev}\ x$		

Fig. 12. ℚASM syntax. For an operator OP, $\texttt{OP}^{[-1]}$ indicates that the operator has a built-in inverse available.

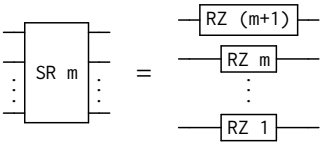


Fig. 13. SR unfolds to a series of RZ instructions

$b \in \{0, 1\}$), which is a computational basis value. A Phi qubit has form $|\Phi(r)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + \alpha(r)\,|1\rangle)$, which is a value of the (A)QFT basis. The number n in Phi n indicates the precision of the state φ. As shown by Beauregard [2003], arithmetic on the computational basis can sometimes be more efficiently carried out on the QFT basis, which leads to the use of quantum operations (like QFT) when implementing circuits with classical input/output behavior.

3.2 ℚASM Syntax, Typing, and Semantics

[Liyi: add RZ gate back]

Figure 12 presents ℚASM's syntax. An ℚASM program consists of a sequence of instructions ι. Each instruction applies an operator to either a variable x, which represents a group of qubits, or a *position* p, which identifies a particular offset into a variable x.

The instructions in the first row correspond to simple single-qubit quantum gates—$\texttt{ID}\ p$, $\texttt{X}\ p$, and $\texttt{RZ}^{[-1]}\ n\ p$ —and instruction sequencing. The instructions in the next row apply to whole variables: $\texttt{QFT}\ n\ x$ applies the AQFT to variable x with n-bit precision and $\texttt{QFT}^{-1}\ n\ x$ applies its inverse. If n is equal to the size of x, then the AQFT operation is exact. $\texttt{SR}^{[-1]}\ n\ x$ applies a series of RZ gates (Figure 13). Operation $\texttt{CU}\ p\ \iota$ applies instruction ι *controlled* on qubit position p. All of the operations in this row—SR, QFT, and CU—will be translated to multiple sqir gates. Function rz_adder in Figure 10(b) uses many of these instructions; e.g., it uses QFT and $\texttt{QFT}^{-1}$ and applies CU to the mth position of variable a to control instruction SR m b.

In the last row of Figure 12, instructions $\texttt{Lshift}\ x$, $\texttt{Rshift}\ x$, and $\texttt{Rev}\ x$ are *position shifting operations*. Assuming that x has d qubits and x_k represents the k-th qubit state in x, $\texttt{Lshift}\ x$ changes the k-th qubit state to $x_{(k+1)\%d}$, $\texttt{Rshift}\ x$ changes it to $x_{(k+d-1)\%d}$, and Rev changes it to x_{d-1-k}. In our implementation, shifting is *virtual* not physical. The ℚASM translator maintains a logical map of variables/positions to concrete qubits and ensures that shifting operations are no-ops, introducing no extra gates.

Other quantum operations could be added to ℚASM to allow reasoning about a larger class of quantum programs, while still guaranteeing a lack of entanglement. In **??**, we show how ℚASM can be extended to include the Hadamard gate H, z-axis rotations Rz, and a new basis Had to reason directly about implementations of QFT and AQFT. However, this extension compromises the property of type reversibility (Theorem 3.5, Section 3.3), and we have not found it necessary in oracles we have developed.

Typing. In ℚASM, typing is with respect to a *type environment* Ω and a predefined *size environment* Σ, which map ℚASM variables to their basis and size (number of qubits), respectively. The typing judgment is written $\Sigma; \Omega \vdash \iota \triangleright \Omega'$ which states that ι is well-typed under Ω and Σ, and transforms the variables' bases to be as in Ω' (Σ is unchanged). **[Liyi: good?]** Σ is fixed because the number of qubits in an execution is always fixed. It is generated in the high level language compiler, such as ℚIMP in **??**. The algorithm generates Σ by taking an ℚIMP program and scanning through all the variable initialization statements. Select type rules are given in Figure 14; the rules not shown (for ID, Rshift, Rev, $\texttt{RZ}^{-1}$, and $\texttt{SR}^{-1}$) are similar.

