Poq: Projection-based Runtime Assertions for Debugging on a Quantum Computer

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ABSTRACT
In this paper, we propose Poq, a runtime assertion scheme for debugging on a quantum computer. The predicates in the assertions are represented by projections (or equivalently, closed subspaces of the state space), following Birkhoff-von Neumann quantum logic. The satisfaction of a projection by a quantum state can be directly checked upon a small number of projective measurements rather than a large number of repeated executions. Several techniques are introduced to rotate the predicates to the computational basis, on which a realistic quantum computer usually supports its measurements, so that a satisfying tested state will not be destroyed when an assertion is checked and multi-assertion per testing execution is enabled. We compare Poq with existing quantum program assertions and demonstrate the effectiveness and efficiency of Poq by its applications to assert two sophisticated quantum algorithms.

1 INTRODUCTION
Quantum computing is a promising computing paradigm with great potential in cryptography [31], database [14], linear systems [15], chemistry simulation [27], etc. Several quantum program languages [1, 2, 12, 13, 26, 29, 32] have been published to write quantum programs for quantum computers. One of the key challenges that must be addressed during quantum program development is to guarantee the correctness of the composed program since it is easy for programmers living in the classical world to make mistakes in the counter-intuitive quantum programming. For example, Huang and Martonosi [16, 17] reported a few bugs found in the example programs from the ScaffCC compiler project [20]. Bugs have also been found in the example programs in IBM’s OpenQASM project [19] and Rigetti’s PyQuil project [28]. These erroneous quantum programs, written and reviewed by professional quantum computing experts, are sometimes even of very small size (with only 3 qubits)1. Such difficulty in writing correct quantum programs hinders practical quantum computing. Thus, effective and efficient quantum program debugging is naturally in urgent demand.

Assertions have demonstrated the ability to capture the bugs in quantum programs. Huang and Martonosi proposed statistical assertions, which employed statistical tests on classical observations [17] to debug quantum programs. Motivated by quantum error correction (QEC), Zhou and Byrd proposed a runtime assertion [42], which introduces ancilla qubits to indirectly detect the system state. However, as early attempts towards quantum program debugging, these assertion schemes suffer from the following drawbacks:

1) Very few assertion types The properties of quantum states can be much more complex than those in classical computing. Expressing the quantum program assertion predicates in a classical logic language leads to very few available assertion types. Existing quantum assertions [17, 42] can only describe three types of states.

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1We checked the issues raised in these projects’ official GitHub repositories for this information.
2) **Limited assertion locations** The behaviors of quantum states can be very complicated inside a quantum program and it requires non-trivial effort to evaluate the predicates even within a quantum program logic system [18, 33, 38, 41, 43]. Existing quantum assertions [17, 42] can only inject assertions at some special locations where the states are within the three supported types.

3) **Repeated executions for one assertion** A general quantum state cannot be duplicated [36], while measurements usually only probe part of the state information and will destroy the tested state immediately. Thus, an assertion, together with the computation before it, must be repeated for a large number of times to achieve a precise estimation [17].

4) **One assertion per execution** Another drawback of the destructive measurement is that the computation after an assertion will become meaningless. Even though multiple assertions can be injected at the same time, only one assertion could be inspected per execution, which will make the assertion testing more prolonged [17].

Limited assertion types and locations will increase the difficulty in debugging as assertions may have to be injected far away from a bug. Moreover, programs with complex intermediate states cannot be checked by the limited assertions. The large number of executions will make the testing process very time-consuming, restricting the size of the program and the number of assertions that could be feasibly checked.

We observe that projection can be the key to address these issues due to its potential logical expressive power and unique mapping property. First used as propositions or predicates in quantum logic by Birkhoff and von Neumann back in 1936 [7], projections can enable reasoning about quantum programs with the power of quantum logic. It has already served as predicates in several existing quantum program logics [5, 9, 33, 40, 43]. Projections correspond to closed subspaces of a Hilbert space, on which logical connectives (e.g., conjunction, disjunction, and negation) can be defined, leading to strong logical expressive power. Moreover, projections naturally match the projective measurement, which may not affect the measured state when the state is in one of some pure states [21]. Such a feature could potentially reduce the testing overhead as a state can be tested for multiple predicates [43].

However, the systematic employment of projections in quantum program debugging remains unexplored. We fill this gap by proposing the first Projection-Operator based Quantum program assertion scheme, namely Poq, for practical runtime debugging on a quantum computer. In particular, we make the following main contributions:

1) We define the **syntax** and **semantics** of a new **assert** primitive for Poq, using projections as predicates. With the help of the expressive power of the logical connectives in Birkhoff-von Neumann quantum logic, this **assert** primitive could represent much more complex properties of quantum programs. Poq also employs applied Quantum Hoare Logic [43] to derive flexible assertions at arbitrary locations in a program.

2) We introduce several **transformation techniques**, including **additional unitary transformation, combination of projections**, and using **auxiliary qubits**, to implement the **assert** primitive on a measurement-restricted quantum computer. The satisfaction of such **assert** primitives can be checked within very few executions with high certainty. Multi-assertion per execution is also allowed since a satisfying tested state will not be destroyed during the assertion checking.

3) We further investigate the trade-off between **efficiency and effectiveness of debugging** by studying the local projection technique, which can relax the constraints in the predicates for a simplified assertion implementation. We also prove the **robustness** of our assertions under small errors.

4) We show that Poq outperforms existing quantum program assertions [17, 42] in both theoretical analysis and practical application, with much stronger expressive power, more flexible assertion location, fewer testing executions, and low implementation overhead. Case studies are performed on two well-known sophisticated quantum algorithms, namely Shor’s algorithm [31] and HHL algorithm [15].

2 **PRELIMINARY**

In this section, we cover the necessary preliminary to help understand the proposed assertion scheme.

2.1 **Quantum computing**

Quantum computing is based on quantum systems which evolve under the law of quantum mechanics. The state space of a quantum system is a Hilbert space (denoted by $\mathcal{H}$), a complete complex vector space with inner product defined. A pure state of a quantum system is described by a unit vector $|\psi\rangle$ in its state space. When the exact state is unknown but we know it could be in one of some pure states $|\psi_i\rangle$, with respective probabilities $p_i$, where $\sum_i p_i = 1$, a density operator $\rho$ can be defined to represent such a mixed state with $\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|$. A pure state is a special mixed state. Hence, in this paper, we adopt the more general density operator formulation most of the time since the state in a quantum program can be mixed upon branches and while-loops.

For example, a qubit (the quantum counterpart of a bit in classical computing) has a two-dimensional state space
We list the definitions of the unitary transformations used in the rest of this paper in Appendix A.

Definition 2.1 (Unitary transformation). A unitary transformation $U$ on a quantum system in the finite-dimensional Hilbert space $\mathcal{H}$ is a linear operator satisfying $UU^\dagger = I_{\mathcal{H}}$, where $I_{\mathcal{H}}$ is the identity operator on $\mathcal{H}$.

After a unitary transformation, a state vector $|\psi\rangle$ or a density operator $\rho$ is changed to $U|\psi\rangle$ or $U\rho U^\dagger$, respectively. We list the definitions of the unitary transformations used in this paper in Appendix A.

Definition 2.2 (Quantum measurement). A quantum measurement on a quantum system in the Hilbert space $\mathcal{H}$ is a collection of linear operators $\{M_m\}$ satisfying $\sum_m M_m^\dagger M_m = I_{\mathcal{H}}$.

After a quantum measurement on a pure state $|\psi\rangle$, an outcome $m$ is returned with probability $p(m) = \langle \psi | M_m^\dagger M_m | \psi \rangle$ and then the state is changed to $|\psi_m\rangle = \frac{M_m|\psi\rangle}{\sqrt{p(m)}}$. Note that $\sum_m p(m) = 1$. For a mixed state $\rho$, the probability that the outcome $m$ occurs is $p(m) = tr(M_m^\dagger M_m \rho)$, and then the state will be changed to $\rho_m = \frac{M_m \rho M_m^\dagger}{tr(M_m^\dagger M_m \rho)}$.

2.2 Quantum programming language

For simplicity of presentation, this paper adopts the quantum while-language [38] to describe the quantum algorithms. This language is purely quantum without classical variables but this selection will not affect the generality since the quantum while-language, which has been proved to be universal [38], only keeps basic quantum computation elements that can be easily implemented by other quantum programming languages [1, 2, 12, 13, 26, 29, 32]. Thus, our debugging scheme based on this language can also be easily extended to other quantum programming languages.

Definition 2.3 (Syntax [38]). The quantum while-programs are defined by the grammar:

\[
S ::= \text{skip} \mid S_1 ; S_2 \mid q ::= |0\rangle \mid \overline{q} ::= U|\overline{q}\rangle \\
|\text{if } (\square m \cdot M|\overline{q}\rangle = m \rightarrow S_m) \text{ fi} \\
|\text{while } M|\overline{q}\rangle = 1 \rightarrow S \text{ od}
\]

The language grammar is explained as follows. $q$ represents a quantum variable while $\overline{q}$ means a quantum register, which consists of one or more variables with its corresponding Hilbert space denoted by $\mathcal{H}_q$. $q ::= |0\rangle$ means that quantum variable $q$ is initialized to be $|0\rangle$. $\overline{q} := U|\overline{q}\rangle$ denotes that a unitary transformation $U$ is applied to $\overline{q}$. Case statement if $\cdots$ $\cdot$ fi means a quantum measurement $M$ is performed on $\overline{q}$ to determine which subprogram $S_m$ should be executed based on the measurement outcome $m$. The loop while $\cdots$ od means a measurement $M$ with two possible outcomes 0, 1 will determine whether the loop will terminate or the program will re-enter the loop body.

2.3 Projection and projective measurement

One type of quantum measurement of particular interest is the projective measurement, which is directly supported on realistic quantum computers. We first introduce projections and then define the projective measurement.

For each closed subspace $X$ of $\mathcal{H}$, we can define a projection $P_X$. Note that every $|\psi\rangle \in \mathcal{H}$ ($|\psi\rangle$ does not have to be normalized) can be written as $|\psi\rangle = |\psi_X\rangle + |\psi_0\rangle$ with $|\psi_X\rangle \in X$ and $|\psi_0\rangle \in X^\perp$ (the orthocomplement of $X$).

Definition 2.4 (Projection). The projection $P_X : \mathcal{H} \rightarrow X$ is defined by $P_X|\psi\rangle = |\psi_X\rangle$ for every $|\psi\rangle \in \mathcal{H}$.

Note that $P$ is Hermitian ($P^\dagger = P$) and $P^2 = P$. If a pure state $|\psi\rangle$ (or a mixed state $\rho$) is in the corresponding subspace of a projection $P$, we have $P|\psi\rangle = |\psi\rangle$ ($P\rho P = \rho$). There is a one-to-one correspondence between the closed subspaces of a Hilbert space and the projections in it. For simplicity, we do not distinguish a projection $P$ with its corresponding subspace. Then the rank of a projection $P$ is defined by the dimension of its corresponding subspace.

