A Logic for Recursive Quantum Programs

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Abstract

Most modern (classical) programming languages support recursion. Recursion has also been successfully applied to the design of several quantum algorithms and introduced in a couple of quantum programming languages. So, it can be expected that recursion will become one of the fundamental paradigms of quantum programming. Several program logics have been developed for verification of non-recursive quantum programs. However, there are as yet no general methods for reasoning about recursive procedures in quantum computing. We fill the gap in this paper by presenting a logic for recursive quantum programs. This logic is an extension of quantum Hoare logic for quantum while-programs. The (relative) completeness of the logic is proved, and its effectiveness is shown by a running example: fixed-point Grover’s search.

1 Introduction

Quantum programming has been extensively investigated for the past two decades, including both imperative and functional languages and their semantics [2, 22, 26, 27, 28], as surveyed in [28, 13, 33]. In the last few years, a number of mature quantum programming languages have been proposed, for example, Quipper [14], Scaffold [1], LIQUi|> [31], Q# [30], and QWIRE [24]. At the same time, various techniques for program analysis and verification have been extended to quantum programs [4, 7, 34, 19].

Quantum Hoare Logic: Hoare logic [16] has been a cornerstone of classical programming theory. The basic idea is based on intermediate assertion method [12] — attach each program point with an assertion and whenever the data flow reaches a program point the attached assertion would be satisfied — called Floyd-Hoare’s Principle. This logic has had a significant impact upon the methods of both designing and verifying programs. It has also been used as a way of specifying program semantics. Several logics for reasoning about quantum programs have been developed by Floyd-Hoare’s Principle [5, 10, 18, 32]; for the landscape of these quantum logics, cf. Rand [25]. Among them, D’Hondt and Panangaden [23] proposed the notion of weakest precondition. The attractiveness of this approach is that both preconditions and postconditions are

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modelled by Hermitian operators and thus have natural interpretation as physical observables. Based on this, a quantum Hoare-like logic was built and, in particular, its (relative) completeness was established, by Ying in [32].

Recursion in Classical Programming: Historically, the mechanism of recursion was first proposed as a basic operator in generating (partial) recursive functions; later on, it was introduced to various classical programming languages; for now, while-programs extended with recursion have formed the core of modern high-level programming languages. Moreover, it induces the problem-solving strategy of “divide and conquer”, which has become one of the most important algorithm design paradigms; for example, recursion has been successfully used in designing sorting algorithms, such as quicksort and mergesort. Verification techniques for recursive programs have also been systematically developed since Hoare’s pioneering work [17] (see for example, Chapters 4 and 5 of [3] and Chapter 6 of [11]).

Recursion in Quantum Computing: A natural question is whether recursion, if applied to quantum algorithm design, brings similar advantages to quantum computation? Actually, this question has been partially answered by a few positive examples. The first one is Grover’s fixed-point search algorithm [15, 35], which, by applying recursion, supplements the original search algorithm with a feature that the moving state converges monotonically to the target state without drifting away. (We adopt this algorithm as a running example throughout the paper.) As another example, Recursive Fourier Sampling [6] requires exponentially fewer queries than the classical one, and has extensive applications in research on quantum complexity theory (cf. the Introduction of [20]).

As such, recursion is promised to be one of the fundamental paradigms of quantum programming. Indeed, recursive procedures were already introduced by Selinger in his quantum programming language QPL [28]. Furthermore, the literature [33] defined an expansion of quantum while-language and its operational and denotational semantics. But there are as yet no general methods for reasoning about recursive quantum programs. Such methods are certainly needed to help guide design and verification of recursive quantum programs.

Contributions of the Paper: The aim of this paper is to develop a logic for reasoning about recursive quantum programs. It is built upon D’Hondt and Panangaden’s quantum weakest preconditions [23] and Ying’s quantum Hoare logic [32]. Generally speaking, this paper extends quantum while-programs defined in [32] with recursive procedures, and presents a (relatively) complete logic for both partial and total correctness of recursive quantum programs. Concretely speaking, four main contributions are highlighted as follows.

• We formulate the underlying model for formalizing quantum program correctness as a typed first-order infinite model. Quantum predicates — Hermitian operators between zero and identity operators — are simply employed in [23, 32] as pre- and post-conditions of quantum programs. We elevate quantum predicates to the syntactical level, by introducing the concept of quantum predicate terms with variables. The introduction of quantum predicate variables lays the foundation of the Substitution Rule, which is crucial in dealing with recursion. We choose the (Schrödinger-Heisenberg) dual of a quantum operation (super-operator)
as a basic construct of quantum predicate terms, for all quantum programs can be interpreted as a quantum operation. This makes sure the strong expressiveness of quantum predicate terms.

- We define syntax and semantics of quantum Hoare’s triple and weakest (liberal) preconditions. By using quantum predicate terms (rather than quantum predicates) as pre- and post-conditions, we further define the partial and total correctness formulas of a quantum program. Such syntactical Hoare’s triples can be interpreted as the semantical counterparts used in \cite{23, 32}. Weakest (liberal) preconditions are ideal candidates for all intermediate assertions in proving program correctness, especially in establishing the completeness of our proof systems. In virtue of quantum predicate terms, we also implement separating syntactical weakest (liberal) preconditions from their semantical counterparts.

- We propose the proof rule for partial correctness of recursive quantum procedures, and show the proof rule is sound and complete w.r.t. partial correctness semantics. Similar to the classical case, the proof rule, here, can be readily established by resorting to Floyd-Hoare’s principle. The approach of proving its soundness is to reduce to the nonrecursive case by approximating every recursive procedure with its finite syntactic unrolling. For the completeness proof, we introduce the notion of the most general partial correctness formula, which, together with the Substitution Rule, produces all desired partial correctness formulas.

- Reasoning about total correctness of recursive quantum programs requires some novel ideas fundamentally differently from those for classical recursive programs. Our fourth and last contribution is to invent proof rules for total correctness of quantum loop statements and recursive quantum procedures, and argue their soundness and completeness w.r.t. total correctness semantics. The proof rules for total correctness can be adapted from those for partial correctness coupled with the constraint of guaranteeing termination upon satisfaction of precondition. The difficulty is how to apply Löwner comparison between quantum predicate terms to resolving issues of termination. Our solution is to introduce an infinite non-decreasing sequence of quantum predicate terms \( \{Q_n\}_{n \geq 0} \) with \( Q_0 = 0 \). Intuitively speaking, if current assertion is \( Q_{n+1} \), then, after one iteration or (re)invocation, the assertion will be strengthened to \( Q_n \), and assertion \( Q_0 \) is used to ensure exiting the loop body or ceasing (re)invocation.