$$\text{X}\quad \frac{\Omega(x) = \texttt{Nor} \qquad n < \Sigma(x)}{\Sigma;\Omega \vdash \texttt{X}\ (x,n) \triangleright \Omega}$$

$$\text{RZ}\quad \frac{\Omega(x) = \texttt{Nor} \qquad n < \Sigma(x)}{\Sigma;\Omega \vdash \texttt{RZ}\ q\ (x,n) \triangleright \Omega}$$

$$\text{SR}\quad \frac{\Omega(x) = \texttt{Phi}\ n \qquad m < n}{\Sigma;\Omega \vdash \texttt{SR}\ m\ x \triangleright \Omega}$$

$$\text{QFT}\quad \frac{\Omega(x) = \texttt{Nor} \qquad n \le \Sigma(x)}{\Sigma;\Omega \vdash \texttt{QFT}\ n\ x \triangleright \Omega[x \mapsto \texttt{Phi}\ n]}$$

$$\text{RQFT}\quad \frac{\Omega(x) = \texttt{Phi}\ n \qquad n \le \Sigma(x)}{\Sigma;\Omega \vdash \texttt{QFT}^{-1}\ n\ x \triangleright \Omega[x \mapsto \texttt{Nor}]}$$

$$\text{CU}\quad \frac{\Omega(x) = \texttt{Nor} \qquad \texttt{fresh}\ (x,n)\ \iota \qquad \Sigma;\Omega \vdash \iota \triangleright \Omega \qquad \texttt{neutral}(\iota)}{\Sigma;\Omega \vdash \texttt{CU}\ (x,n)\ \iota \triangleright \Omega}$$

$$\text{LSH}\quad \frac{\Omega(x) = \texttt{Nor}}{\Sigma;\Omega \vdash \texttt{Lshift}\ x \triangleright \Omega}$$

$$\text{SEQ}\quad \frac{\Sigma;\Omega \vdash \iota_1 \triangleright \Omega' \qquad \Sigma;\Omega' \vdash \iota_2 \triangleright \Omega''}{\Sigma;\Omega \vdash \iota_1\ ;\ \iota_2 \triangleright \Omega''}$$

Fig. 14. Select ⓞQASM typing rules

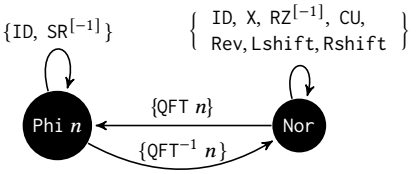


Fig. 15. Type rules' state machine

The type system enforces three invariants. First, it enforces that instructions are well-formed, meaning that gates are applied to valid qubit positions (the second premise in X) and that any control qubit is distinct from the target(s) (the `fresh` premise in CU). This latter property enforces the quantum *no-cloning rule*. For example, we can apply the CU in `rz_adder'` (Figure 10) because position `a,m` is distinct from variable `b`.

Second, the type system enforces that instructions leave affected qubits in a proper basis (thereby avoiding entanglement). The rules implement the state machine shown in Figure 15. For example, QFT n transforms a variable from Nor to Phi n (rule QFT), while $\texttt{QFT}^{-1}$ n transforms it from Phi n back to Nor (rule RQFT). Position shifting operations are disallowed on variables x in the Phi basis because the qubits that make up x are internally related (see Definition 3.1) and cannot be rearranged. Indeed, applying a Lshift and then a $\texttt{QFT}^{-1}$ on x in Phi would entangle x's qubits.

Third, the type system enforces that the effect of position shifting operations can be statically tracked. The `neutral` condition of CU requires that any shifting within ι is restored by the time it completes. For example, CU p (Lshift x) ; X $(x, 0)$ is not well-typed, because knowing the final physical position of qubit $(x, 0)$ would require statically knowing the value of p. On the other hand, the program CU c (Lshift x ; X $(x, 0)$; Rshift x) ; X $(x, 0)$ is well-typed because the effect of the Lshift is "undone" by an Rshift inside the body of the CU.

Semantics. We define the semantics of an ⓞQASM program as a partial function $[\![\ ]\!]$ from an instruction ι and input state φ to an output state φ', written $[\![\iota]\!]\varphi = \varphi'$, shown in Figure 16.