Definition 2.5 (Projective measurement). A projective measurement $M$ is a quantum measurement in which all the measurement operators are projections ($0_{\mathcal{H}}$ is the zero operator on $\mathcal{H}$):

$M = \{P_m\},$ where $\sum_m P_m = I_{\mathcal{H}}, P_m P_n = \begin{cases} P_m & \text{if } m = n, \\
0_{\mathcal{H}} & \text{otherwise.}
\end{cases}$

Note that if a state $|\psi\rangle$ (or $\rho$) is in the corresponding subspace of $P_m$, then a projective measurement with observed outcome $m$ will not change the state since:

$$|\psi_m\rangle = \frac{P_m|\psi\rangle}{\sqrt{\langle \psi | P_m^\dagger P_m | \psi \rangle}} = \frac{|\psi\rangle}{\sqrt{\langle \psi | P_m^\dagger P_m | \psi \rangle}} = |\psi\rangle$$

$$\text{resp. } \rho_m = \frac{P_m \rho P_m^\dagger}{\text{tr}(P_m^\dagger P_m \rho)} = \frac{\rho}{\text{tr}(\rho)} = \rho$$
2.4 Applied Quantum Hoare Logic

To reason about a quantum program with projective measurements, applied Quantum Hoare Logic (aQHL) was introduced in [43] as a variant of the Quantum Hoare Logic [38] for convenient applications. In aQHL, both the precondition $P$ and the postcondition $Q$ of a Hoare triple $\{P\}S\{Q\}$ are assumed to be projections. A state $\rho$ is said to satisfy a predicate $P$ (written $\rho \models P$) corresponding to subspace $X$ if $\text{supp}(\rho) \subseteq X$ where $\text{supp}(\rho)$ is the subspace spanned by the eigenvectors of $\rho$ with non-zero eigenvalues. A projective Hoare triple $\{P\}S\{Q\}$ is true in the sense of partial correctness in aQHL if for all $\rho$, $\rho \models P \Rightarrow \|S\|\rho \models Q$, where $\|S\|$ is the semantic function of program $S$. It was proved that aQHL is (relatively) complete for quantum programs in which all the measurements are projective.

In addition, aQHL can reason about the robustness of quantum programs, i.e., error bounds of the outputs of programs, with robust (projective) Hoare triples. A robust Hoare triple is a formula of the form: $\{(P, \epsilon)\}S\{(Q, \delta)\}$ where $P, Q$ are projections, $S$ is a program, and $0 \leq \epsilon, \delta < 1$.

**Definition 2.6 (Trace distance of states).** For two states $\rho$ and $\sigma$, the trace distance $D$ between $\rho$ and $\sigma$ is defined as $D(\rho, \sigma) = \frac{1}{2}\text{tr}|\rho - \sigma|$, where $\text{tr}X = \text{tr}X^{\dagger}X$.

A state $\rho$ is said to approximately satisfy (projective) predicate $P$ with error parameter $\epsilon$, written $\rho \models^\epsilon P$ if there exists a $\sigma$ with the same trace such that $\sigma \models P$ and $D(\rho, \sigma) \leq \epsilon$. A robust Hoare triple $\{(P, \epsilon)\}S\{(Q, \delta)\}$ is true (written $\models^R \{(P, \epsilon)\}S\{(Q, \delta)\}$) if for all $\rho$, $\rho \models^\epsilon P \Rightarrow \|S\|\rho \models^\delta Q$.

2.5 Measurement-restricted quantum computer

Although aHQL has restricted all the measurements in a quantum program to be projective measurements, most realistic quantum computers which run on the well-adopted quantum circuit model [25] usually only support projective measurement in the computational basis. For $n$ qubits, such a measurement is described as $M = \{P_i\}$, where $P_i = |i\rangle\langle i|$ is the projection onto the 1-dimensional subspace spanned by the basis state $|i\rangle$, and $i$ ranges over all $n$-bit strings; in particular, for a single qubit, this measurement is simply $M = \{P_0, P_1\}$ with $P_0 = |0\rangle\langle 0|$ and $P_1 = |1\rangle\langle 1|$.

3 ASSERTION DESIGN AND IMPLEMENTATION

In this section, we introduce Poq, a projection-based assertion scheme. We first define the syntax and semantics of a new projection-based assert primitive. Then we introduce several techniques to implement the new assert primitives on measurement-restricted machines. The proof of all the propositions, lemmas, and theorems in this and the next sections are in Appendix B.

3.1 Syntax and semantics

In classical computing, a runtime assertion is checked during execution. If the program state satisfies the predicate in the assertion, the program will continue with the state unchanged. Otherwise, an exception is raised. Such property can be achieved with projection based quantum predicates.

A quantum state $\rho$ will not be affected by a projection $P$ if it is in the subspace of $P$. We can construct a projective measurement $M = \{M_{\text{true}} = P, M_{\text{false}} = I - P\}$. When $\rho$ is in the subspace of $P$, the outcome of this projective measurement is always "true" with probability of 1 and the state is still $\rho$. Then we can know that $\rho$ satisfies $P$ without changing the state. When $\rho$ is not in the subspace of $P$, which means that $\rho$ does not satisfy $P$, the probability of outcome "true" or "false" in the constructed projective measurement is $\text{tr}(P\rho)$ or $1 - \text{tr}(P\rho)$, respectively. Suppose we perform such procedure $k$ times, the probability that we do not observe any "false" outcome is $\text{tr}(P\rho)^k$. Since $\text{tr}(P\rho) < 1$, this probability approaches 0 very quickly and we can conclude if $\rho$ satisfies $P$ with high certainty within very few executions.

Thus, quantum runtime assertions can be designed with projections as predicates. We first add a new assertion statement to the quantum while-language grammar.

**Definition 3.1 (Syntax of the assertion statement).** A quantum assertion is defined as

$$\text{assert}(\overline{q}; P) \equiv P[q_1, \ldots, q_n]$$

where $\overline{q} = q_1, \ldots, q_n$ is a collection of quantum variables and $P$ is a projection onto a (closed) subspace of the state space $\mathcal{H}_q$.

**Semantics of the assertion statement** When executing a assertion statement $\text{assert}(\overline{q}; P)$, a constructed projective measurement $M = \{M_{\text{true}} = P, M_{\text{false}} = I - P\}$ will be performed on the quantum variables $\overline{q}$. If the outcome is "true", the execution continues. Otherwise an error message is reported and the execution will terminate.

With Poq’s runtime assertion defined above, we can inject several assertions in a program since a passed assertion will not affect the state. And with just a few executions, we can conclude whether the predicates are satisfied with high certainty. However, we still need to know what predicate $P$ we should use at what place in a program.

Poq cooperates with aQHL to resolve this problem and is able to derive and inject assertions at arbitrary places in a quantum program. Suppose we have a program $S$. We divide the it into $n$ segments $S_1; S_2; \cdots; S_n$ and hope to inject assertion between consecutive program segments. In Poq, we first derive a series of Hoare triples $\{P_0\}S_1\{P_1\}, \{P_1\}S_2\{P_2\}, \cdots, \{P_{n-1}\}S_n\{P_n\}$ with aQHL where all $P_i$s are projections.
Then we can define a debugging scheme to check whether $S$ is correct in the sense of Hoare triple $\{P_0\}S\{P_n\}$.

**Definition 3.2.** A debugging scheme for $S$ is a new program $S'$ with assertions being added between consecutive subprograms $S_i$ and $S_{i+1}$:

$$S' \equiv \text{assert} (\overline{q}_0; P_0);$$

$$S_1;$$

$$\text{assert} (\overline{q}_1; P_1);$$

$$\vdots$$

$$\text{assert} (\overline{q}_{n-1}; P_{n-1});$$

$$S_{n};$$

$$\text{assert} (\overline{q}_n; P_n)$$

where $\overline{q}_i$ is the collection of quantum variables and $P_i$ is a projection on $H_{q_i}$ for all $0 \leq i \leq n$.

The following theorem shows that this debugging scheme is theoretically feasible.

**Theorem 3.1 (Feasibility of debugging scheme).** Suppose we execute $S'$ for $l$ times with input $\rho$ satisfying $P_0$ and collect all the error messages.

1. If an error message occurs in $\text{assert} (\overline{q}_m; P_m)$ with $m \neq 0$, we conclude that subprogram $S_m$ is not correct according to Hoare triple $\{P_m\}S_{m-1}\{P_m\}$;
2. If no error message is reported, we claim that program $S$ is close to the bug-free standard program; more precisely, $\min_{\text{std}} D(\|S\|_\rho; \|S_{\text{std}}\|_\rho) \leq \frac{1}{\sqrt{n}}$, where the minimum is taken over all bug-free standard program $S_{\text{std}}$ that satisfies $\{P_0\}S_{\text{std}}\{P_n\}$.

Moreover, any error detection does not significantly affect a later detection; that is, even if $S_m$ is wrong, the error detection $S_{m'}$ will still be efficient for all $m' > m$.

### 3.2 Transformation techniques for implementation on quantum computers

Although the debugging scheme is theoretically feasible, the constructed projective measurement may not be directly supported on a realistic quantum computer. In aQHL, there is no constraint on the derived projections and the projective measurement in the assertions can be in any basis. However, only projective measurements in the computational basis is supported on a realistic quantum computer, which makes the assertions not directly executable on the measurement-restricted quantum computers. In this section, we introduce several transformation techniques to overcome this obstacle.

#### 3.2.1 Additional unitary transformation

Suppose the assertion $\text{assert}(\overline{q}; P)$ we want to implement is over $n$-qubit, that is, $\overline{q} = q_1, q_2, \cdots, q_n$, each of $q_i$ is a single qubit variable. The simplest case is rank $P = 2^m$ for some integer $m$ with $0 \leq m \leq n$.

**Proposition 3.1.** For projection $P$ with rank $P = 2^m$, there exists unitary transformation $U_P$ such that (here $I_{q_i} = I_{H_{q_i}}$):

$$U_P U_P^\dagger = Q_{q_1} \otimes Q_{q_2} \otimes \cdot \cdot \cdot \otimes Q_{q_n} = \bigotimes_{i=1}^{n} Q_{q_i} \triangleq Q_P,$$

where $Q_{q_i}$ is either $|0\rangle_q \langle 0|$ or $|1\rangle_q \langle 1|$ or $I_{q_i}$, for each $1 \leq i \leq n$.

We call the pair $(U_P, Q_P)$ an implementation in computational basis (ICB for short of $\text{assert}(\overline{q}; P)$). Generally, ICB is not unique. According to this proposition, we have the following procedure to implement $\text{assert}(\overline{q}; P)$:

1. Apply $U_P$ on $\overline{q}$;
2. Check $Q_P$ in the following steps: For each $1 \leq i \leq n$, if $Q_{q_i} = |0\rangle_q \langle 0|$ or $|1\rangle_q \langle 1|$, then measure $q_i$ in the computational basis to see whether the outcome $k$ is consistent with $Q_{q_i}$; that is, $Q_{q_i} = |k\rangle_q \langle k|$. If all outcomes are consistent, go ahead; otherwise, we terminate the program with an error message;
3. Apply $U_P^\dagger$ on $\overline{q}$.

**Example 3.1.** Given a two-qubit register $\overline{q} = q_1, q_2$, if we want to test whether it is in the Bell state (maximally entangled state) $|\Phi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, we can use the assertion $\text{assert}(\overline{q}; P = |\Phi\rangle \langle \Phi|)$. To implement it in the computational basis, noting that

$$\text{CNOT}[q_1, q_2]H[q_1] \cdot P \cdot H[q_1] \cdot \text{CNOT}[q_1, q_2]$$

$$= |0\rangle_q \langle 0| \otimes |0\rangle_q \langle 0|$$

we can first apply CNOT gate on $\overline{q}$ and $H$ gate on $q_1$, then measure $q_1$ and $q_2$ in the computational basis. If both outcomes are “0”, we apply $H$ on $q_1$ and CNOT on $\overline{q}$ again to recover the state; otherwise, we terminate the program and report that the state is not Bell state $|\Phi\rangle$.