**Organization of the Paper:** We present preliminaries on quantum computation in Section 2; recursive quantum programs are defined in Section 3; quantum program correctness and weakest (liberal) preconditions are defined in Section 4; proof systems for partial and total correctness are shown in Sections 5 and 6, respectively. Section 7 concludes the paper.
2 Preliminaries

2.1 Quantum states

The state space of a quantum system is a Hilbert space $\mathcal{H}$. For any finite integer $n$, an $n$-dimensional Hilbert space is essentially the space $\mathbb{C}^n$ of complex vectors. We use Dirac’s notation, $|\psi\rangle$, to denote a complex vector in $\mathbb{C}^n$. The inner product of two vectors $|\psi\rangle$ and $|\phi\rangle$ is denoted by $\langle\psi|\phi\rangle$, which is the product of the Hermitian conjugate of $|\psi\rangle$, denoted by $\langle\psi|$, and vector $|\phi\rangle$. The norm of a vector $|\psi\rangle$ is denoted by $|\langle\psi|\psi\rangle|$. We define (linear) operators as linear mappings over $\mathcal{H}$. For $\mathbb{C}^n$, operators are represented by $n \times n$ matrices. The Hermitian conjugate of operator $A$ is denoted by $A^\dagger$. $A$ is Hermitian if $A = A^\dagger$. Let $I_\mathcal{H}$ be the identity matrix over $\mathcal{H}$. The trace of an operator $A$ is

$$tr(A) = \sum_i A_{ii}$$

(the sum of the entries on the main diagonal). A Hermitian operator $A$ is positive semidefinite (resp., positive definite) if for all vector $|\psi\rangle \in \mathcal{H}$,

$$\langle\psi|A|\psi\rangle \geq 0 \; \text{(resp.,} > 0)$$

It induces the L"owner order $\sqsubseteq$ among operators:

1. $A \sqsubseteq B$ if $B - A$ is positive semidefinite;
2. $A \sqsubseteq B$ if $B - A$ is positive definite.

The least upper bound (resp. greatest lower bound) operator in the complete partial order generated by L"owner comparison is denoted as $\biguplus$ (resp. $\bigsqcap$).

A pure quantum state is represented by a unit vector, i.e., a vector $|\psi\rangle$ with $||\psi|| = 1$. For example, a qubit, or quantum bit, system refers to the case when $\mathcal{H} = \mathbb{C}^2$. An important basis of a qubit system is the computational basis with $|0\rangle = (1, 0)^T$ and $|1\rangle = (0, 1)^T$, which corresponds to the 0/1 in a classical bit. One can represent multi-qubits by tensor-producting each qubit. For instance, classical two-bit string 01 can be represented by $|0\rangle \otimes |1\rangle$ (or $|01\rangle$ for short). Thus an $m$-qubit system lives in the space $\mathbb{C}^{2^m} = (\mathbb{C}^2)^\otimes m$ that is the $m$-time tensor-product of a single qubit system $\mathbb{C}^2$.

A mixed state can be represented by a probability distribution over an ensemble of pure states $\mathcal{E} = \{(p_i, |\psi_i\rangle)\}_i$, i.e., the system is in state $\psi_i$ with probability $p_i$. One can also use density operators to represent both pure and mixed quantum states. A density operator $\rho$ for a mixed state represented by the ensemble $\mathcal{E}$ is a positive semidefinite operator

$$\rho = \Sigma_i p_i |\psi_i\rangle\langle\psi_i|,$$

where $|\psi_i\rangle\langle\psi_i|$ is the outer-product of $|\psi_i\rangle$; in particular, a pure state $|\psi\rangle$ can be identified with the density operator $\rho = |\psi\rangle\langle\psi|$. Note that $tr(\rho) = 1$ holds for all density operators. A positive semidefinite operator $\rho$ on $\mathcal{H}$ is said to be a partial density operator if $tr(\rho) \leq 1$. The set of partial density operators on $\mathcal{H}$ is denoted by $\mathcal{D}(\mathcal{H})$.
2.2 Quantum operations

Operations (or evolutions) on (closed) quantum systems can be characterized by unitary operators. An operator $U$ is a unitary operator if its Hermitian conjugate is its own inverse, i.e., $U^*U = 1$. For a pure state $|\psi\rangle$, it describes the evolution $|\psi\rangle \rightarrow U|\psi\rangle$. For a density operator $\rho$, the corresponding evolution is $\rho \rightarrow U \rho U^*$.

More generally, the evolution of (open) quantum systems can be characterized by an (admissible) super operator (or alternatively quantum operation) $\mathcal{E}$, a completely postive and trace-non-increasing linear mapping from $\mathcal{D}(\mathcal{H})$ to $\mathcal{D}(\mathcal{H})$. Namely, for any initial state $\rho$, $\mathcal{E}(\rho)$ is the final state after the evolution and $0 \leq \text{tr}(\mathcal{E}(\rho)) \leq \text{tr}(\rho)$. For every such super-operator $\mathcal{E} : \mathcal{D}(\mathcal{H}) \rightarrow \mathcal{D}(\mathcal{H})$, there exists a set of Kraus operators $\{E_k\}_k$ such that

$$\mathcal{E}(\rho) = \sum_k E_k \rho E_k^\dagger$$

for any input $\rho$. We denote the Kraus form of $\mathcal{E}$ by writing $\mathcal{E} = \sum_k E_k \circ E_k^\dagger$.

Since $\mathcal{E}$ is nonnegative and trace-non-increasing, it holds that $0 \subseteq \sum_k E_k^\dagger E_k \subseteq I$. For example, a unitary evolution can also be represented by a super-operator $\mathcal{E} = U \circ U^\dagger$. An identity (resp. zero) operation refers to the super-operator $I_\mathcal{H} = I_\mathcal{H} \circ I_\mathcal{H}$ (resp. $0_\mathcal{H} = 0_\mathcal{H} \circ 0_\mathcal{H}$). The Schrödinger-Heisenberg dual of a super-operator $\mathcal{E} = \sum_k E_k \circ E_k^\dagger$, denoted by $\mathcal{E}^*$, is defined as follows: for every state $\rho \in \mathcal{D}(\mathcal{H})$ and any operator $A$, $\text{tr}(A\mathcal{E}(\rho)) = \text{tr}(\mathcal{E}^*(A)\rho)$. The Kraus form of $\mathcal{E}^* = \sum_k E_k^\dagger \circ E_k$.

The way to extract information about a quantum system is called a quantum measurement. Mathematically, a quantum measurement on a system over $\mathcal{H}$ can be described by a set of linear operators $\{M_m\}_m$ with

$$\sum_m M_m^\dagger M_m = I_\mathcal{H}.$$  

If we perform a measurement $\{M_m\}$ on a state $\rho$, the outcome $m$ is observed with probability $p_m = \text{tr}(M_m \rho M_m^\dagger)$ for each $m$. After the measurement, the state collapses to a post-measurement state $M_m \rho M_m^\dagger / p_m$. To characterize quantum measurement as a super operator, we remark that the probability $p_m$ can be encoded into the post-measurement state $M_m \rho M_m^\dagger / p_m$, resulting in $M_m \rho M_m^\dagger$. Such an evolution can be written as a super operator $\mathcal{E} = M_m \circ M_m^\dagger$. A major difference between classical and quantum computation is that a quantum measurement changes the state. For example, a measurement in the computational basis is described as $M = \{M_0 \equiv |0\rangle \langle 0|, M_1 \equiv |1\rangle \langle 1|\}$. If we perform the computational basis measurement $M$ on state $\rho = |\pm\rangle \langle +|$, where $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, then with probability $\frac{1}{2}$ the outcome is 0 and the state becomes $|0\rangle \langle 0|$; with probability $\frac{1}{2}$, the outcome is 1 and the state becomes $|1\rangle \langle 1|$.

3 Recursive quantum programs

Recursive quantum programs can be viewed as a recursive extension of the quantum while-programs $\text{PL}$ defined in [32, 33]. In this section, we define syntax and semantics of recursive quantum programs.
3.1 Syntax

We assume a set $\mathbf{Var}$ of quantum variables annotated with a type $\mathbf{Bool}$ or $\mathbf{Int}$, and $\bar{q} \subseteq \mathbf{Var}$. For each $q \in \mathbf{Var}$, its state Hilbert space is denoted by $\mathcal{H}_q$. Then $\bar{q}$ is associated with the Hilbert space $\mathcal{H}_{\bar{q}} = \bigotimes_{q \in \bar{q}} \mathcal{H}_q$.