Recall that a state φ is a tuple of d qubit values, modeling the tensor product $q_1 \otimes \cdots \otimes q_d$. The rules implicitly map each variable x to a range of qubits in the state, e.g., $\varphi(x)$ corresponds to some sub-state $q_k \otimes \cdots \otimes q_{k+n-1}$ where $\Sigma(x) = n$. Many of the rules in Figure 16 update a *portion* of a state. We write $\varphi[(x,i) \mapsto q_{(x,i)}]$ to update the i-th qubit of variable x to be the (single-qubit) state $q_{(x,i)}$, and $\varphi[x \mapsto q_x]$ to update variable x according to the qubit *tuple* q_x. $\varphi[(x,i) \mapsto \uparrow q_{(x,i)}]$ and $\varphi[x \mapsto \uparrow q_x]$ are similar, except that they also accumulate the previous global phase of $\varphi(x,i)$ (or $\varphi(x)$). We use $\downarrow$ to convert a qubit $\alpha(b)\overline{q}$ to an unphased qubit $\overline{q}$.

Function xg updates the state of a single qubit according to the rules for the standard quantum gate X. cu is a conditional operation depending on the Nor-basis qubit (x, i). **[Liyi: good?]** RZ (or $\texttt{RZ}^{-1}$) is an z-axis phase rotation operation. Since it applies to Nor-basis, it applies a global phase.

$$
\begin{array}{lll}
[\![\texttt{ID}\ p]\!]\varphi & = \varphi & \\
[\![\texttt{X}\ (x,i)]\!]\varphi & = \varphi[(x,i) \mapsto \uparrow \texttt{xg}(\downarrow \varphi(x,i))] & \text{where } \texttt{xg}(|0\rangle) = |1\rangle \quad \texttt{xg}(|1\rangle) = |0\rangle \\
[\![\texttt{CU}\ (x,i)\ \iota]\!]\varphi & = \texttt{cu}(\downarrow \varphi(x,i), \iota, \varphi) & \text{where } \texttt{cu}(|0\rangle, \iota, \varphi) = \varphi \quad \texttt{cu}(|1\rangle, \iota, \varphi) = [\![\iota]\!]\varphi \\
[\![\texttt{RZ}\ m\ (x,i)]\!]\varphi & = \varphi[(x,i) \mapsto \uparrow \texttt{rz}(m, \downarrow \varphi(x,i))] & \text{where } \texttt{rz}(m, |0\rangle) = |0\rangle \quad \texttt{rz}(m, |1\rangle) = \alpha(\frac{1}{2^m})\,|1\rangle \\
[\![\texttt{RZ}^{-1}\ m\ (x,i)]\!]\varphi & = \varphi[(x,i) \mapsto \uparrow \texttt{rrz}(m, \downarrow \varphi(x,i))] & \text{where } \texttt{rrz}(m, |0\rangle) = |0\rangle \quad \texttt{rrz}(m, |1\rangle) = \alpha(-\frac{1}{2^m})\,|1\rangle \\
[\![\texttt{SR}\ m\ x]\!]\varphi & = \varphi[\forall i \le m.\ (x,i) \mapsto \uparrow |\Phi(r_i + \frac{1}{2^{m-i+1}})\rangle] & \text{when } \downarrow \varphi(x,i) = |\Phi(r_i)\rangle \\
[\![\texttt{SR}^{-1}\ m\ x]\!]\varphi & = \varphi[\forall i \le m.\ (x,i) \mapsto \uparrow |\Phi(r_i - \frac{1}{2^{m-i+1}})\rangle] & \text{when } \downarrow \varphi(x,i) = |\Phi(r_i)\rangle \\
[\![\texttt{QFT}\ n\ x]\!]\varphi & = \varphi[x \mapsto \uparrow \texttt{qt}(\Sigma(x), \downarrow \varphi(x), n)] & \text{where } \texttt{qt}(i, |y\rangle, n) = \bigotimes_{k=0}^{i-1}(|\Phi(\frac{y}{2^{n-k}})\rangle) \\
[\![\texttt{QFT}^{-1}\ n\ x]\!]\varphi & = \varphi[x \mapsto \uparrow \texttt{qt}^{-1}(\Sigma(x), \downarrow \varphi(x), n)] & \\
[\![\texttt{Lshift}\ x]\!]\varphi & = \varphi[x \mapsto \texttt{pm}_l(\varphi(x))] & \text{where } \texttt{pm}_l(q_0 \otimes q_1 \otimes \cdots \otimes q_{n-1}) = q_{n-1} \otimes q_0 \otimes q_1 \otimes \cdots \\
[\![\texttt{Rshift}\ x]\!]\varphi & = \varphi[x \mapsto \texttt{pm}_r(\varphi(x))] & \text{where } \texttt{pm}_r(q_0 \otimes q_1 \otimes \cdots \otimes q_{n-1}) = q_1 \otimes \cdots \otimes q_{n-1} \otimes q_0 \\
[\![\texttt{Rev}\ x]\!]\varphi & = \varphi[x \mapsto \texttt{pm}_a(\varphi(x))] & \text{where } \texttt{pm}_a(q_0 \otimes \cdots \otimes q_{n-1}) = q_{n-1} \otimes \cdots \otimes q_0 \\
[\![\iota_1; \iota_2]\!]\varphi & = [\![\iota_2]\!]([\![\iota_1]\!]\varphi) &
\end{array}
$$