#### 3.2.2 Combining assertions

The method introduced above only applies to the case that rank $P = 2^m$ with some integer $m$. The following proposition provides us a way for dealing with the more general case rank $P \leq 2^{n-1}$: split the assertion into multiple sub-assertions that satisfy the above conditions.

**Proposition 3.2.** For projection $P$ with rank $P \leq 2^{n-1}$, there exist projections $P_1, P_2, \cdots, P_l$ satisfying rank $P_i = 2^{n_i}$ for all $1 \leq i \leq l$, such that $P = P_1 \cap P_2 \cap \cdots \cap P_l$.

Essentially, this way works for our scheme because conjunction can be defined in Birkhoff-von Neumann quantum logic. Theoretically, $l = 2$ is sufficient; but in practice a larger $l$ allows us to choose simpler $P_i$ for each $i \leq l$. 
Using the above proposition, to implement \( \text{assert}(\overline{q}; P) \), we may sequentially apply \( \text{assert}(\overline{q}; P_1), \text{assert}(\overline{q}; P_2), \ldots, \text{assert}(\overline{q}; P_l) \). Suppose \((U_{P_i}, Q_{P_i})\) is an ICB of \( \text{assert}(\overline{q}; P_i) \) for \( 1 \leq i \leq l \), we have the following scheme to implement \( \text{assert}(\overline{q}; P) \):

1. Set counter \( i = 1 \);
2. If \( i = 1 \), apply \( U_{P_1} \); else if \( i = l \), apply \( U_{P_l}^\dagger \); return;
3. otherwise, apply \( U_{P_{i-1}}^\dagger U_{P_i} \);
4. Check \( Q_{P_i} ; i := i + 1 \); go to step 2.

Example 3.2. Given register \( \overline{q} = q_1, q_2, q_3 \), how to implement \( \text{assert}(\overline{q}; P) \) where \( P = |0\rangle_q |0\rangle_q |0\rangle_q \otimes I_{\overline{q}} + |111\rangle_{q_1,q_2,q_3} \)?

Observe that \( P = P_1 \cap P_2 \) where

\[
P_1 = (|0\rangle_{q_1,q_2} |0\rangle_q + |11\rangle_{q_1,q_2}) \otimes I_{\overline{q}},
\]

\[
P_2 = |0\rangle_{q_1,q_2} |0\rangle_q \otimes I_{\overline{q}} + |100\rangle_{q_1,q_2,q_3} |100\rangle_q + |111\rangle_{q_1,q_2,q_3} |111\rangle_q, \tag{1}
\]

with following properties:

\[
\text{CNOT}[q_1, q_2] \cdot \text{CNOT}[q_1, q_2] = I_{\overline{q}} \otimes |0\rangle_q |0\rangle_q \otimes I_{\overline{q}}.
\]

\[
\text{Toffoli}[q_1, q_2, q_3] \cdot \text{Toffoli}[q_1, q_2, q_3] = I_{\overline{q}} \otimes |0\rangle_q |0\rangle_q \otimes I_{\overline{q}}.
\]

Therefore, we are able to implement \( \text{assert}(\overline{q}; P) \) by:

- Apply \( \text{CNOT}[q_1, q_2] \);
- Measure \( q_1 \) and check if the outcome is “0”; if not, terminate and report the error message;
- Apply \( \text{CNOT}[q_1, q_2] \) and then \( \text{Toffoli}[q_1, q_2, q_3] \);
- Measure \( q_3 \) and check if the outcome is “0”; if not, terminate and report the error message;
- Apply \( \text{Toffoli}[q_1, q_2, q_3] \).

3.2.3 Auxiliary qubits. A case still remains unsolved: rank \( P > 2^{n-1} \). To handle this case, the auxiliary qubit is necessary. Without the auxiliary qubit, any measurement divides the entire space into multiple subspaces with dimension at most \( 2^{n-1} \), which leads to the impossibility of implementing \( \text{assert}(\overline{q}; P) \). Introducing an auxiliary qubit can solve this difficulty.

Specifically, we introduce an auxiliary qubit \( a \) which is initialized to basis state \( |0\rangle_a \), then implement

\[
\text{assert}(a, \overline{q}; |0\rangle_a |0\rangle_a \otimes P)
\]

instead of original \( \text{assert}(\overline{q}; P) \). Noting that rank \( |0\rangle_a |0\rangle_a \otimes P ) = rank P \leq 2^n \) and the number of qubits is \( n+1 \) including auxiliary qubit \( a \), therefore the methods introduced before is enough to complete the rest steps. Here is a trick to reduce the complexity: we may split \(|0\rangle_a |0\rangle_a \otimes P\) with \( P = |0\rangle_a |0\rangle_a \otimes I_q, P_1, \ldots, P_l \) such that \(|0\rangle_a |0\rangle_a \otimes P = \bigcap_{i=1}^l P_i \). Since the auxiliary qubit is initialized to \( |0\rangle \), \( P_0 \) automatically holds and thus we only need to sequentially apply \( \text{assert}(a, \overline{q}; P_1), \ldots, \text{assert}(a, \overline{q}; P_l) \).

In fact, \( l = 1 \) is enough.

Example 3.3. Given register \( \overline{q} = q_1, q_2 \), we aim to implement \( \text{assert}(\overline{q}; P) \) where \( P = |0\rangle_{q_1} |0\rangle_q \otimes I_{\overline{q}} + |11\rangle_{q_1,q_2} |11\rangle_q \). We may have the decomposition \( |0\rangle_a |0\rangle \otimes P = P_0 \cap P_1 \), where

\[
P_0 = |0\rangle_a |0\rangle \otimes I_q,
\]

\[
P_1 = |0\rangle_a |0\rangle \otimes I_q + |011\rangle_{a,q_1,q_2} |011\rangle_q + |100\rangle_{a,q_1,q_2} |100\rangle_q,
\]

and an ICB of \( P_1 \) is:

\[
\text{Fredkin}[q_2, a, q_1] \cdot P_1 \cdot \text{Fredkin}[q_2, a, q_1] = I_q \otimes |0\rangle_q |0\rangle \otimes I_q.
\]

Note that \( P_0 \) automatically holds since the auxiliary qubit \( a \) is in \( |0\rangle \), we only need to execute:

- Introduce auxiliary qubit \( a \), initialize it to \( |0\rangle \);
- Apply \( \text{Fredkin}[q_2, a, q_1] \);
- Measure \( q_1 \) and check if the outcome is “0”; if not, terminate and report the error message;
- Apply \( \text{Fredkin}[q_2, a, q_1] \); free the auxiliary qubit \( a \).

4 EFFICIENCY AND ROBUSTNESS OF DEBUGGING

In this section, we discuss efficient assertion designs and the decomposition of the introduced unitary transformation. We also prove the robustness of our debugging scheme. In other words, the accumulated error from the assertions is bounded when the error from each assertion is small.

4.1 Local projection: trade-off between efficiency and effectiveness

For projections over multiple qubits, it is quite common to be highly entangled, which leads to the difficulty of implementing the unitary transformation in ICB. It is possible to slightly relax the constraints in the predicates for simplified assertion implementation. To achieve this trade-off, we employ a commonly used approach in quantum information science, namely the quantum state tomography via local measurements \([10, 22, 37]\).

We first introduce the notion of partial trace to describe the state (operator) of a subsystem. Let \( \overline{q}_1 \) and \( \overline{q}_2 \) be two disjoint registers with corresponding state Hilbert space \( \mathcal{H}_{\overline{q}_1} \) and \( \mathcal{H}_{\overline{q}_2} \), respectively. The partial trace over \( \mathcal{H}_{\overline{q}_1} \) is a mapping \( \text{tr}_{\overline{q}_1}(\cdot) \) from operators on \( \mathcal{H}_{\overline{q}_1} \otimes \mathcal{H}_{\overline{q}_2} \) to operators in \( \mathcal{H}_{\overline{q}_2} \) defined by:

\[
\text{tr}_{\overline{q}_1}(|\phi\rangle_{\overline{q}_1} \langle \psi|_{\overline{q}_2}) = \langle \psi_1| \phi_1 \rangle \langle \psi_2| \phi_2 \rangle_{\overline{q}_2}
\]

for all \( |\phi_1\rangle, |\psi_1\rangle \in \mathcal{H}_{\overline{q}_1} \) and \( |\phi_2\rangle, |\psi_2\rangle \in \mathcal{H}_{\overline{q}_2} \) together with linearity. The partial trace \( \text{tr}_{\overline{q}_1}(\cdot) \) over \( \mathcal{H}_{\overline{q}_1} \) can be defined dually.

To illustrate this idea, we need the following definition of local projection:

**Definition 4.1 (Local Projection).** Given \( \text{assert}(\overline{q}; P) \), a local projection \( P_{\overline{q}} \) over \( \overline{q} \subseteq \overline{q} \) is defined as:

\[
P_{\overline{q}} = \text{supp} \left( \text{tr}_{\overline{q} \setminus \overline{q}}(P) \right).
\]

Realizing that \( \overline{q} \subseteq P_{\overline{q}} \otimes I_{\overline{q} \setminus \overline{q}} \), the implementation of \( \text{assert}(\overline{q}; P_{\overline{q}}) \) can partially test whether the state satisfies
P. Moreover, if the number of qubits of $\overline{q}$ is small, the implementation of $\text{assert}(\overline{q}^i; P_q^j)$ can be efficiently achieved. Therefore, we have the following implementation strategy which is essentially a trade-off between checking efficiency and effectiveness:

- Find a sequence of local projection $P_{q_1}, P_{q_2}, \ldots, P_{q_l}$ of $\text{assert}(\overline{q}^i; P)$;
- Instead of implementing the original assertion $\text{assert}(\overline{q}^i; P)$, we sequentially apply $\text{assert}(q_1^i; P_{q_1}), \text{assert}(q_2^i; P_{q_2}), \ldots, \text{assert}(q_l^i; P_{q_l})$.

**Example 4.1.** Given register $\overline{q} = q_1, q_2, q_3, q_4$, we want to check if the state is the superposition of following states:

$|\psi_1\rangle = |+\rangle_{q_1}|111\rangle_{q_2,q_3,q_4}$, $|\psi_2\rangle = |000\rangle_{q_2,q_3,q_4}|-\rangle_{q_1}$,

$|\psi_3\rangle = \frac{1}{\sqrt{2}}(|0\rangle_{q_1}(|00\rangle_{q_2,q_3} + |11\rangle_{q_2,q_3})|1\rangle_{q_4}$.

To accomplish this, we may apply the assertion $\text{assert}(\overline{q}^i; P)$ with $P = \text{supp} (\sum_{i=0}^{3} |\psi_i\rangle \langle \psi_i|)$. However, projection $P$ is highly entangled which prevents efficient implementation. Observe the following local projections:

$P_{q_4,q_3} = \text{tr}_{q_4,q_3}(P) = |0\rangle_{q_4} \otimes |11\rangle_{q_2,q_3}$,

$P_{q_2,q_1} = \text{tr}_{q_2,q_1}(P) = |00\rangle_{q_2,q_1} \otimes |11\rangle_{q_3,q_4}$,

$P_{q_4,q_2} = \text{tr}_{q_4,q_2}(P) = |00\rangle_{q_4,q_2} \otimes |11\rangle_{q_3,q_1}$.

To avoid implementing $\text{assert}(\overline{q}^i; P)$ directly, we may apply $\text{assert}(q_1^i; P_{q_1}), \text{assert}(q_2^i; P_{q_2}), \text{assert}(q_3^i; P_{q_3}), \text{assert}(q_4^i; P_{q_4})$ instead. Though these assertions do not fully characterize the required property, their implementation requires only relatively low cost, i.e., each of them only acts on two qubits.