If $\text{type}(q) = \mathbf{Bool}$ then $\mathcal{H}_q$ is the two-dimensional Hilbert space $\{|0\rangle, |1\rangle\}$. If $\text{type}(q) = \mathbf{Int}$ then $\mathcal{H}_q$ is the infinite-dimensional Hilbert space $\{|n\rangle : n \in \mathbb{Z}\}$.

Now we are able to define the generalized recursive procedural extension of quantum while-programs $\mathbf{PL}$, denoted by $\mathbf{RPL}$. Note, here, that a program $P$ consists of a recursive procedural declaration $D$, associating some body with a recursive procedure name, followed by some statement $S$ containing activation statements to declared recursive procedures. Formally, $\mathbf{RPL}$ is generated by the following grammar:

$$
P \doteq D; S
$$

$$
D \doteq \text{recursion} \langle \text{rec}_1 \rangle : S_1, \ldots, \text{recursion} \langle \text{rec}_n \rangle : S_n
$$

$$
S \doteq \text{skip} \mid q := 0 \mid \bar{q} := U[q] \mid S_1; S_2 \mid
$$

$$
\begin{array}{l}
\text{if } \square m \cdot M[q] = m \rightarrow S_m \text{ fi } \\
\text{while } M[q] = 1 \text{ do } S_0 \text{ od }
\end{array}
$$

$$
\text{call } \langle \text{rec}_i \rangle, \quad 1 \leq i \leq n
$$

where for each recursion declaration $\text{recursion} \langle \text{rec}_i \rangle : S_i, 1 \leq i \leq n$, rec$_i$ is the name, $S_i$ is the body. We stipulate that the calling graph, here, is generated by connecting rec$_i$ to rec$_j$ iff $S_i$ contains a statement $\text{call } \langle \text{rec}_j \rangle$. To ensure recursiveness of these procedures, we require that every such procedure lie on a cycle of the calling graph. We say a recursion is simple if its calling graph is a self cycle, and non-simple otherwise. A typical non-simple recursion is mutual recursion of several procedures, for example where proc$_1$ and proc$_2$ (assumed different) invoke each other.

The intended semantics of language constructs above is similar to that of their classical counterparts.

1. skip does nothing.
2. “$q := |0\rangle$” sets quantum variable $q$ to the basis state $|0\rangle$.
3. “$\bar{q} := U[q]$” applies the unitary $U$ to the qubits in $\bar{q}$.
4. Sequencing has the same behavior as its classical counterpart.
5. “if $\square m \cdot M[q] = m \rightarrow S_m$ fi” performs the measurement $M \doteq \{M_m\}$ on the qubits in $\bar{q}$, and executes program $S_m$ depending on the outcome of the measurement.
6. “while $M[q] = 1 \text{ do } S_0 \text{ od}$” performs the measurement $M \doteq \{M_0, M_1\}$ on the qubits in $\bar{q}$, and either executes $S_0$ or terminates depending on the outcome of the measurement.
7. “call $\langle \text{rec}_i \rangle$” activates the procedure rec$_i$, executes the body $S_i$, and resumes with the statement immediately following call $\langle \text{rec}_j \rangle$ (if any), whenever the execution of $S_i$ terminates.
As a special example, quantum program \texttt{abort}, which on any input never terminates, can be implemented as an endless loop, each iterative step doing nothing after the (true) measurement \( M_t = \{ M_0 \neq 0, M_1 \neq I \} \), whose outcome is always 1. That is,

\[
\text{abort} \triangleq \text{while } M_t[q] = 1 \text{ do skip od}
\]

We need to highlight two differences between quantum and classical \texttt{while}-programs: (1) Qubits may only be initialized to the basis state \(|0\rangle\). There is no quantum analogue for initialization to any expression (i.e. \( x := e \)) because of the no-cloning theorem of quantum states. Any state \(|\psi\rangle \in \mathcal{H}_q\), however, can be constructed by applying some unitary \( U \) to \(|0\rangle\). (2) Evaluating the guard of a conditional or loop, which performs a measurement, potentially disturbs the state of the system.

### 3.2 Running Example: Fixed-point Grover’s Search

We now present an example program written in our recursive quantum programming language. Grover’s search is a quantum algorithm of finding a target item in an unsorted database, which has a square-root speedup over the corresponding classical algorithm. The original idea is to design the iterative transformations in a way that each iteration results in a small rotation of the moving state in a two-dimensional Hilbert space spanned by the initial and target vectors. If we choose the right number of iterative steps, the moving state will stop just at the target state, otherwise it will drift away. Fixed-point Grover’s search supplements the original search algorithm by permitting the moving state converges monotonically to the target state irrespective of the number of iteration. This feature leads to robust search algorithms and also to new schemes for quantum control and error correction.

**Example 3.1** (Fixed-point Grover’s search). Define the search space \( \mathcal{H}_s \) to be the \( N \)-dimensional Hilbert space with orthonormal basis states \(|n\rangle: n \in [N - 1]\), for encoding an \( N \)-element database with solutions represented as \(|t\rangle\). Define the counting space \( \mathcal{H}_c \) to be the infinite-dimensional Hilbert space with orthonormal basis states \(|n\rangle: n \in \mathbb{Z}\), for indexing the depth of the recursive search engine. Now the state space of the search is \( \mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_s \) and the initial state is \(|0\rangle|0\rangle\). For convenience of following description, define the \( \frac{\pi}{3} \) phase shift \( R_x \) for \(|x\rangle \in \mathcal{H}_s \) as

\[
R_x \triangleq I - \exp(i \frac{\pi}{3}) \langle x|x| \]

define \((+n)\)-operator \( U_{+n} \) of \( \mathcal{H}_c \) by \( U_{+n}: |x\rangle \rightarrow |x + n\rangle \), and similarly for \((-n)\)-operator \( U_{-n} \).

In each step of the search procedure:

1. Prepare the counting state \(|n\rangle\) and source state \(|s\rangle\) by applying unitary operator \( U_{+n} \otimes U_s \) to \(|0\rangle|0\rangle\).
2. Apply the search engine \( V_n \) — a sequence of unitary operators recursively defined as

\[
V_{n+1} \triangleq V_n R_x V_n^\dagger R_t V_n
\]
Table 1: (a) $q\text{Search}$ and $q\text{Search}_\text{dag}$ implement the search engine $V_n$ together with its adjoint $V_n^\dagger$.

| recursion $q\text{Search} \cdot S$ | recursion $q\text{Search}_\text{dag} \cdot S$ |
|----------------------------------|----------------------------------|
| $S \triangleq \text{if } \lceil m \cdot M[q_1] \rceil = m \rightarrow S_m$ | $S \triangleq \text{if } \lceil m \cdot M[q_1] \rceil = m \rightarrow S_m$ |
| $S_0 \triangleq q_2 := V \cdot q_2$ | $S_0 \triangleq q_2 := V \cdot q_2$ |
| $S_1 \triangleq \text{call } q\text{Search}$; | $S_1 \triangleq \text{call } q\text{Search}$; |
| $q_2 := R_s \cdot q_2$; | $q_2 := R_s \cdot q_2$; |
| $\text{call } q\text{Search}_\text{dag}$; | $\text{call } q\text{Search}_\text{dag}$; |
| $q_2 := U_s \cdot q_2$; | $q_2 := U_s \cdot q_2$; |
| $\text{call } q\text{Search}$; | $\text{call } q\text{Search}$; |
| $q_1 := U_{++} \cdot q_1$; | $q_1 := U_{++} \cdot q_1$; |
| $S_2 \triangleq \text{while } M_1[q_1] = 1 \text{ do skip od}$ | $S_2 \triangleq \text{while } M_1[q_1] = 1 \text{ do skip od}$ |

Table 2: (b) The main program $FGS$ implements the search procedure.