$$
\begin{array}{l}
\downarrow \alpha(b)\overline{q} = \overline{q} \qquad \downarrow (q_1 \otimes \cdots \otimes q_n) = \downarrow q_1 \otimes \cdots \otimes \downarrow q_n \\
\varphi[(x,i) \mapsto \uparrow \overline{q}] = \varphi[(x,i) \mapsto \alpha(b)\overline{q}] \quad \text{where } \varphi(x,i) = \alpha(b)\overline{q_i} \\
\varphi[(x,i) \mapsto \uparrow \alpha(b_1)\overline{q}] = \varphi[(x,i) \mapsto \alpha(b_1 + b_2)\overline{q}] \quad \text{where } \varphi(x,i) = \alpha(b_2)\overline{q_i} \\
\varphi[x \mapsto q_x] = \varphi[\forall i < \Sigma(x).\ (x,i) \mapsto q_{(x,i)}] \\
\varphi[x \mapsto \uparrow q_x] = \varphi[\forall i < \Sigma(x).\ (x,i) \mapsto \uparrow q_{(x,i)}]
\end{array}
$$

Fig. 16. 𝒪QASM semantics

By Theorem 3.4, when we compiles it to SQIR, the global phase might be turned to a local one. For example, to prepare the state $\sum_{j=0}^{2^n}(-i)^x\,|x\rangle$ [Childs et al. 2007], we apply a series of Hadamard gates following by several controlled-RZ gates on x, where the controlled-RZ gates are definable by 𝒪QASM. SR (or $\texttt{SR}^{-1}$) applies an $m+1$ series of RZ (or $\texttt{RZ}^{-1}$) rotations where the i-th rotation applies a phase of $\alpha(\frac{1}{2^{m-i+1}})$ (or $\alpha(-\frac{1}{2^{m-i+1}})$). qt applies an approximate quantum Fourier transform; $|y\rangle$ is an abbreviation of $|b_1\rangle \otimes \cdots \otimes |b_i\rangle$ (assuming $\Sigma(y) = i$) and n is the degree of approximation. If $n = i$, then the operation is the standard QFT. Otherwise, each qubit in the state is mapped to $|\Phi(\frac{y}{2^{n-k}})\rangle$, which is equal to $\frac{1}{\sqrt{2}}(|0\rangle + \alpha(\frac{y}{2^{n-k}})\,|1\rangle)$ when $k < n$ and $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$ when $n \le k$ (since $\alpha(n) = 1$ for any natural number n). $\texttt{qt}^{-1}$ is the inverse function of qt. Note that the input state to $\texttt{qt}^{-1}$ is guaranteed to have the form $\bigotimes_{k=0}^{i-1}(|\Phi(\frac{y}{2^{n-k}})\rangle)$ because it has type Phi n. $\texttt{pm}_l$, $\texttt{pm}_r$, and $\texttt{pm}_a$ are the semantics for Lshift, Rshift, and Rev, respectively.