### 4.2 Unitary transformation decomposition

The additional unitary transformation, which is essential in $P_{oq}$, is usually decomposed into a directly supported gate set when being implemented on a quantum computer. We focus on assertion scheme design while detailed unitary transformation decomposition is out of the scope of this paper. Here we only briefly discuss common target gate sets for decomposition, and the metrics to evaluate a decomposition. It has been proved that arbitrary unitary transformation can be decomposed into a gate set consisting of CNOT gates and single-qubit gates [4]. CNOT gate count is a commonly used metric due to the high implementation overhead of a CNOT gate under state-of-the-art technology [23].

After considering quantum error correction, the set of the elementary logical gates allowed is dictated by the fault tolerance techniques that limit the efficiency of implementing an arbitrary transformation. Recent studies suggest that the fault-tolerant library should consist of Clifford (single-qubit Pauli, Hadamard, Phase, CNOT gates) and T logical gates, with the understanding that the T gate requires considerably more resources than any of the Clifford gates. It has become widely accepted that the T-gate count/depth serves as a good first-order approximation of the resource count required to physically implement a quantum circuit [3, 30].

### 4.3 Robust debugging scheme

Similar to the debugging scheme defined in Section 3, we can still use the projections $P$ and $Q$ appeared in a robust Hoare triple $(P, \epsilon, S)(Q, \delta)$ [43] to define the robust debugging scheme for approximate quantum programs while ignoring the parameter $\epsilon$ and $\delta$. However, it is worthwhile to show this robust debugging scheme is still correct and efficient to detect possible errors of the program when $\epsilon$ and $\delta$ is small.

We first study a special case of the gentle measurement lemma [35] with projections. The result is slightly stronger than the original one in [35] under the constraint of projection.

**Lemma 4.1 (Gentle measurement with projections).** For projection $P$ and density operator $\rho$, if $\text{tr}(P \rho) \geq 1 - \epsilon$, then

$$D(\rho, \frac{P \rho P}{\text{tr}(P \rho)}) \leq \epsilon + \sqrt{\epsilon(1-\epsilon)}.$$

Suppose a state $\rho$ satisfies $P$ with error $\epsilon$, then $\text{tr}(P \rho) \geq 1 - \epsilon$ which ensures that, applying the projection measurement $M_P = \{M_{\text{true}} = P, M_{\text{false}} = I - P\}$, we have the outcome "true" with probability at least $1 - \epsilon$. Moreover, if the outcome is "true", the post-measurement state is $|\frac{P \rho P}{\text{tr}(P \rho)}\rangle$, which is actually close to the original state $\rho$ in the sense that their trace distance is at most $\epsilon + \sqrt{\epsilon(1-\epsilon)}$.

Consider a program $S = S_1; S_2; \ldots; S_n$ with desired robust Hoare triples

$$\{(P_0, \epsilon_0)\} S_1((P_1, \epsilon_1)) \cdots \{(P_{n-1}, \epsilon_{n-1})\} S_n((P_n, \epsilon_n))$$

which are used to conclude the correctness formula $\{(P_0, \epsilon_0)\} S((P_n, \epsilon_n))$ of $S$. The following theorem states that the debugging scheme defined in Definition 3.2 is still efficient for robust debugging.

**Theorem 4.1 (Feasibility of robust debugging).** Assume that all $\epsilon_i$ are small. Execute $S'$ for $k$ times, and we count $k_m$ for the occurrence of error message for assertion $\text{assert}(\overline{q}^i, P_m)$.

(1) If $\frac{k_m}{k - \sum_{i=1}^{m-1} k_i}$ is significantly larger than $\epsilon_m$, we conclude that $S_m$ is not valid for $\{(P_{m-1}, \epsilon_{m-1})\} S_m((P_m, \epsilon_m))$ with high confidence.

(2) If $\frac{k_m}{k - \sum_{i=1}^{m} k_i}$ are close to or smaller than $\epsilon_m$ for all $m \geq 1$, we can conclude that $\{(P_0, 0)\} S((P_n, \delta))$ is valid with high probability, where $\delta = \sum_{i=1}^{n} (\epsilon_i + \sqrt{\epsilon_i(1 - \epsilon_i)}) \approx \sum_{i=1}^{n} \sqrt{\epsilon_i}$ which is explained as the accumulated error of applying assertions.
5 OVERALL COMPARISON

We evaluate Poq in the Section 5 and 6. In this section, we focus on an overall comparison among Poq and two other quantum program assertions in terms of assertion coverage (i.e., the expressive power of the predicates, the assertion locations in a program) and debugging overhead (i.e., the number of measurements, executions, and auxiliary qubits).

**Baseline** We use the statistical assertions (Stat) [17] and the QEC-inspired assertions (QECA) [42] as the baseline assertion schemes. To the best of our knowledge, they are the only published quantum program assertions till now. Stat employs classical statistical test on the measurement results to check if a state satisfies a predicate. QECA introduces auxiliary qubits to indirectly measure the tested state.

5.1 Coverage analysis

Poq employs projections which are able to represent a wide variety of predicates in the derived assertions. However, both Stat and QECA only support three types of assertions: classical assertion, superposition assertion, and entanglement assertion. All these three types of assertions can be considered as 1-dimensional special cases in Poq. The corresponding projections are

\[
P = |t \rangle \langle t|, \quad t \text{ ranges over all n-bit strings}
\]

for classical assertion (suppose n qubits are asserted)

\[
P = |+++ \ldots \rangle \langle +++ \ldots| \quad \text{for superposition assertion}
\]

\[
P = (|00 \ldots 0 \rangle + |11 \ldots 1 \rangle)(|00 \ldots 0 \rangle + |11 \ldots 1 \rangle)
\]

for entanglement assertion

Thus, all the three types of assertions are covered in Poq. The expressive power of the assertions in Poq, which can support many more complicated cases as introduced in Section 3, is much more than that of the baseline schemes.

For the assertion location, Poq can inject assertions at arbitrary place in a program with the help of the proof system proposed in aQHL [43]. But the baseline schemes can only inject assertions in those places with states that can be checked with the very limited types of assertions. Therefore, the number of potential assertion injection locations of Poq is much larger than that of the baseline schemes.

Table 1: Asymptotic overhead comparison for Poq, Stat [17], and QECA [42], \(m\) assertions, \(n\) qubits, and \(N \gg 2^n\)

| # of       | Poq   | Stat   | QECA |
|------------|-------|--------|------|
| Measure    | \(O(nm)\) | \(O(nmN)\) | N/A  |
| Execution  | \(O(1)\) | \(mN\)  | N/A  |
| Aux. Qbit  | 0 or 1 | 0      | \(\geq 1\) |
For HHL algorithm, instead of just asserting a concrete circuit implementation, we will show that Poq could derive non-trivial assertions that cannot be supported by the baselines. In these non-trivial assertions, we will illustrate how the proposed techniques, i.e., combining assertions, auxiliary qubits, local projection, can be applied in implementing the projections. Numerical simulation confirms that Poq-derived assertions can work correctly.

### 6.1 Shor’s algorithm

Shor’s algorithm was proposed to factor a large integer [31]. Given an integer \( N \), Shor’s algorithm can find its non-trivial factors within \( O(\text{poly}(\log(N))) \) time. In this paper, we focus on its quantum order finding subroutine and omit the classical part which is assumed to be correctly implemented.

#### 6.1.1 Shor’s algorithm program

Figure 1 shows the program of the quantum subroutine in Shor’s algorithm with the injected assertions in the quantum while-language. Briefly, it leverages Quantum Fourier Transform (QFT) to find the period of the function \( f(x) = a^x \mod N \) where \( a \) is a random number selected by a preceding classical subroutine. The transformation \( U_f \), the measurement \( M \), and the result set \( R \) are defined as follows:

\[
U_f : |x\rangle_p |0\rangle_q \mapsto |x\rangle_p |a^x \mod N\rangle_q
\]

\[
M = \left\{ M_0 = \sum_{r \in R} |r\rangle \langle r|, M_1 = I - M_0 \right\}
\]

\[
R = \{ r | gcd(a^2 + 1, N) \text{ or } gcd(a^2 - 1, N) \text{ is a non-trivial factor of } N \}
\]

For the measurement, the set \( R \) consists of the expected values that can be accepted by the follow-up classical subroutine. For a comprehensive introduction, please refer to [25].

#### 6.1.2 Assertions for a concrete example

The circuit implementation we select for the subroutine is for factoring \( N = 15 \) with the random number \( a = 11 \) [34]. This will not lose the generality since the overall circuit structures for other configurations are similar. We apply Poq on this circuit and derive four assertions, \( A_0, A_1, A_2, \) and \( A_3 \), as shown in Figure 1. The proof outline is in Appendix C.

Figure 2 shows the final assertion-injected circuit with 5 qubits. The circuit blocks labeled with `assert` are for the four assertions with four projections defined as follows:

\[
A_0 = |00000\rangle_{0,1,2,3,4};
\]

\[
A_1 = |++\rangle_{0,1,2} (+++) \otimes |00\rangle_{3,4};
\]

\[
A_2 = |+\rangle_{0,1} (+r) \otimes (|0000\rangle + |1111\rangle)_{3,4};
\]

\[
A_3 = (|00\rangle + |01\rangle)_{0,1,2}(|00\rangle + |11\rangle)_{3,4};
\]

\[
p := |0\rangle^\otimes n;
\]

while \( M[p] = 1 \) do

\[
p := |0\rangle^\otimes n; \quad q := |0\rangle^\otimes n;
\]

assert\( (p, q); A_0\);

\[
p := H^\otimes n[p];
\]

assert\( (p, q); A_1\);

\[
p, q := U_f[p, q];
\]

assert\( (p, q); A_2\);

\[
p := \text{QFT}^{-1}[p];
\]

assert\( (p, q); A_3\);

od

![Figure 1: Shor's algorithm program with assertions](image)

We detail the implementation of the assertion circuit blocks on the upper half of Figure 2. For each assertion, we list its projection, the additional unitary transformations, with the complete implementation circuit diagram. For \( A_1, A_2, \) and \( A_3 \), since the qubits not fully entangled, we only assert part of the qubits without affecting the results. The unitary transformations are decomposed into the combinations of CNOT gates and single-qubit gates by hand.

#### 6.1.3 Assertion comparison

Similar to Section 5, we first compare the coverage of assertions derived for this realistic algorithm, and then detail the implementation cost in terms of the number of additional gates, measurements, and auxiliary qubits.

**Assertion Support** All four assertions are supported in Stat and Poq. For QECA, \( A_0, A_1, \) and \( A_2 \) are covered but \( A_3 \) is not yet supported even if it is an entanglement state. Because the assertion from QECA for the two-qubit entanglement state cannot be directly extended to cases with more qubits.

**Implementation Cost** We compare the circuit cost when implementing the assertions between Poq and QECA. Stat is not included because it only requires some additional measurements and we have already shown the inefficiency of Stat with respect to the numbers of executions in Section 5.

Table 2 shows the implementation cost of the three assertions supported by both Poq and QECA. In particular, we compare the number of H gates, CNOT gates, measurements, and auxiliary qubits. It can be observed that Poq use no CNOT gates and auxiliary qubits for the three considered assertions, while QECA always needs to use additional CNOT gates and auxiliary qubits. This reason is that QECA always measure auxiliary qubits to indirectly probe the qubit information. So that additional CNOT gates are always required to couple the auxiliary qubits with existing qubits.
This design significantly increases the implementation cost when comparing with Poq.