$V_0 \triangleq V$ — to the source state $|s\rangle$ with the counting state $|n\rangle$ to determine the recursion depth. We perform measurement

$$M \triangleq \{M_0 \triangleq \{0\}\langle0|, M_1 \triangleq \sum_{i \geq 1} |i\rangle\langle i|, M_2 \triangleq \sum_{i \leq 1} |i\rangle\langle i|\}$$

on the counting state $|n\rangle$; then execute the following depending on the measurement outcome. If the outcome is 0, the search procedure apply $V$; if the outcome is 1, the search procedure apply $V_{n-1}R_s V_{n-1}^\dagger R_s V_{n-1}$; if the outcome is 2, the search procedure collapses (implemented by \textbf{abort}).

(3) Measure the resulting state $V_n|s\rangle$ to obtain the solution $|t\rangle$. We use the measurement

$$M' = \{|t\rangle\langle t|, |t^\dagger\rangle\langle t^\dagger| \triangleq (I - |t\rangle\langle t|)\}.$$ 

Suppose that $V$ drives the state vector from $s$ to $t$ with a probability of $(1 - \epsilon)$, i.e. $||\langle t|V|s\rangle||^2 = 1 - \epsilon$. It is straightforward to show that the resulting state $V_n|s\rangle$ after applying $V_n$ deviates from $t$ with a probability of $e^{3\epsilon}$, i.e. $||\langle t|V_n|s\rangle||^2 = (1 - e^{3\epsilon})$, hence reducing the error probability from $\epsilon$ to $e^{3\epsilon}$.

The program for the search procedure is shown as follows.

### 3.3 Operational semantics

The operational semantics of quantum programs can be defined as a transition relation $\rightarrow$ between quantum configurations $\langle S, \rho \rangle$ — the global description for quantum program $S$ on current state represented as partial density operator $\rho$. Note that $S$ could be the empty statement $E$. By a transition $\langle S, \rho \rangle \rightarrow \langle S', \rho' \rangle$, we mean that program $S$ on input state $\rho$ is evaluated in one step to program $S'$ with output state $\rho'$.

The transition relation $\rightarrow$ for RPL is defined by adding the rule

$$\langle \text{Proc} \rangle \rightarrow \langle \text{call rec}, \rho \rangle \quad \text{if } D \text{ contains recursion } \text{rec} : S$$

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3.4 Denotational semantics

The denotational semantics of a quantum program, denoted \([\_\_\_\_\_\_\_\_]\), is defined as a superoperator that acts on \(\rho \in \mathcal{H}_{Var}\). The semantics of each term is given in a compositional way. To handle the statement of while, we need to define its \(k\)th syntactic approximation (i.e., unrolling) \((\text{while})^k\) as

\[
\begin{align*}
(\text{while } M[\bar{q}] = 1 \text{ do } S)^0 & \triangleq \text{abort} \\
(\text{while } M[\bar{q}] = 1 \text{ do } S)^{k+1} & \triangleq \text{if } \Box m \cdot M[\bar{q}] = m \rightarrow S_m \text{ fi, } \rho \end{align*}
\]
$[\text{skip}](\rho) = \rho$

$[q := |0\rangle](\rho) = \left\{ \begin{array}{ll} |0\rangle\langle 0|\rho|0\rangle\langle 0| + |0\rangle\langle 1|\rho|1\rangle\langle 0|, & \text{if type}(q) = \text{Bool} \\ \sum_{n=-\infty}^{\infty} |0\rangle\langle n|\rho|n\rangle\langle 0|, & \text{if type}(q) = \text{Int} \end{array} \right.$

$[S_1; S_2](\rho) = [S_2][[S_1](\rho)]$

$[\text{if } n \cdot M[q] = m \rightarrow S_m \text{ fi}](\rho) = \Sigma_m [[S_m](M_m\rho M_m^\dagger)]$

$[\text{while } M[q] = 1 \text{ do } S](\rho) = \prod_{n=0}^{\infty}[\text{while}]^{(n)}(\rho)$

$[\text{call } \langle \text{rec} \rangle](\rho) = \prod_{n=0}^{\infty}[[\text{call } \text{rec}_1, \ldots, \text{call } \text{rec}_n]]$

Table 4: Denotational semantics of recursive quantum while-programs

where $S \triangleq \{S_0, S_1\}$ with

$S_0 \triangleq \text{skip}$

$S_1 \triangleq S; (\text{while } M[q] = 1 \text{ do } S)^k$

For all declared recursive procedures $\text{rec}_i$ with body $S_i$, $1 \leq i \leq n$, the $k$th syntactic approximation $S_i^{(k)}$ is defined as:

$S_i^{(0)} \triangleq \Omega$

$S_i^{(k+1)} \triangleq S_i[S_1^{(k)}/\text{call } \text{rec}_1, \ldots, S_n^{(k)}/\text{call } \text{rec}_n]$

where $[S_1^{(k)}/\text{call } \text{rec}_1, \ldots, S_n^{(k)}/\text{call } \text{rec}_n]$ stands for simultaneous substitution of $S_i^{(k)}$ for $\text{call } \text{rec}_i$ for all $1 \leq i \leq n$.

The denotational semantics $[\cdot]$ for $\text{RPL}$ is defined by adding the equation

$[\text{call } \langle \text{rec} \rangle](\rho) = \prod_{n=0}^{\infty}[[S^{(n)}]]$

handling recursive procedural activation, to that for base quantum language $\text{PL}$ (cf. Figure 3).

The following proposition reveals the connection between operational and denotational semantics. Namely, the meaning of running program $S$ on input state $\rho$ is the sum of all possible output states, weighted by their probabilities.

**Proposition 3.1.** For any recursive quantum while-program $S$

$[S](\rho) = \sum_{\rho'} [\langle S, \rho \rangle \rightarrow^* \langle E, \rho' \rangle]$

where $\rightarrow^*$ is the reflexive, transitive closure of $\rightarrow$ and $[\cdot]$ stands for a multiset.

## 4 Correctness and expressiveness

As defined by D’Hondt and Panangaden in [23], a quantum predicate on $\mathcal{H}$ is a Hermitian operator $M$ such that $0_{\mathcal{H}} \subseteq M \subseteq I_{\mathcal{H}}$. Intuitively, $tr(M\rho)$ is the expectation of the truth value of predicate $M$ on state $\rho$. Note that restricting $M$ to be between $0_{\mathcal{H}}$ and $I_{\mathcal{H}}$ ensures that $0 \leq tr(M\rho) \leq 1$ for any $\rho \in D(\mathcal{H})$.

For example, the identity matrix corresponds to the true predicate; the zero matrix corresponds to the false predicate; $|0\rangle\langle 0|$ is the predicate that says that
a state is in the subspace spanned by $|0\rangle$. We write $\mathcal{P}(\mathcal{H})$ for the set of quantum predicates on $\mathcal{H}$.