3.3 𝒪QASM Metatheory

Soundness. We prove that well-typed 𝒪QASM programs are well defined; i.e., the type system is sound with respect to the semantics. We begin by defining the well-formedness of an 𝒪QASM state.

Definition 3.1 (Well-formed 𝒪QASM state). A state φ is *well-formed*, written $\Sigma; \Omega \vdash \varphi$, iff:

- For every $x \in \Omega$ such that $\Omega(x) = \texttt{Nor}$, for every $k < \Sigma(x)$, $\varphi(x,k)$ has the form $\alpha(r)\,|b\rangle$.
- For every $x \in \Omega$ such that $\Omega(x) = \texttt{Phi}\ n$ and $n \le \Sigma(x)$, there exists a value v such that for every $k < \Sigma(x)$, $\varphi(x,k)$ has the form $\alpha(r)\,|\Phi(\frac{v}{2^{n-k}})\rangle$.[4]

Type soundness is stated as follows; the proof is by induction on ι, and is mechanized in Coq.

[4]Note that $\Phi(x) = \Phi(x+n)$, where the integer n refers to phase $2\pi n$; so multiple choices of v are possible.

$$\texttt{X}\ (x,n) \xrightarrow{\text{inv}} \texttt{X}\ (x,n) \qquad \texttt{SR}\ m\ x \xrightarrow{\text{inv}} \texttt{SR}^{-1}\ m\ x \qquad \texttt{QFT}\ n\ x \xrightarrow{\text{inv}} \texttt{QFT}^{-1}\ n\ x \qquad \texttt{Lshift}\ x \xrightarrow{\text{inv}} \texttt{Rshift}\ x$$

$$\frac{\iota \xrightarrow{\text{inv}} \iota'}{\texttt{CU}\ (x,n)\ \iota \xrightarrow{\text{inv}} \texttt{CU}\ (x,n)\ \iota'} \qquad \frac{\iota_1 \xrightarrow{\text{inv}} \iota_1' \qquad \iota_2 \xrightarrow{\text{inv}} \iota_2'}{\iota_1\ ;\ \iota_2 \xrightarrow{\text{inv}} \iota_2'\ ;\ \iota_1'}$$

Fig. 17. Select 𝒪QASM inversion rules

Theorem 3.2. [𝒪QASM type soundness] If $\Sigma; \Omega \vdash \iota \triangleright \Omega'$ and $\Sigma; \Omega \vdash \varphi$ then there exists φ' such that $[\![\iota]\!]\varphi = \varphi'$ and $\Sigma; \Omega' \vdash \varphi'$.

Algebra. Mathematically, the set of well-formed d-qubit 𝒪QASM states for a given Ω can be interpreted as a subset $\mathcal{S}^d$ of a 2^d-dimensional Hilbert space $\mathcal{H}^d$,[5] and the semantics function $[\![\ ]\!]$ can be interpreted as a $2^d \times 2^d$ unitary matrix, as is standard when representing the semantics of programs without measurement [Hietala et al. 2021a]. Because 𝒪QASM's semantics can be viewed as a unitary matrix, correctness properties extend by linearity from $\mathcal{S}^d$ to $\mathcal{H}^d$—an oracle that performs addition for classical Nor inputs will also perform addition over a superposition of Nor inputs. We have proved that $\mathcal{S}^d$ is closed under well-typed 𝒪QASM programs.

[Liyi: good?] Given a qubit size map Σ and type environment Ω, the set of 𝒪QASM programs that are well-typed with respect to Σ and Ω (i.e., $\Sigma; \Omega \vdash \iota \triangleright \Omega'$) form a algebraic structure $(\{\iota\}, \Sigma, \Omega, \mathcal{S}^d)$, where $\{\iota\}$ defines the set of valid program syntax, such that there exists Ω', $\Sigma; \Omega \vdash \iota \triangleright \Omega'$ for all ι in $\{\iota\}$; $\mathcal{S}^d$ is the set of d-qubit states on which programs $\iota \in \{\iota\}$ are run, and are well-formed $(\Sigma; \Omega \vdash \varphi)$ according to Definition 3.1. From the 𝒪QASM semantics and the type soundness theorem, for all $\iota \in \{\iota\}$ and $\varphi \in \mathcal{S}^d$, such that $\Sigma; \Omega \vdash \iota \triangleright \Omega'$ and $\Sigma; \Omega \vdash \varphi$, we have $[\![\iota]\!]\varphi = \varphi'$, $\Sigma; \Omega' \vdash \varphi'$, and $\varphi' \in \mathcal{S}^d$. Thus, $(\{\iota\}, \Sigma, \Omega, \mathcal{S}^d)$, where $\{\iota\}$ defines a groupoid.