To summarize, we demonstrate the complete assertion-injected circuit for a quantum program of Shor’s algorithm and the implementation details of the assertions. We compare the implementation cost between Poq and QECA to show that Poq has lower cost even for the limited assertions that are supported by both assertion schemes.

### 6.2 HHL algorithm

In the first example of Shor’s algorithm, we focus the assertion implementation on a concrete circuit example and compare against other assertions due to the simplicity of the derived assertions. In the next HHL algorithm example, we will have non-trivial assertions that are not supported in the baselines and demonstrate how to implement the projection with the techniques introduced in Section 3 and 4.1.

The HHL algorithm was proposed for solving linear systems of equations [15]. Given a matrix $A$ and a vector $\vec{b}$, the algorithm produces a quantum state $|x\rangle$ which is corresponding to the solution $\vec{x}$ such that $A\vec{x} = \vec{b}$. It is well-known that the algorithm offers up to an exponential speedup over the fastest classical algorithm if $A$ is sparse and has a low condition number $\kappa$.

#### 6.2.1 HHL program. The HHL algorithm has been formulated to the quantum while-language and formally statically verified in the sense of both partial and total correctness in [45]. We adopt the assumptions and symbols there. Briefly speaking, $A$ is a Hermitian and full-rank matrix with dimension $N = 2^m$, which has the diagonal decomposition $A = \sum_{j=1}^{N} \lambda_j |u_j\rangle \langle u_j|$ with corresponding eigenvalues $\lambda_j$ and eigenvectors $|u_j\rangle$. We assume for all $j$, $\delta_j = \frac{\lambda_j}{2\pi} \in \mathbb{N}^+$ and set $T = 2^m = \lceil \max_j \delta_j \rceil$, where $t_0$ is a time parameter to perform unitary transformation $U_f$. Moreover, the input vector $\vec{b}$ is presumed to be unit and corresponding to state $|b\rangle$ with the linear combination $|b\rangle = \sum_{j=1}^{N} \beta_j |u_j\rangle$. It is straightforward

| # of | $A_0$ | $A_1$ | $A_3$ |
|------|------|------|------|
| H    | 0    | 0    | 6    |
| CNOT | 0    | 5    | 0    |
| Measure | 5    | 5    | 3    |
| Aux. Qbit | 0    | 1    | 0    | 1    |
\( p := |0\>^r; \; q := |0\>^m; \; r := |0\>; \)
while \( M[r] = 1 \) do
\[\begin{align*}
  \text{assert}(p, r; P); \\
  q := |0\>^m; \; q := U_b[q]; \; p := H^m[p]; \\
  p, q := U_f[p, q]; \; p := \text{QFT}\{p\}; \\
  \text{assert}(p; S); \\
  p, r := U_s[p, r]; \; p := \text{QFT}[p]; \\
  p, q := U_f[p, q]; \; p := H^m[p]; \\
  \text{assert}(p, q, r; R); \\
  \text{od}
\]
\text{assert}(q; Q);

Figure 3: HHL algorithm program with assertions

to find the solution state \(|x\> = c \sum_{j=1}^N \frac{\beta_j}{\sqrt{\delta_j}} |u_j\>\) where \( c \) is for normalization.

The HHL program has three registers \( p, q, r \) which are \( n, m, 1 \)-qubit systems and used as the control system, state system and indicator of while loop, respectively. For details of unitary transformations \( U_b, U_f \) and QFT and measurement \( M \), please refer to Appendix D or \([15, 43]\).

6.2.2 Debugging scheme for HHL program. According to the proof outline for HHL program in \([43]\) (also in Appendix D), we introduce the debugging scheme shown in Figure 3. The projections \( R, P, Q, S \) are defined as follows:

\[\begin{align*}
  P &= |0\>_p |0\>_r \otimes |0\>_q; \quad Q = |x\>_q |x\>; \\
  R &= |0\>_p |0\>_r \otimes (|x\>_q |x\> \otimes |1\>_q + I_q \otimes |0\>_r, |0\>); \\
  S &= \text{supp} \left( \sum_{j=1}^N |\delta_j\>_p |\delta_j\>_r \right)
\]

Projection \( R \) is the same as in \([43]\) while \( P \) is focused on register \( p, r \) and \( Q \) is focused on the output register \( q \). These projections can be implemented using the techniques introduced in Section 3; more precisely:

1. Implementation of \text{assert}(p, r; P):
   - measure register \( p \) and check if the outcomes are all "0";
2. Implementation of \text{assert}(q; Q):
   - apply \( U_x \) on \( q \);
   - measure register \( q \) and check if the outcome is "0";
   - apply \( U_x^\dagger \) on \( q \);
3. Implementation of \text{assert}(p, q, r; R):
   - measure register \( p \) directly to see if the outcome is "0";
   - introduce an auxiliary qubit \( a \), initialize it to \( |0\> \);
   - apply \( U_x \) on \( q \) and \( U_b \) on \( r, q, a \);

measure register \( a \) and check if the outcome is "0";
 apply \( U_x^\dagger \) on \( r, q, a \) and \( U_x^\dagger \) on \( q \);

where \( U_x \) is defined by \( U_x|x\> = |0\> \) and \( U_R \) is defined by
\( U_R|1\>_r \otimes (|1\>_q |0\>_k) \otimes |0\>_r(0) \), which is a highly entangled projection over register \( p \) and \( q \). We discussed in Section 4.1, in order to avoid the hardness of implementing \( S' \), we introduce \( S = \text{supp}(\text{tr}_{q_r} S') \) which is actually the reduced projection of \( S' \) over \( p \). Though \text{assert}(p; S) is strictly weaker than original \text{assert}(p, q, r; S'), it can be efficiently implemented and partially test the state.

6.2.3 Numerical simulation results. For illustration, we choose \( m = n = 2 \) as an example. Then the matrix \( A \) is \( 4 \times 4 \) matrix and \( b \) is \( 4 \times 1 \) vector. We first randomly generate four orthonormal vectors for \(|u_j\>\) and then select \( \delta_j \) to be either 1 or 0. Such configuration will demonstrate the applicability of all four derived assertions. Finally, \( A \) and \( b \) are generated as follows.

\[A = \begin{bmatrix}
  1.951 & -0.863 & 0.332 & -0.377 \\
  -0.863 & 2.239 & -0.011 & -0.444 \\
  0.332 & -0.011 & 1.301 & -0.634 \\
  -0.377 & -0.444 & -0.634 & 2.509
\end{bmatrix}, \quad b = \begin{bmatrix}
  -0.486 \\
  -0.345 \\
  -0.494 \\
  -0.633
\end{bmatrix}\]

Assertion Support We have four assertions, labeled \( P, Q, R, \) and \( S \) for the HHL program. Only \( P \) is for a classical state and supported by the baselines and Poq. \( Q, R, \) and \( S \) are more complex and not supported in the baselines.

Figure 4 shows the amplitude distribution of the states during the execution of the four assertions and each block corresponds to one assertion. Since our experiments are performed in simulation, we can directly obtain the state vector \(|\psi\>\). The X-axis represents that basis states of which the amplitudes are not zero. The Y-axis is the probability of the measurement outcome, This probability can be calculated by \(|\langle \psi | x \rangle|^2\), where \(|x\>\) is the corresponding basis state.

Assertion \( P \) is at the beginning of the loop body \( D \). The predicate is \( P = |000\> \otimes |000\> \), which has a simple classical form but requires non-trivial efforts to find that the quantum register \( p \) is always in state \(|0\> \) at the beginning of the loop body. This fact could be found with Poq but it is hard to derive such assertions in Stat and QECA. Figure 4 shows that when the program enter the loop \( D \) at the first and second time, the assertion is satisfied and the quantum registers \( r \) and \( q \) are 0.

Assertion \( Q \) is at the end of the program. Figure 4 shows that there are non-zero amplitudes at 4 possible measurement
Before and after the assertion

Assertion Q
Before unitary transformation

Assertion P
1st time enter the loop
2nd time enter the loop

Assertion R
Before unitary transformation
After unitary transformation

Assertion S
Before and after the assertion

Figure 4: Numerical simulation results for the states around the assertions in HHL algorithm

outcomes at the assertion location. But after the applied unitary transformation, the only possible outcome is 10000. Such an assertion is hard for Stat and QECA to describe but it is easy to define this assertion using projection in Poq.

Assertion R is at the end of the loop body D. Figure 4 confirms that the basis states with non-zero amplitudes are in the subspace defined by the projection in assertion R. Its projection implementation involves the techniques of combining assertions and using auxiliary qubits. Assertions with such complex predicates cannot be defined in Stat and QECA while Poq can decompose and implement it.

Assertion S is in the middle of the loop body D. At this place the state is highly entangled as mentioned above and directly implementing this projection will be expensive. We employ the local projection technique in Section 4.1. Since δ,s are selected to be either 1 or 3, the projection S becomes |01⟩ₚ⟨01| + |11⟩ₚ⟨11|. This simple form of local projection that can be easily implemented. Figure 4 confirms that the tested highly entangled state is not affected in this local projective measurement.

To summarize, we derive four assertions for the program of HHL algorithm with Poq. Among them, only P can be defined in Stat and QECA but it is hard to realize the predicate in this assertion without the help of quantum logic. The rest three assertions, which cannot be defined in Stat or QECA, demonstrate that Poq can help assert and debug realistic quantum algorithms on a quantum computer.

7 DISCUSSION

Program debugging has been an active research topic for a long time because it reflects the practical application requirements for reliable software. Compared with its counterpart in classical computing, quantum program debugging is still at a very early stage. Basic debugging approaches, such as assertions [11], static code analysis [6], and design by contract [24], which have been invented for classical program debugging in the last few decades, are not yet available or well-developed for quantum programs. This paper made efforts towards practical quantum program debugging through studying how to design and implement effective and efficient
quantum program assertions. Specifically, we select projections as predicates and use aQHL [43] to derive assertions. Several techniques are proposed to implement the projection under machine constraints. To the best of our knowledge, this is the first runtime assertion scheme for quantum program debugging with such flexible assertions and low testing overhead. The proposed assertion technique would benefit future quantum program development, testing, and verification.

Although we have demonstrated the feasibility and advantages of the proposed assertion scheme, there are several future research directions that can be explored as with any initial research.

**Projection Implementation Optimization** We have shown that our assertion-based debugging scheme can be implemented with several techniques in Section 3 and demonstrated concrete examples in Section 6. However, further optimization of the projection implementation is not yet well studied. One assertion can be split into several sub-assertions but different sub-assertion selections would have different implementation overhead. We showed that one auxiliary qubit is enough but employing more auxiliary qubits may yield fewer sub-assertions. For the circuit implementation of an assertion, the decomposition of the assertion-introduced unitary transformations can be optimized for several possible objectives, e.g., gate count, circuit depth. A systematic approach to generate optimized assertion implementations is thus important for more efficient assertion-based quantum program debugging in the future.

**More Efficient Checking** Assertions derived from Poq for a complicated highly entangled state may require significant effort for its precise implementation. However, the goal of assertions is to check if a tested state satisfies the predicates rather than to prove the correctness of a program. It is possible to trade-in checking accuracy for simplified assertion implementation by relaxing the constraints in the predicates. Local projection can be a solution to approximate a complex projective measurement as we discussed in Section 4.1 and demonstrated in one of the assertions for the HHL algorithm in Section 6. However, the degree of predicate relaxation and its effect on the robustness of the assertions in realistic erroneous program debugging need to be studied. Other possible directions, like non-demolition measurement [8], are also worth exploring.