Quantum predicates are simply employed in $[23, 32]$ as the pre- and post-conditions of quantum Hoare triples. However, to develop quantum program logic, we have to formally define the underlying model $\mathcal{M}$ for formalizing quantum program correctness. It can be defined as a typed first-order infinite model — the domains including the set of partial density operators, over which the input-output relation of a quantum program is defined, and the set of quantum predicates, with which the properties of input and output states are specified, together with the standard interpretation $I$ of the associated symbols. In this view, the syntactic counterpart of quantum predicates is described by terms generated from constant symbols and variables after applying function symbols finite or (sometimes) infinite times. Thus the (partial or total) correctness formula of a quantum program will be expressed by a Hoare’s triple, where the the pre- and post-conditions are given by quantum predicate terms instead of quantum predicates.

To ensure a broad scope of applicability of our quantum program logic, we require that $\mathcal{M}$ have enough power of expressibility so that both quantum predicates of practical interest and all the intermediate predicates, e.g. weakest (liberal) preconditions, in proving program correctness can be expressed thereof. Thus the terms for quantum predicate can be defined as follows.

**Definition 4.1.** Let $\mathcal{H}$ be the Hilbert space $\mathcal{H}_q$ associated with quantum variables $\bar{q}$. Let $I_\mathcal{H}$ be the constant symbol denoting the identity operator on $\mathcal{H}$, $X_\mathcal{H}$ a metavariable ranging over all first-order variables on $\mathcal{P}(\mathcal{H})$, and $\sum_k M_k^\dagger \circ M_k$ the dual of a quantum operation on $\mathcal{H}$.

Quantum predicate term $P_\mathcal{H}$ and L"owner ordering formula $F_\mathcal{H}$ on $\mathcal{H}$ are defined as:

$$P_\mathcal{H} \triangleq I_\mathcal{H} | X_\mathcal{H} | P_{\mathcal{H}_1} \otimes P_{\mathcal{H}_2} | I_\mathcal{H} - P_\mathcal{H} | \sum_k M_k^\dagger P_k M_k | \bigcup_l Q_l^\dagger$$

$$F_\mathcal{H} \triangleq P_\mathcal{H} \subseteq Q_\mathcal{H}$$

where $P_{\mathcal{H}_1}$ and $P_{\mathcal{H}_2}$ denote resp. quantum predicate terms on $\mathcal{H}_1 = \mathcal{H}_{q_1}$ and $\mathcal{H}_2 = \mathcal{H}_{q_2}$ with $q = q_1 \cup q_2$ (if any); each of $P_k, Q_k^\dagger$ and $Q_\mathcal{H}$ denotes a (possibly different) quantum predicate term on $\mathcal{H}$ with $Q_\mathcal{H}^\dagger \subseteq Q_\mathcal{H}^\dagger$, $\forall l$.

To show reasonability of quantum operation used as a construct of quantum predicate terms, we remark that any quantum operation can be obtained by tracing out the environmental part of a global unitary operation, and any unitary operation can be approximated to arbitrary accuracy by a quantum circuit involving only finite one-qubit operations, e.g. Hadamard, CNOT and $\pi/8$ $[21]$. Alternatively, an arbitrary quantum operation can be (approximately) represented by denotational semantics $[S]$, for some program $S$ of a procedural extension of $PL$ with local variables (cf. Subsec. 3.3.6 of $[32]$).

**Definition 4.2.** Let symbols occurring in this definition be as in Definition 4.1. Let $v$ be an assignment of quantum predicate variables to quantum predicates, i.e. $v(X_\mathcal{H}) \in \mathcal{P}(\mathcal{H})$. 

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The denotation of $P_H$ under interpretation $\ll$ and assignment $v$, denoted $P^{I,v}_{H}$, is defined as

$$P^{I,v}_{H} = \left\{ \begin{array}{ll} I_H & P_H = I_H \\
v(X_H) & P_H = X_H \\
P^{I,v}_{H1} \otimes P^{I,v}_{H2} & P_H = P_{H1} \otimes P_{H2} \\
I_H - P^{I,v}_{H} & P_H = I_H - P_H \\
\sum_k M^1_k P^{I,v}_{H,k} M_k & P_H = \sum_k M^1_k P^0_{H,k} M_k \\
\bigwedge Q^i_{H,v} & P_H = \bigwedge Q^i_{H} \\
\end{array} \right. $$

where the notational abuse between semantics (the left) and syntax (the right) is allowed, e.g., the left $I_H$, or strictly $I^3_H$, is the denotation of the right $I_H$ under interpretation $\ll$. We shall follow this convention in the following.

The truth of Löwner ordering formula $P_H \subseteq Q_H$ under interpretation $\ll$, denoted $\models_{\ll} P_H \subseteq Q_H$, is defined by

$$P^{I,v}_{H} \subseteq Q^{I,v}_{H}, \forall v$$

To see well-definedness of quantum predicate terms, we remark that the existence of $\bigwedge Q^i_{H}$ with $Q^i_{H} \equiv Q^i_{H} + 1$, $\forall l$, is justified by the fact that $(\mathcal{P}(H), \subseteq)$ is a complete partial order, as shown in [33]. In addition, to show $\sum_k M^1_k P^{I,v}_{H,k} M_k \in \mathcal{P}(H)$, we note that it is Hermitian and $0_H = \sum_k M^1_k 0_H M_k \subseteq \sum_k M^1_k P^0_{H,k} M_k \subseteq \sum_k M^1_k I_H M_k \subseteq I_H$.

Introduction of variables into quantum predicate terms lays the foundation of the Substitution Rule, which is indispensable to ensure that both partial and total correctness rules for recursion are complete. The set of quantum predicate terms on $\mathcal{H}$ is written as $\mathcal{T}(\mathcal{H})$. We shall omit the subscript of $P_H$ if it is obvious from the context. Note that the term $0$, whose denotation is the zero matrix, can be defined by $0 \equiv I - I$; the term $\bigwedge Q^i$ with $Q^i \equiv Q^i + 1$, $\forall l$, whose denotation is the greatest lower bound of a decreasing sequence of quantum predicates, can be defined by $\bigwedge Q^i \equiv I - \bigvee (I - Q^i)$.

The whole formal assertions on quantum predicates considered in this paper are all true Löwner ordering formulas $Tr_I$ under interpretation $\ll$, i.e.

$$Tr_I \equiv \bigvee \{ P \subseteq Q : P, Q \in \mathcal{T}(H) \} \text{ and } \models_{\ll} P \subseteq Q.$$ 

For now, a quantum partial (resp. total) correctness formula can be the Hoare’s triple $\{ P \} S \{ Q \}$ (resp. $\langle P \rangle S \{ Q \}$), where $S$ is a quantum program, and $P,Q$ are quantum predicate terms. Since quantum programs can be viewed semantically as quantum operations, to define the semantics of quantum Hoare’s triple, we first define the correctness semantics of quantum operations.

**Definition 4.3.** Let $M, N$ be quantum predicates and $E$ a quantum operation. We say that

- $E$ is partially correct w.r.t. precondition $M$ and postcondition $N$, written $\{ M \} E \{ N \}$, if

$$tr(M \rho) \leq tr(N E(\rho)) + \left[ tr(\rho) - tr(E(\rho)) \right], \; \forall \rho.$$ (1)

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• $\mathcal{E}$ is totally correct w.r.t. precondition $M$ and postcondition $N$, written $\langle M \rangle \mathcal{E} \langle N \rangle$, if
  \[ \text{tr}(M\rho) \leq \text{tr}(N\mathcal{E}(\rho)), \ \forall \rho. \]

According to the interpretation of quantum mechanics, $\text{tr}(M\rho)$ (resp. $\text{tr}(N\mathcal{E}(\rho))$) is the expectation (average value) of observable $M$ (resp. $N$) in state $\rho$ (resp. $\mathcal{E}(\rho)$). Then inequality (a) can be seen as the quantum version of the following statement: if state $\rho$ satisfies predicate $M$, then, applying the operator $\mathcal{E}$ to $\rho$, either $\mathcal{E}$ fails to terminate or the resulting state $\mathcal{E}(\rho)$ should satisfy predicate $N$. Note that total correctness is a stronger version of partial correctness by guaranteeing termination once the precondition is satisfied.