We can certainly extend the groupoid to another algebraic structure $(\{\iota'\}, \Sigma, \mathcal{H}^d)$, where $\mathcal{H}^d$ is a general 2^d dimensional Hilbert space $\mathcal{H}^d$ and $\{\iota'\}$ is a universal set of quantum gate operations. Clearly, we have $\mathcal{S}^d \subseteq \mathcal{H}^d$ and $\{\iota\} \subseteq \{\iota'\}$, because sets $\mathcal{H}^d$ and $\{\iota'\}$ can be acquired by removing the well-formed $(\Sigma; \Omega \vdash \varphi)$ and well-typed $(\Sigma; \Omega \vdash \iota \triangleright \Omega')$ definitions for $\mathcal{S}^d$ and $\{\iota\}$, respectively. $(\{\iota'\}, \Sigma, \mathcal{H}^d)$ is a groupoid because every 𝒪QASM operation is valid in a traditional quantum language like SQIR. We then have the following two two theorems to connect 𝒪QASM operations with operations in the general Hilbert space:

Theorem 3.3. $(\{\iota\}, \Sigma, \Omega, \mathcal{S}^d) \subseteq (\{\iota\}, \Sigma, \mathcal{H}^d)$ is a subgroupoid.

Theorem 3.4. Let $|y\rangle$ be an abbreviation of $\bigotimes_{m=0}^{d-1} \alpha(r_m)\,|b_m\rangle$ for $b_m \in \{0,1\}$. If for every $i \in [0, 2^d)$, $[\![\iota]\!]\,|y_i\rangle = |y_i'\rangle$, then $[\![\iota]\!](\sum_{i=0}^{2^d-1} |y_i\rangle) = \sum_{i=0}^{2^d-1} |y_i'\rangle$.

We prove these theorems as corollaries of the compilation correctness theorem from 𝒪QASM to SQIR (**??**). Theorem 3.3 suggests that the space $\mathcal{S}^d$ is closed under the application of any well-typed 𝒪QASM operation. Theorem 3.4 says that 𝒪QASM oracles can be safely applied to superpositions over classical states.[6]

𝒪QASM programs are easily invertible, as shown by the rules in Figure 17. This inversion operation is useful for constructing quantum oracles; for example, the core logic in the QFT-based subtraction circuit is just the inverse of the core logic in the addition circuit (Figure 17). This allows us to reuse

[5] A *Hilbert space* is a vector space with an inner product that is complete with respect to the norm defined by the inner product. $\mathcal{S}^d$ is a sub*set*, not a sub*space* of $\mathcal{H}^d$ because $\mathcal{S}^d$ is not closed under addition: Adding two well-formed states can produce a state that is not well-formed.

[6] Note that a superposition over classical states can describe *any* quantum state, including entangled states.

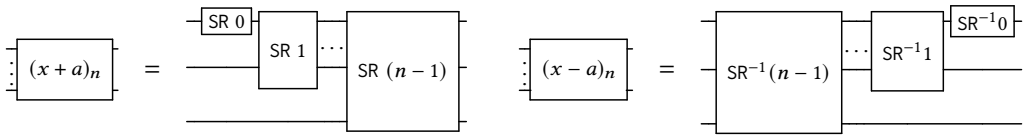


Fig. 18. Addition/subtraction circuits are inverses

the proof of addition in the proof of subtraction. The inversion function satisfies the following properties:

Theorem 3.5. [Type reversibility] For any well-typed program ι, such that $\Sigma; \Omega \vdash \iota \triangleright \Omega'$, its inverse ι', where $\iota \xrightarrow{\text{inv}} \iota'$, is also well-typed and we have $\Sigma; \Omega' \vdash \iota' \triangleright \Omega$. Moreover, $[\![\iota; \iota']\!]\varphi = \varphi$.