8 RELATED WORK

Recently, two types of assertions have been proposed for debugging on quantum computers. Huang and Martonosi proposed quantum program assertions based on statistical tests on classical observations [17]. For each assertion, the program executes from the beginning to the place of the injected assertion followed by measurements. This process is repeated many times to extract the statistical information about the state. The advantage of this work is that, for the first time, assertion is used to reveal bugs in realistic quantum programs and help discover several bug patterns. But in this debugging scheme, each time only one assertion can be tested due to the destructive measurements. Therefore, the statistical assertion scheme is very time consuming. Poq circumvents this issue by choosing to use projective assertions.

Zhou and Byrd further improved the assertion scheme by proposing dynamic assertion circuits inspired by quantum error correction [42]. They introduce ancilla qubits and indirectly collect the information of the qubits of interest. The success rate can also be improved since some unexpected states can be detected and corrected in the noisy scenarios. However, their approach always relies on ancilla qubits, which will increase the implementation overhead as discussed in Section 6.1.

Moreover, both of these assertion schemes can only inspect very few types of states that can be considered as some 1-dimensional special cases of our proposed projection based assertions, leading to limited applicability.

Poq presents one more improvement over the previous work. The debugging schemes discussed above do not cooperate with a logic system and fail to derive the assertions automatically. But our scheme is based on a program logic, called aQHL (applied Quantum Hoare logic) [43]. Although it is a simplified version of quantum Hoare logic defined in [40], aQHL is (relative) complete for projective assertions, which makes out our debugging scheme more powerful comparing with existing assertion schemes [17, 42].

9 CONCLUSION

The demand for bug-free quantum programs calls for efficient and effective debugging scheme on quantum computers. This paper enables assertion-based quantum program debugging by proposing Poq, a projection-based runtime assertion scheme. In Poq, predicates in the `assert` primitives are projective operators, which significantly increase the expressive power compared with existing quantum assertion scheme. Cooperating with aQHL, in which the preconditions and postconditions are also projections, we can derive assertions at arbitrary place of a quantum program. Several techniques are introduced to rotate the predicates to the computational basis, on which a realistic quantum computer usually supports its measurements, so that the measurements in our assertions do not destroy the state when the assertion is satisfied. Therefore, multiple assertions can be tested in one execution. The superiority of Poq is demonstrated by its applications to derive assertions for two well-known sophisticated quantum algorithms.
REFERENCES

[1] Ali Javadi Abhari, Arvin Faruque, Mohammad Javad Dousti, Lukas Svec, Oana Catu, Amlan Chakrabati, Chen-Fu Chiang, Seth Vanderwilt, John Black, Fred Chong, Margaret Martonosi, Martin Suchara, Ken Brown, Massoud Pedram, and Todd Brun. 2012. scaffold: Quantum programming language. Technical report, Technical Report TR-934-12. Princeton University.

[2] Héctor Abraham, Ismail Yunus Akhalwaya, Gadi Aleksandrowicz, Thomas Alexander, Gadi Aleksandrowicz, Eli Arbel, Abraham Asfaw, Carlos Azaustre, Panagiotis Barkoutsos, George Barron, Luciano Bello, Yael Ben-Haim, Daniel Bevenius, Lev S. Berezin, Samuel Bosch, David Bucher, CZ. Fran Cabrera, Padraic Calpin, Lauren Capelluto, Jorge Carbulo, Ginés Carrascal, Adrian Chen, Chun-Fu Chen, Richard Chen, Jerry M. Chow, Christian Claus, Christian Clauss, Abigail J. Cross, Andrew W. Cross, Juan Cruz-Benito, Cryoris, Chris Culver, Antonio D. Córcoles-Gonzales, Sean Dague, Matthieu Dartiailh, Abdón Rodríguez Davila, Delton Ding, Eugene Dumitrescu, Karel Dumon, Ivan Duran, Pieter Eendebak, Daniel Egger, Mark Everitt, Paco Martín Fernández, Albert Frisch, Andreas Furher, IAN GOULD, Gadi, Borja Godoy Gago, Jay M. Gambetta, Luis García, Shelly Garion, Gaylor-Kus, Juan Gomez-Mosquera, Salvador de la Puente González, Donny Greenberg, John A. Gunning, Isabel Haide, Ikko Hamamura, Vojtech Havlicek, Joe Hellmers, Lukasz Herok, Hiroshi Hirai, Connor Howington, Haochen Hu, Wei Hu, Haruki Imai, Takashi Immachi, Rabin Iten, Toshinori Ito, Ali Javadi-Abhari, Jessica, Konnor Johns, Naoki Kanazawa, Anton Karazeev, Paul Kassebaum, Arvin Faruque, Mohammad Javad Dousti, Lukas Svec, Oana Catu, Amlan Chakrabati, Seth Vanderwilt, John Black, Fred Chong, Margaret Martonosi, Martin Suchara, Ken Brown, Massoud Pedram, and Todd Brun. 2012. scaffold: Quantum programming language. Technical report, Technical Report TR-934-12. Princeton University.

[3] Al Bessey, Ken Block, Ben Chelf, Andy Chou, Bryan Fulton, Seth Hallem, Charles Henri-Gros, Asya Kamsky, Scott McPeak, and Dawson Engler. A few billion lines of code later: using static analysis to find bugs in the real world. Communications of the ACM, 53(2):66–73, 2010.

[4] Oliver Brunet and Philippe Jorrand. Dynamic quantum logic for quantum programs. International Journal of Quantum Information, 2(01):45–54, 2004.

[5] Jiaxin Chen, Zhengfeng Ji, Bei Zeng, and D. L. Zhou. From ground states to local Hamiltonians. Phys. Rev. A, 86:022339, Aug 2012.

[6] Google. Announcing Cirq: An Open Source Framework for NISQ Algorithms. https://ai.googleblog.com/2018/07/announcing-cirq-open-source-framework.html, 2018.

[7] Geoffrey W. Adenilton Silva, Yukio Siraichi, Seyon Sivarajah, John A. Smolin, Matthew Treinish, Trisha Pe, Yael Ben-Haim, Daniel Bevenius, Lev S. Bishop, Samuel Bosch, David Jerry M. Chow, Christian Claus, Christian Clauss, Abigail J. Cross, Albert Frisch, Andreas Furher, IAN GOULD, Gadi, Borja Godoy Gago, Jay M. Gambetta, Luis Garcia, Shelly Garion, Gaylor-Kus, Juan Gomez-Mosquera, Salvador de la Puente González, Donny Greenberg, John A. Gunning, Isabel Haide, Ikko Hamamura, Vojtech Havlicek, Joe Hellmers, Lukasz Herok, Hiroshi Hirai, Connor Howington, Haochen Hu, Wei Hu, Haruki Imai, Takashi Immachi, Rabin Iten, Toshinori Ito, Ali Javadi-Abhari, Jessica, Konnor Johns, Naoki Kanazawa, Anton Karazeev, Paul Kassebaum, Arvin Faruque, Mohammad Javad Dousti, Lukas Svec, Oana Catu, Amlan Chakrabati, Seth Vanderwilt, John Black, Fred Chong, Margaret Martonosi, Martin Suchara, Ken Brown, Massoud Pedram, and Todd Brun. 2012. scaffold: Quantum programming language. Technical report, Technical Report TR-934-12. Princeton University.

[8] Garth A Clarke and David S Rosenblum. A historical perspective on runtime assertion checking in software development. ACM SIGSOFT Software Engineering Notes, 33(3):25–37, 2006.

[9] Google. Announcing Cirq: An Open Source Framework for NISQ Algorithms. https://ai.googleblog.com/2018/07/announcing-cirq-open-source-framework.html, 2018.

[10] Alexander S Green, Peter LeFanu Lumsdaine, Neil J Ross, Peter Selinger, and Benoît Valiron. Quipper: a scalable quantum programming language. In ACM SIGPLAN Notices, volume 48, pages 333–342. ACM, 2013.

[11] Lov K Grover. A fast quantum mechanical algorithm for database search. In Proceedings of the twenty-eighth annual ACM symposium on Theory of computing, pages 212–219. ACM, 1996.

[12] Aram W Harrow and Avinatan Hassidim, and Seth Lloyd. Quantum algorithm for linear systems of equations. Physical review letters, 103(15):150502, 2009.

[13] Yipeng Huang and Margaret Martonosi. Qdb: From quantum algorithms towards correct quantum programs. In 9th Workshop on Evaluation and Usability of Programming Languages and Tools (PLATEAU 2018). Schloss Dagstuhl-Leibniz-Zentrum fuer Informatik, 2019.

[14] Yipeng Huang and Margaret Martonosi. Statistical assertions for validating patterns and finding bugs in quantum programs. In Proceedings of the 46th International Symposium on Computer Architecture, pages 541–553. ACM, 2019.

[15] Shih-Han Hung, Kesha Hietala, Shaoqeng Zhu, Mingsheng Ying, Michael Hicks, and Xiaodi Wu. Quantitative robustness analysis of quantum programs. Proceedings of the ACM on Programming Languages, 3(POPL):31, 2019.

[16] IBM. Gate and operation specification for quantum circuits. https://github.com/Qiskit/openqasm, 2019.

[17] Ali JavadiAbhari, Shrutii Patil, Daniel Kudrow, Jeff Heckey, Alexey Lvov, Frederic T Chong, and Margaret Martonosi. Scaffcc: Scalable compilation and analysis of quantum programs. Parallel Computing, 45:2–17, 2015.

[18] Yangja Li and Mingsheng Ying. Debugging quantum processes using runtime assertion checking in software development. ACM SIGSOFT Software Engineering Notes, 33(3):25–37, 2006.

[19] Panos Aliferis, Daniel Gottesman, and John Preskill. Quantum accuracy threshold for concatenated distance-3 codes. Quantum Info. Comput., 6(2):97–165, March 2006.

[20] Adriano Barenco, Charles H Bennett, Richard Cleve, David P DiVincenzo, Norman Margolus, Peter Shor, Tycho Sleator, John A Smolin, and Harald Weinfurter. Elementary gates for quantum computation. Physical review A, 52(5):3457, 1995.

[21] Gilles Barthe, Justin Hsu, Mingsheng Ying, Nengkun Yu, and Li Zhou. Coupling techniques for reasoning about quantum programs. arXiv preprint arXiv:1901.05184, 2019.

[22] Google. Announcing Cirq: An Open Source Framework for NISQ Algorithms. https://ai.googleblog.com/2018/07/announcing-cirq-open-source-framework.html, 2018.

[23] Norbert M Linke, Dmitri Maslov, Martin Roetteler, Shantanu Debnath, Bertrand Meyer. Applying’design by contract’. Journal of Object Technology, 25(10):40–51, 1999.
[25] Michael A Nielsen and Isaac L Chuang. Quantum computation and quantum information. Quantum Computation and Quantum Information, by Michael A. Nielsen, Isaac L. Chuang, Cambridge, UK: Cambridge University Press, 2010, 2010.

[26] Jennifer Paykin, Robert Rand, and Steve Zdancewic. Qwire: A core language for quantum circuits. In Proceedings of the 44th ACM SIGPLAN Symposium on Principles of Programming Languages, POPL 2017, pages 846–858, New York, NY, USA, 2017. ACM.

[27] Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J Love, Alán Aspuru-Guzik, and Jeremy L O’Brien. A variational eigenvalue solver on a photonic quantum processor. Nature communications, 5:4213, 2014.

[28] Rigetti. A Python library for quantum programming using Quil. https://github.com/rigetti/pyquil, 2019.

[29] Rigetti Forest team. Forest SDK. https://www.rigetti.com/forest, 2019.

[30] Neil J. Ross and Peter Selinger. Optimal ancilla-free clifford+t approximation of z-rotations. Quantum Info. Comput., 16(11-12):901–953, September 2016.