The above definition for semantical Hoare triples can be easily lifted to the case of syntactic Hoare triples.

**Definition 4.4.** Let $P$, $Q$ be quantum predicate terms and $S$ a quantum program. We say that

1. $S$ is partially correct w.r.t. precondition $P$ and postcondition $Q$ under interpretation $I$, written $\models_I \langle P \rangle S \langle Q \rangle$, if $\forall v, \langle P^{I,v} \rangle[S] \langle Q^{I,v} \rangle$.

2. $S$ is totally correct w.r.t. precondition $P$ and postcondition $Q$ under interpretation $I$, written $\models_I \langle P \rangle S \langle Q \rangle$, if $\forall v, \langle P^{I,v} \rangle[S] \langle Q^{I,v} \rangle$.

As in classical Hoare logic, the notion of weakest (liberal) preconditions can be used as an ideal choice for defining intermediate assertions involved in proving program correctness, and will play a key role in establishing the completeness of quantum program logic. The semantical weakest (liberal) preconditions are defined as:

**Definition 4.5.** Let $N$ be a quantum predicate and $\mathcal{E}$ a quantum operation.

1. The weakest precondition $WP(\mathcal{E}, N)$ of $\mathcal{E}$ w.r.t. $N$ is defined to be the quantum predicate $M \in \mathcal{P}(\mathcal{H})$ such that:
   a. $\langle M \rangle \mathcal{E} \langle N \rangle$;
   b. for any $M' \in \mathcal{P}(\mathcal{H})$, if $\langle M' \rangle \mathcal{E} \langle N \rangle$, then $M' \subseteq M$.

2. The weakest liberal precondition $WLP(\mathcal{E}, N)$ of $\mathcal{E}$ with respect to $N$ is defined to be the quantum predicate $M \in \mathcal{P}(\mathcal{H})$ such that:
   a. $\{ M \} \mathcal{E} \{ N \}$;
   b. for any $M' \in \mathcal{P}(\mathcal{H})$, if $\{ M' \} \mathcal{E} \{ N \}$, then $M' \subseteq M$.

The following proposition shows that the weakest precondition of a quantum operation can be represented by its dual.

**Proposition 4.1.** Let $N$ be a quantum predicate and $\mathcal{E}$ a quantum operation.

1. $WP(\mathcal{E}, N) = \mathcal{E}^*(N)$;
2. $WLP(\mathcal{E}, N) = I - \mathcal{E}^*(I - N)$.

Following is the structural representation of weakest (liberal) preconditions of quantum programs.
Let $S$ be a quantum program, and $P$ a quantum predicate term. For any assignment $v$, it is the case that

1. $WP([S], P^L_v) = [wp.S.P]^L_v$, where $wp.S.P$ is defined in Table 5

2. $WLP([S], P^L_v) = [wlp.S.P]^L_v$, where $wlp.S.P$ is defined in Table 6

It is worth noting that both $wp.S.P$ and $wlp.S.P$ in the above theorem are quantum predicate terms. We present the proof sketch by induction on $S$.

- For the base case, $wp.S.P$ (resp. $wlp.S.P$) is either $P$ itself or obtained by applying the dual of a quantum operation to $P$.
- For $S = S_1; S_2$, the proof is by applying induction hypothesis first to $S_2$ and then to $S_1$.
- For $S = \text{if}$, the proof is by applying the dual of a quantum operation to $wp.S_m.P$ (resp. $wlp.S_m.P$) which, by induction hypothesis, are quantum predicate terms.
- For $S = \text{while}$, we first show that $wp.(\text{while})^n.P$ (resp. $wlp.(\text{while})^n.P$) is a quantum predicate term by induction on $n$ and by induction hypothesis to sub-statements; then show that $wp.(\text{while})^n.P \subseteq wp.(\text{while})^{n+1}.P$ (resp. $wlp.(\text{while})^n.P \supseteq wlp.(\text{while})^{n+1}.P$) by induction on $n$; finally apply the least upper bound (resp. greatest lower bound) operator.
- For the activation statement, the proof is as previous.

Combining Theorem 4.1 and Proposition 4.1, we have an alternative definition of $wp.S.P$ and $wlp.S.P$ as follows.
Corollary 4.1. Let $S$ be a quantum program, and $P$ a quantum predicate term. It is the case that

1. $wp.S.P = [S]^*(P)$;
2. $wlp.S.P = I - [S]^*(I - P)$.

5 Proof system for partial correctness

In this section, we aim to introduce the axiom system $QPR$ for proving partial correctness of recursive quantum programs $RPL$.

Our first step is to give a proof system $qPW$ for proving partial correctness of syntactical quantum Hoare triples; that is, quantum Hoare triples with quantum predicate terms as pre- and post-conditions. It is obtained by appending to its counterpart $qPD$ of [22] the proof rule

\[
\frac{\{P\}S\{Q\}}{\{P[R/X]\}S\{Q[R/X]\}}
\]

handling the substitution in quantum predicate terms, where $R$ (resp. $X$) is an arbitrary quantum predicate term (resp. variable), and $P[R/X]$ stands for the result of simultaneously substituting $R$ for each occurrence of $X$ in $P$. For proof system $qPW$, the reader is referred to Table 7.

For presentational convenience, we introduce some notations and definitions. We only allow formulas of Hoare’s triple and Löwner order comparison in the sequel. For sets of formulas $A$ and $B$, $A \models I B$ means that if $\models I A$ then $\models I B$, where by $\models I A$ is meant that for all formulas $F$ of $A$, $\models I F$. For a proof system $H$, e.g. $qPW$, by $Tr_I, A \models H B$ is meant that every formula of $B$ can be deduced from $Tr_I, A$ and axioms of $H$ by finite applications of proof rules of $H$. We say that $H$ is sound if for any Hoare’s triple $F$ with $Tr_I \vdash_H F$, $\models I F$; $H$ is (relatively) complete if for any Hoare’s triple $F$ with $\models I F$, $Tr_I \vdash_H F$. Note
that \( T_{\text{I}} \) provide all possible Löwner ordering formulas used as antecedents of the (Order Rule), which, together with the condition of expressiveness, is a prerequisite to make \( H \) complete \([9,5]\). As with \( qPD \) of \([32]\), \( qPW \) is sound and complete.

We are now in a position to present the proof rule — (Partial REC Rule) — for proving the partial correctness of recursive procedure \( \text{rec} \) with body \( S \). Consider first the case of simple recursion, that is, \( S \) should itself contain the (re)invocation statement \( \text{call} \langle \text{rec} \rangle \), but retain the exclusion of invoking other recursive procedures. (The case of complex recursion is deferred to the end of this section.)

\[
\begin{array}{c}
\text{(Partial REC Rule)} \\
T_{\text{I}}, \{P\}\text{call} \text{rec}\{Q\} \vdash_{qPW} \{P\}S\{Q\} \\
\hline
\{P\}\text{call} \text{rec}\{Q\}
\end{array}
\]

The intuition of the (Partial REC Rule) is that, to derive the correctness assertion \( \{P\}\text{call} \text{rec}\{Q\} \) about \text{call rec}, it suffices to derive \( \{P\}S\{Q\} \) for its body \( S \); since \( S \) itself contains the (re)invocation statement (or inner) \text{call rec}, it suffices to derive correctness assertions about the inner \text{call rec}, say \( \{P'\}\text{call} \text{rec}\{Q'\} \); by Floyd-Hoare’s Principle, \( \{P'\}\text{call} \text{rec}\{Q'\} \) should be adapted from the premise \( \{P\}\text{call} \text{rec}\{Q\} \) possibly by using Substitution Rule. This reveals the reason for introducing the (Substitution Rule): without which the above derivation might not proceed as desired.

Then proof system \( qPR \) for recursive quantum programs can be obtained from \( qPW \) by adding the (Partial REC Rule).

We show in the following soundness and completeness of \( qPR \).

**Theorem 5.1 (Soundness).** \( qPR \) is sound. That is, for any quantum program \( S \in RPL \) and any quantum predicate terms \( P,Q \), we have

\[ T_{\text{I}} \vdash_{qPR} \{P\}S\{Q\} \text{ implies } \models \{P\}S\{Q\}. \]

**Proof.** By induction on the length of proof of theorems of \( qPR \). We consider the cases of the last step of the proof. The only nontrivial case is when \( \{P\}\text{call} \text{rec}\{Q\} \) is deduced by means of (Partial REC Rule). Let \( S \) be the body of \text{rec}. Then we have

\[ T_{\text{I}}, \{P\}\text{call} \text{rec}\{Q\} \vdash_{qPW} \{P\}S\{Q\}. \]

Let \( D \) denote the union of \( \{\{P\}S^{(0)}\{Q\}\} \) with the set of formulas \( \{P'\}S'\{Q'\} \) occurring in the above proof of \( \{P\}S\{Q\} \), \( S' \) containing no occurrence of \text{call rec}. By easy calculation, together with induction hypothesis, it follows that \( \models \emptyset \).

**Claim 1.** For every \( n \geq 0 \), \( T_{\text{I}}, D \vdash_{qPW} \{P\}S^{(n)}\{Q\} \).

**Proof.** By induction on \( n \).

The proof for the base case is immediate from definition of \( D \).

As the inductive step, suppose that Claim 1 holds for \( n = k \). That is, \( T_{\text{I}}, D \vdash_{qPW} \{P\}S^{(k)}\{Q\} \). Then we have to show that \( T_{\text{I}}, D \vdash_{qPW} \{P\}S^{(k+1)}\{Q\} \).

Consider any application of a rule in \( qPW \) using \( \{P\}\text{call} \text{rec}\{Q\} \) as one of its premises. In its conclusion, there is some occurrence of \text{call rec} in the program part. By the definition of \( S^{(k+1)} \), the corresponding program section is obtained by replacing that occurrence with \( S^{(k)} \). Thus, the same rules in the proof of \( \{P\}S\{Q\} \) with \( \{P\}\text{call} \text{rec}\{Q\} \) as one of its premises can be applied in the proof of \( \{P\}S^{(k+1)}\{Q\} \) by using the assumption \( \{P\}S^{(k)}\{Q\} \) instead. \( \Box \)
Since $|= I \ D$, by Claim\textsuperscript{11}, jointly with soundness of $\vdash qPW$, it follows that

$$|= I \ \{P\} S^{(n)} \{Q\},$$

for every $n \geq 0$. Fix $n \geq 0$. By definition of partial correctness, it follows that

$$tr(P\rho) \leq tr(Q[S^{(n)}](\rho)) + [tr(\rho) - tr([S^{(n)}](\rho))],$$

for all $\rho \in D(H)$. Let $n \rightarrow \infty$. By semantics of recursive procedure, it follows that

$$tr(P\rho) \leq tr(Q[\text{call \ rec}](\rho)) + [tr(\rho) - tr([\text{call \ rec}](\rho))],$$

for all $\rho \in D(H)$. By definition of partial correctness, it follows that

$$|= I \ \{P\}\text{call \ rec}\{Q\}.$$

And we are done. □

**Theorem 5.2.** $qPR$ is complete. That is, for any quantum program $S \in RPL$ and any quantum predicate terms $P, Q$, we have

$$|= I \ \{P\} S\{Q\} \implies TrI \vdash_{qPR} \{P\} S\{Q\}.$$ 

**Proof.** We proceed by induction on $S$, where the only interesting case is for $S$ equal to $\text{call \ rec}$. Assume that $|= I \ \{P\}\text{call \ rec}\{Q\}$. Then we have to show that

$$TrI \vdash_{qPR} \{P\}\text{call \ rec}\{Q\}.$$

Let $S$ be the body of $\text{rec}$. As a preliminary step, we consider a proof of $\{P\} S\{Q\}$ from a recursive assumption of a special form, known also as the most general partial correctness formula, namely

$$\{\text{wlp.}(\text{call \ rec}).X\}\text{call \ rec}\{X\},$$

where $X$ is a fresh quantum predicate variable. To this end, we first show that for any quantum predicate terms $P'$ and $Q'$ with $|= I \ \{P'\}\text{call \ rec}\{Q'\}$,

$$TrI, \{\text{wlp.}(\text{call \ rec}).X\}\text{call \ rec}\{X\} \vdash_{qPW} \{P'\}\text{call \ rec}\{Q'\}. \tag{2}$$

By (Substitution Rule), with $Q'$ in place of $X$, it follows that

$$TrI, \{\text{wlp.}(\text{call \ rec}).X\}\text{call \ rec}\{X\} \vdash_{qPW} \{\text{wlp.}(\text{call \ rec}).Q'\}\text{call \ rec}\{Q'\}.$$

Since $|= I \ \{P'\}\text{call \ rec}\{Q'\}$, it follows that

$$|= I \ P' \subseteq \text{wlp.}(\text{call \ rec}).Q'.$$

By (Order Rule), Assertion (2) follows. Since $|= I \ \{P\}\text{call \ rec}\{Q\}$, by Assertion (2), it follows that

$$TrI, \{\text{wlp.}(\text{call \ rec}).X\}\text{call \ rec}\{X\} \vdash_{qPW} \{P\}\text{call \ rec}\{Q\}.$$ 

Since $|= I \ \{\text{wlp.}(\text{call \ rec}).X\}\text{call \ rec}\{X\}$, by semantics of recursion, we have

$$|= I \ \{\text{wlp.}(\text{call \ rec}).X\} S\{X\}.$$
Applying Assertion 2 to each occurrence of call rec in S, it follows that

\[ Tr_I, \{ wlp.(call rec).X \} call \ rec\{X\} \vdash_{qPR} \{ wlp.(call rec).X \} S\{X\}. \]

By (Partial REC Rule), it follows that

\[ Tr_I \vdash_{qPR} \{ wlp.(call rec).X \} call \ rec\{X\}. \]

Finally, \( Tr_I \vdash_{qPR} \{ P \} call \ rec\{Q\} \) follows.

We now extend the (Partial REC Rule) for simple recursion to the general case. For arbitrary (simple or complex) recursive procedures \( rec_i \) with body \( S_i \), \( 1 \leq i \leq n \), the proof rule — generalized (Partial REC Rule) — for their partial correctness can be given, in a uniform way, by

\[
\text{Soundness and completeness of the generalized (Partial REC Rule) can be shown similarly to the case of simple recursion.}
\]

**Example 5.1** (Partial correctness of fixed-point Grover’s search). Recall from Example 3.1 that if \( V \) drives the state vector from \( s \) to \( t \) with a probability of \( 1 - \epsilon \), i.e. \( \|\langle t|V|s\rangle\|^2 = 1 - \epsilon \), then the resulting state \( V_n|s\rangle \) after applying \( V_n \) deviates from \( t \) with a probability of \( \epsilon^{3^n} \), i.e. \( \|\langle t|V_n|s\rangle\|^2 = (1 - \epsilon^{3^n}) \).