[31] Peter W Shor. Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer. SIAM review, 41(2):303–332, 1999.

[32] Dominique Unruh. Quantum relational hoare logic. Proceedings of the ACM on Programming Languages, 3(POPL):33, 2019.

[33] Lieven MK Vandersypen, Matthias Steffen, Gregory Breyta, Costantino S Yannoni, Mark H Sherwood, and Isaac L Chuang. Experimental realization of shor’s quantum factoring algorithm using nuclear magnetic resonance. Nature, 414(6866):883, 2001.

[34] A. Winter. Coding theorem and strong converse for quantum channels. IEEE Transactions on Information Theory, 45(7):2481–2485, Nov 1999.

[35] William K Wootters and Wojciech H Zurek. A single quantum cannot be cloned. Nature, 299(5886):802, 1982.

[36] Tao Xin, Dawei Lu, Joel Klassen, Nengkun Yu, Zhengfeng Ji, Jianxin Chen, Xian Ma, Guifu Long, Bei Zeng, and Raymond Laflamme. Quantum state tomography via reduced density matrices. Phys. Rev. Lett., 118:020401, Jan 2017.

[37] Nengkun Yu. Quantum temporal logic, 2019.

[38] MS Ying, RY Duan, Yuan Feng, and ZF Ji. Predicate transformer semantics of quantum programs. ACM Transactions on Programming Languages and Systems (TOPLAS), 33(6):19, 2011.

[39] Mingsheng Ying. Foundations of Quantum Programming. Morgan Kaufmann, 2016.

[40] Mingsheng Ying. Floyd–hoare logic for quantum programs. ACM Transactions on Programming Languages and Systems (TOPLAS), 33(6):19, 2011.

[41] Nengkun Yu. Quantum temporal logic, 2019.

[42] H. Zhou and G. T. Byrd. Quantum circuits for dynamic runtime assertions in quantum computation. IEEE Computer Architecture Letters, 18(2):111–114, July 2019.

[43] Li Zhou, Nengkun Yu, and Mingsheng Ying. An applied quantum hoare logic. In Proceedings of the 40th ACM SIGPLAN Conference on Programming Language Design and Implementation, pages 1149–1162. ACM, 2019.
A DEFINITION OF THE UNITARY TRANSFORMATIONS USED IN THIS PAPER

Single-qubit gate:

\[ H (\text{Hadamard}) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \]

Two-qubit gate CNOT(Controlled-NOT, Controlled-X):

\[ \text{CNOT} = |0\rangle\langle 0| \otimes I_2 + |1\rangle\langle 1| \otimes X = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \]

Swap = \[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

Three-qubit gate Toffoli:

\[ \text{Toffoli} = |0\rangle\langle 0| \otimes I_4 + |1\rangle\langle 1| \otimes \text{CNOT} \]

\[ = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \]

Three-qubit gate Fredkin (Controlled-Swap, CSwap):

\[ \text{Fredkin} = |0\rangle\langle 0| \otimes I_4 + |1\rangle\langle 1| \otimes \text{Swap} \]

\[ = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \]

B PROOF OF THE THEOREMS, PROPOSITIONS, AND LEMMAS

B.1 Proof of Theorem 3.1

**Theorem:** Suppose we execute \( S' \) for \( k \) times with input state \( \rho \) that satisfies \( P_0 \), and collect all the error messages.

1. (Posterior) If an error message occurs in \( \text{assert}(\overline{q}_m, P_m) \) with \( m \neq 0 \), we conclude that subprogram \( S_m \) is not correct according to Hoare triple \( \{P_{m-1}\}S_m\{P_m\} \).
2. (Posterior) If no error message is reported, we claim that program \( S \) is close to the bug-free standard program; more precisely, for the input \( \rho \),

\[
\min_{\text{Std}} D([S] (\rho), [S_{\text{std}}] (\rho)) \lesssim \frac{n}{\sqrt{k}}
\]

where the minimum is taken over all bug-free standard program \( S_{\text{std}} \) that satisfies \( \{P_0\}S_{\text{std}}\{P_n\} \).

Moreover, any error detection does not significantly affect a later detection; that is, even if \( S_m \) is wrong, the error detection \( S'_m \) will still be efficient for all \( m > m' \).

**Proof.** The proof has three parts.

- **Error message occurred in \( \text{assert}(\overline{q}_m, P_m) \).**

  Obviously, no error message occurred in \( \text{assert}(\overline{q}_{m-1}, P_{m-1}) \), which ensures that the current state \( \rho \) after the assertion \( \text{assert}(\overline{q}_m, P_m) \) indeed satisfies \( \rho = P_{m-1} \).

  After executing the subprogram \( S_m \), the state becomes \([S_m](\rho)\). The error message occurred in \( \text{assert}(\overline{q}_m, P_m) \) indicates that \([S_m](\rho) \not\equiv P_m \), which implies the violation of Hoare triple \( \{P_{m-1}\}S_m\{P_m\} \).

- **No error message is reported.**

  We assume that for the original program \( S \) with the first assertion \( \text{assert}(\overline{q}_0, P_0) \), the state before and after \( S_m \) is \( \rho_{m-1} \) and \( \rho_m \) for \( 1 \leq m \leq n \); and for the debugging scheme \( S' \), the state after \( \text{assert}(\overline{q}_m, P_m) \) is \( \rho'_m \) for \( 0 \leq m \leq n \). We first show by induction that \( D(\rho_{m'}, \rho'_m) \lesssim \frac{m}{\sqrt{k}} \) with high probability when \( k \) is large.

  For the basis, it is trivial \( \rho_0 = \rho'_0 \).

  If \( D(\rho_{m-1}, \rho'_{m-1}) \lesssim \frac{m-1}{\sqrt{k}} \) with high probability, then after execution of \( S_m \) and \( \text{assert}(\overline{q}_m, P_m) \), we have:

\[
\rho_m = [S_m](\rho_{m-1}), \quad \rho'_m = \frac{P_m[S_m](\rho'_{m-1})P_m}{\text{tr}(P_m[S_m](\rho'_{m-1})P_m)}.
\]

Moreover, as no error message is reported for \( k \)-round execution, it is reasonable that

\[
1 - \text{tr}(P_m[S_m](\rho'_{m-1})P_m) \lesssim \frac{1}{k}.
\]

According to Lemma 4.1, we obtain:

\[
D([S_m](\rho'), \rho'_{m-1}) \lesssim \frac{1}{k} + \sqrt{\frac{k-1}{k^2}} \lesssim \frac{1}{\sqrt{k}}.
\]
Moreover, by the contractiveness of quantum operations [25] and the fact that semantic functions are quantum operations [39], it holds that
\[ D(\|S_m\|, \|S_m\|, \rho_{m-1}, \rho_m) \leq D(\rho_{m-1}, \rho_m). \]
Therefore, we conclude that
\[ D(\rho_m, \rho_m) \leq D(\|S_m\|, \rho_{m-1}, \rho_m) + D(\rho_m, \|S_m\|, \rho_{m-1}) \]
\[ \leq \frac{1}{\sqrt{k}} + \frac{m-1}{\sqrt{k}} = \frac{m}{\sqrt{k}}. \]

Nothing that \( \rho_m \models P_m \), we have \( \rho_m \models \phi \) with \( \phi = \frac{m}{\sqrt{k}} \); in other words, for the input \( \rho \) satisfying \( P_0, D(\|S\|, \rho) \), we hold that \[ S_{\text{std}} \] is the bug-free standard program of \( S \).
• Even if some \( S_m \) is not correct, if the execution of \( S' \) does not terminate at \( \text{assert}(\overline{q}_m; P_m) \), then the state after \( \text{assert}(\overline{q}_m; P_m) \) is changed and satisfies \( P_m \), which is actually the correct input for testing the next Haole triple \( \{P_m\} \subset S_{\text{std}} \). Therefore, the rest of the execution is still good enough for debugging other errors. \( \square \)

### B.2 Proof of Proposition 3.1

**Proposition:** For projection \( P \) with rank \( P = 2^m \), there exists unitary transformation \( U_P \) such that
\[ U_P P U_P^\dagger = Q_{\lambda_1} \otimes Q_{\lambda_2} \otimes \cdots \otimes Q_{\lambda_n} = \bigotimes_{i=1}^n Q_{\lambda_i} \triangleq Q_P, \]
where \( Q_{\lambda_i} \) is either \( |0\rangle_{\lambda_i}, |1\rangle_{\lambda_i} \), or \( I_{\lambda_i} \) for each \( 1 \leq i \leq n \).

**Proof.** \( U_P \) and \( Q_P \) can be obtained immediately after we diagonalize the projection \( P \). \( \square \)

### B.3 Proof of Proposition 3.2

**Proposition:** For projection \( P \) with rank \( P \leq 2^{n-1} \), there exist projections \( P_1, P_2, \cdots, P_l \) satisfying rank \( P_i = 2^n \) for all \( 1 \leq i \leq l \), such that \( P = P_1 \cap P_2 \cap \cdots \cap P_l \). Theoretically, \( l = 2 \) is sufficient.

**Proof.** After we diagonalize the projection \( P \) with the form \( U \Lambda U^\dagger \), where the diagonal matrix
\[ \Lambda = \text{diag}(1, \cdots, 1, 0, \cdots, 0). \]

Choose following two diagonal matrix
\[ \Lambda_1 = \text{diag}(1, \cdots, 1, 0, \cdots, 0), \]
\[ \Lambda_2 = \text{diag}(1, \cdots, 1, 0, \cdots, 0, 1, \cdots, 1, 0, \cdots, 0), \]
which satisfy \( \Lambda_1 \cap \Lambda_2 = \Lambda \) and rank \( \Lambda_1 = \text{rank} \Lambda_2 = 2^{n-1} \). Therefore, we set \( P_1 = U \Lambda_1 U^\dagger \) and \( P_2 = U \Lambda_2 U^\dagger \) as desired. \( \square \)

### B.4 Proof of Lemma 4.1

**Lemma:** For projection \( P \) and density operator \( \rho \), if \( \text{tr}(\rho P \rho P) \geq 1 - \epsilon \), then
\[ D(\rho, \frac{P \rho P}{\text{tr}(P \rho P)}) \leq \epsilon + \sqrt{\epsilon(1-\epsilon)}. \]

**Proof.** For pure state \( |\psi\rangle \), we have:
\[ \text{tr} |P\rangle \langle \psi| P \langle P| = \text{tr} \sqrt{P \rho P} \langle \psi| P \rho P \langle P| \]
\[ = \sqrt{\langle \psi| P \rho P \langle P|} \sqrt{\langle \psi| P \rho P \langle P|}. \]
Therefore, for any density operators \( \rho \) with spectral decomposition \( \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \), we have:
\[ \text{tr} P \rho P \]
\[ = \text{tr} \left| \sum_i p_i |\psi_i\rangle \langle \psi_i| \right| \left| P \rho P \right| \]
\[ \leq \sum_i p_i \text{tr} |P\rangle \langle \psi_i| P \langle \psi_i| P \]
\[ = \sum_i \sqrt{\text{tr} \langle P| \psi_i \rangle \langle \psi_i| P \rangle} \sqrt{\text{tr} |P\rangle \langle \psi_i| P \langle \psi_i| P \rangle} \]
\[ = \sqrt{\text{tr} \langle P| \psi \rangle \langle \psi| P \rangle} \text{tr} (P \rho P) \]
using the Cauchy-Schwarz inequality. Now, it is straightforward to have:
\[ D(\rho, \frac{P \rho P}{\text{tr}(P \rho P)}) \]
\[ = \frac{1}{2} \text{tr} |P \rho P + P^\perp \rho P + P \rho P^\perp + P^\perp \rho P^\perp - P \rho P| \]
\[ \leq \frac{1}{2} \text{tr} |P \rho P| \left| 1 - \frac{\text{tr}(P \rho P)}{2} \right| \]
\[ + \frac{1}{2} \left| P \rho P^\perp \right| \]
\[ \leq \frac{1}{2} \left( 1 - \text{tr}(P \rho P) \right) + \frac{1}{2} \text{tr}(I - P) \rho \]
\[ \leq \frac{\epsilon}{2} + \sqrt{\text{tr}(\rho)} \text{tr}(P \rho P) + \frac{\epsilon}{2} \]
\[ \leq \epsilon + \sqrt{\epsilon(1-\epsilon)}. \]

The restriction of \( P \) makes it a slightly stronger than the original one in [35]. \( \square \)

### B.5 Proof of Theorem 4.1

**Theorem:** Assume that all \( \epsilon_i \) are small. Execute \( S' \) for \( k \) times, and we count \( k_m \) for the occurrence of error message for assertion \( \text{assert}(\overline{q}_m; P_m). \)
(1) If \( \frac{k_m}{k - \sum_{i=0}^{m-1} k_i} \) is significantly larger than \( \epsilon_m \), we conclude that \( S_m \) is not valid for \( \{(P_{m-1}, \epsilon_{m-1})\}S_m\{(P_m, \epsilon_m)\} \) with high confidence.

(2) If all \( \frac{k_m}{k - \sum_{i=0}^{m-1} k_i} \) are close to or smaller than \( \epsilon_m \) for all \( m \geq 1 \), we can conclude that \( \{(P_0, 0)S\{(P_n, \delta)\}\} \) is valid with high probability, where \( \delta = \sum_{i=1}^{n} (\epsilon_i + \sqrt{\epsilon_i(1-\epsilon_i)}) \approx \sum_{i=1}^{n} \sqrt{\epsilon_i} \) is explained as the accumulated error of applying assertions.

**Proof.** The proof is similar to Appendix B.1.

- If \( \frac{k_m}{k - \sum_{i=0}^{m-1} k_i} \) is significantly larger than \( \epsilon_m \). This implies for some \( \rho \models P_{m-1} \), after executing \( S_m \), we have

\[
1 - \text{tr}(P_m[S_m](\rho)) \approx \frac{k_m}{k - \sum_{i=0}^{m-1} k_i}.
\]

On the other hand, if \( \{(P_{m-1}, \epsilon_{m-1})\}S_m\{(P_m, \epsilon_m)\} \) is valid, then

\[
1 - \text{tr}(P_m[S_m](\rho)) \leq \epsilon_m,
\]

which is a contradiction.

- If all \( \frac{k_m}{k - \sum_{i=0}^{m-1} k_i} \) are close to or smaller than \( \epsilon_m \) for all \( m \geq 1 \). Again, for the original program \( S \) with the first assertion \( \text{assert}(\overline{q}_0; P_0) \), we denote the state before and after \( S_m \) by \( \rho_{m-1} \) and \( \rho_m \) for \( 1 \leq m \leq n \); and for the debugging scheme \( S' \), the state after \( \text{assert}(\overline{q}_m; P_m) \) is denoted by \( \rho'_m \) for \( 0 \leq m \leq n \). We first show by induction that

\[
D(\rho_m, \rho'_m) \lesssim \sum_{i=1}^{m} (\epsilon_i + \sqrt{\epsilon_i(1-\epsilon_i)})
\]

with high probability when \( k \) is large.

For the basis, it is trivial \( \rho_0 = \rho'_0 \).

If \( D(\rho_{m-1}, \rho'_{m-1}) \lesssim \sum_{i=1}^{m-1} (\epsilon_i + \sqrt{\epsilon_i(1-\epsilon_i)}) \) with high probability, then after execution of \( S_m \) and \( \text{assert}(\overline{q}_m; P_m) \), we have:

\[
\rho_m = [S_m](\rho_{m-1}), \quad \rho'_m = \frac{P_m[S_m](\rho'_{m-1})P_m}{\text{tr}(P_m[S_m](\rho'_{m-1})P_m)}.
\]

Moreover, as the error message is reported for \( k_m \) times in \((k - \sum_{i=0}^{m-1} k_i)\)-round execution of \( S_m; \text{assert}(\overline{q}_m; P_m) \), it is reasonable that

\[
1 - \text{tr}(P_m[S_m](\rho'_{m-1})P_m) \approx \frac{k_m}{k - \sum_{i=0}^{m-1} k_i} \lesssim \epsilon_m.
\]

According to Lemma 4.1, we obtain:

\[
D([S_m](\rho'_{m-1}), \rho'_m) \lesssim \epsilon_m + \sqrt{\epsilon_m(1-\epsilon_m)}.
\]

Moreover, by the contractiveness of quantum operations [25] and the fact that semantic functions are quantum operations [39], it holds that

\[
D([S_m](\rho'_{m-1}), [S_m](\rho'_{m-1})) \leq D(\rho_{m-1}, \rho'_{m-1}).
\]

Therefore, we conclude that

\[
D(\rho_m, \rho'_m) \leq D([S_m](\rho'_{m-1}), \rho'_m) + D(\rho_m, [S_m](\rho'_{m-1}))
\]

\[
\lesssim \epsilon_m + \sqrt{\epsilon_m(1-\epsilon_m)} + \sum_{i=1}^{m-1} (\epsilon_i + \sqrt{\epsilon_i(1-\epsilon_i)})
\]

\[
= \sum_{i=1}^{m} (\epsilon_i + \sqrt{\epsilon_i(1-\epsilon_i)}).
\]

Observe that

\[
D(\rho_n, \rho'_n) \lesssim \sum_{i=1}^{n} (\epsilon_i + \sqrt{\epsilon_i(1-\epsilon_i)}) \equiv \delta
\]

and \( \rho'_n \models P_n \), thus \( \rho_n \models \delta P_n \), which implies the correctness of robust Hoare triple \( \{(P_0, 0)S\{(P_n, \delta)\}\} \) as we desired. \( \Box \)
C PROOF OUTLINE FOR SHOR'S ALGORITHM QUANTUM SUBROUTINE EXAMPLE

Figure 5 shows the proof outline of the circuit example in Figure 2. The measurement \( M \) is defined as:

\[
M = \{ M_0 = |010\rangle_{0.1.2} |010\rangle + |001\rangle_{0.1.2} |001\rangle + |011\rangle_{0.1.2} |011\rangle, M_1 = I_q|0.1.2\rangle - M_0 \}
\]

Since the loop in Shor’s algorithm initializes all the qubits at the beginning of the loop body, executions of the loop body are uncorrelated. We can treat the loop body like a sequential program without loops. There are only unitary transformations in the loop so we can derive all the predicates with the (Ax.UT) axiom in aQHL [43].

\[
q := |0\rangle^\otimes5;
\]

while \( M[q[0], q[1], q[2]] = 1 \) do

\[
q := |0\rangle^\otimes5;
\]

\[
\{ |00000\rangle_{0.1.2.3.4} (00000) \}
\]

\[
q[0], q[1], q[2] := H^\otimes3[q[0], q[1], q[2]];
\]

\[
\{ |++\rangle_{0.1} (++ \otimes (000) + |111\rangle_{3.4.5} (000) + |111\rangle) \}
\]

\[
q[0], q[1], q[2] := \text{QFT}^{-1}[q[0], q[1], q[2]];
\]

\[
\{ (000) + |001\rangle_{0.1.2} (000) + (001) \}
\]

\[
\otimes (00) + |11\rangle_{3.4.5} (00) + (11) \}
\]

od

Figure 5: Proof outline for the Shor’s algorithm circuit example with \( N = 15 \) and \( a = 11 \). The projections between \{\} are predicates.

D DETAILS AND PROOF OUTLINE FOR HHL ALGORITHM

We give the concrete forms of omitted unitary transformations \( U_b, U_f, \text{QFT} \) and measurement \( M \) here [43]. The measurement \( M = \{ M_0, M_1 \} \) in the loop is a "yes-no" measurement with measurement operators \( M_0 = |1\rangle\langle 1| \) and \( M_1 = |0\rangle\langle 0| \). The unitary operator \( U_b \) is used to generates the input vector \( b \):

\[
U_b |0\rangle^\otimes m = |b\rangle = \sum_{i=1}^N b_i |i\rangle.
\]

\( U_f \) is a controlled unitary operator with control system \( p \) and target system is \( q \); in detail,

\[
U_f = \sum_{r=0}^{T-1} |r\rangle_p \otimes e^{i\pi T r/T}.
\]

\( \text{QFT} \) and \( \text{QFT}^{-1} \) are the quantum Fourier transform and the inverse quantum Fourier transform applied to the control register \( p \); more precisely

\[
\text{QFT} : |k\rangle \mapsto \frac{1}{\sqrt{T}} \sum_{r=0}^{T-1} e^{2\pi i r k/T} |r\rangle, \quad k = 0, 1, \ldots, T - 1,
\]

\[
\text{QFT}^{-1} : |k\rangle \mapsto \frac{1}{\sqrt{T}} \sum_{r=0}^{T-1} e^{-2\pi i r k/T} |r\rangle, \quad k = 0, 1, \ldots, T - 1.
\]

\[
\{ I_p \otimes I_q \otimes I_r \}
\]

\( p := |0\rangle^\otimes n; q := |0\rangle^\otimes m; r := |0\rangle; \)

\[
\{ \text{inv} : |0\rangle_p \otimes (|x\rangle_q \otimes |1\rangle_r \otimes |1\rangle + I_q \otimes |0\rangle_r \otimes |0\rangle) \}
\]

while \( M[r] = 1 \) do

\[
\{ |0\rangle_p \otimes I_q \otimes |0\rangle_r \otimes |0\rangle \}
\]

\[
q := |0\rangle^\otimes m; q := U_b[q]; p := H^\otimes n |p\rangle;
\]

\[
p, q := U_f[p, q]; p := \text{QFT}^{-1}[p];
\]

\[
\{ \sum_{j=1}^N \beta_j \beta_j^* |\delta_j\rangle_p |\delta_j\rangle \otimes |u_j\rangle_q \langle u_j| \otimes |0\rangle_r \langle 0| \}
\]

\[
p, r := U_c[p, r]; p := \text{QFT}[p];
\]

\[
p, q := U_f[p, q]; p := H^\otimes n |p\rangle;
\]

\[
\{ \text{inv} : |0\rangle_p \otimes (|x\rangle_q \otimes |1\rangle_r \otimes |1\rangle + I_q \otimes |0\rangle_r \otimes |0\rangle) \}
\]

od

\[
\{ |0\rangle_p \otimes |x\rangle_q \otimes |1\rangle_r \otimes |1\rangle \}
\]

Figure 6: Proof outline for HHL program [43]. The projections between \{\} are predicates, and inv indicates that the predicate is the loop invariant.
$U_c$ is a controlled unitary with control register $p$ and target register $r$; more specifically, with some proper parameter $C$, $U_c$ is defined as

$$U_c : |0\rangle_p |0\rangle_r \mapsto |0\rangle_p |0\rangle_r$$

$$|i\rangle_p |0\rangle_r \mapsto |i\rangle_p \left( \sqrt{1 - \frac{C^2}{i^2}} |0\rangle_r + \frac{C}{i} |1\rangle_r \right), 1 \leq i \leq T - 1.$$

We summarize the context in [43] as the proof outline shown in Figure 6.