Then we claim that, on any input, the quantum program \( FGS \) executes with output \( V_n|s\rangle \otimes |s\rangle \otimes |t\rangle \) with a probability of \( \epsilon^{3^n} \) (if it terminates). For notational convenience, let \( P_1[X] \equiv |i\rangle_q \otimes X \) with an fresh quantum predicate variable on \( q_2 \). We write the substitution \([Q/X]\) as \([Q] \) for short if \( Q \) is clear from the context. Formally speaking, the claim can be expressed as the partial correctness of a Hoare’s triple:

\[
|\begin{array}{c}
\vdash_I \{ I_{q_1} \otimes I_{q_2} \} FGS \{ \sum_{i=0}^{\infty} P_i[V_i|s\rangle \otimes |s\rangle |V_i'] \}
\end{array}\]

By soundness and completeness of qPR, it is equivalent to show that

\[
Tr_I \vdash_{qPR} \{ I_{q_1} \otimes I_{q_2} \} FGS \{ \sum_{i=0}^{\infty} P_i[V_i|s\rangle \otimes |s\rangle |V_i'] \}.
\]

By (Initialization Axiom), together with (Composition Rule), it follows that

\[
Tr_I \vdash_{qPR} \{ I_{q_1} \otimes I_{q_2} \} q_1 := |0\rangle; q_2 := |0\rangle \{ \sum_{i=0}^{\infty} P_{i-n}[|0\rangle \otimes |0\rangle] \}
\]

By (Unitary Axiom), together with (Composition Rule), it follows that

\[
Tr_I \vdash_{qPR} \{ \sum_{i=0}^{\infty} P_i[|0\rangle \otimes |0\rangle] \} q_{1,2} := U_{+n} \otimes U_s \{ \sum_{i=0}^{\infty} P_i[|s\rangle \otimes |s\rangle] \}
\]

By (Skip Axiom), together with (If Rule), it follows that

\[
Tr_I \vdash_{qPR} \{ \sum_{i=0}^{\infty} P_i[V_i|s\rangle \otimes |s\rangle |V_i'] \} \text{if} \Box m \cdot M'[q_2] = m \rightarrow \text{skip} \{ \sum_{i=0}^{\infty} P_i[V_i|s\rangle \otimes |s\rangle |V_i'] \}
\]
To prove Assertion (3), by (Composition Rule), it suffices to show that

\[ \sum_{i=0}^{\infty} P_i[X] \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\} \]

By (Substitution Rule), it suffices to show that

\[ \sum_{i=0}^{\infty} P_i[X] \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\} \]

By the generalized (Partial REC Rule), it suffices to show that

\[ \sum_{i=0}^{\infty} P_i[X] \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\} \]

illustrated in Table 8 and

\[ \sum_{i=0}^{\infty} P_i[X] \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\} \]

left as an exercise, where

\[ \text{Prem}_1 \equiv \{\sum_{i=0}^{\infty} P_i[X] \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\}\} \]

\[ \text{Prem}_2 \equiv \{\sum_{i=0}^{\infty} P_i[X] \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\}\} \]

Table 8: Part proof for Example 5.1

| (1) | \{\sum_{i=0}^{\infty} P_i[X] \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\}\} | Prem_1 |
| (2) | \{\sum_{i=0}^{\infty} P_i[X] \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\}\} | Prem_2 |
| (3) | \{P_0[X]\}_{q_2 := Vq_2[P_0[V_0X_0^t]]} | Unit. |
| (4) | \{P_0[V_0X_0^t]\} \subseteq \sum_{i=0}^{\infty} P_i[V_iX_i^t] | Tr_l |
| (5) | \{P_0[X]\}_{q_2 := Vq_2[P_0[V_0X_0^t]]} | (3,4),Ord. |
| (6) | \{\sum_{i=0}^{\infty} P_i[X]\}_{q_1 := Uq_1 q_2 [\sum_{i=0}^{\infty} P_i[X]]} | Unit. |
| (7) | \{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\} | (1) |
| (8) | \{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\}_{q_2 := Rq_2 [\sum_{i=0}^{\infty} P_i[V_iX_i^t]]} | Unit. |
| (9) | \{\sum_{i=0}^{\infty} P_1[R_i[V_iX_i^t]R_i]\} \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\} | (2),Subst. |
| (10) | \{\sum_{i=0}^{\infty} P_i[V_i^t R_i[V_iX_i^t]R_i]\}_{q_2 := Rq_2 [\sum_{i=0}^{\infty} P_i[V_iX_i^t]R_i]} | Unit. |
| (11) | \{\sum_{i=0}^{\infty} P_1[R_i[V_iX_i^t]R_i]\} \text{ call } qSearch\{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\} | (1),Subst. |
| (12) | \{\sum_{i=0}^{\infty} P_i[V_iX_i^t]\}_{q_1 := Uq_1 q_2 [\sum_{i=0}^{\infty} P_i[X+iV_iX_i^t]]} | Unit. |
| (13) | \{\sum_{i=0}^{\infty} P_i[X+iV_iX_i^t]\}_{q_2 := Rq_2 [\sum_{i=0}^{\infty} P_i[X+iV_iX_i^t]]} | (6-12),Comp. |
| (14) | \{\sum_{i=0}^{\infty} P_i[X+iV_iX_i^t]\}_{q_2 := Rq_2 [\sum_{i=0}^{\infty} P_i[X+iV_iX_i^t]]} | Tr_l |
| (15) | \{\sum_{i=0}^{\infty} P_i[X]\} S_i [\sum_{i=0}^{\infty} P_i[V_iX_i^t]] | (13,14),Ord. |
| (16) | \{0\}skip[0] | Skip |
| (17) | \{0\}S_2[0] | (16),While |
| (18) | \{0\}S_2[0] | Tr_l |
| (19) | \{0\}S_2[0] | (17,18),Ord. |
| (20) | \{\sum_{i=0}^{\infty} P_i[X]\} S_i [\sum_{i=0}^{\infty} P_i[V_iX_i^t]] | (5,15,19),If |
6 Proof system for total correctness

This section is devoted to presenting the axiom system $qTR$ for proving total correctness of recursive quantum while-programs $RPL$.

Recall the intuition of (Partial While Rule). Each program point of a while-statement is annotated with a different label, say $l_1, l_2, l_3$, and attach program points $l_1, l_2, l_3$ with assertions $R, P, Q$ respectively. We illustrate this as follows.

\[
\{l_1: R\} \text{while} \ M[q] = 1 \{l_2: Q\} \text{do} \ S \ \{l_3: P\}
\]

By Floyd-Hoare’s Principle, we have, for any input $\rho$, that

\[
tr(R\rho) \leq tr(P(M_0\rho M_1)) + tr(Q(M_1\rho M_1))
\]

\[
tr(Q(M_1\rho M_1)) \leq tr(R\llbracket S\rrbracket(M_1\rho M_1))
\]

I.e., $R \subseteq M_1'PM_0 + M_1'QM_1$ and $Q \subseteq [S]^*(R)$. We remark that $R$ can be weakened to $M_1'PM_0 + M_1'QM_1$. Then (Partial While Rule) follows by lifting such a process of reasoning to a proof rule.

To handle termination of while-statement, introduce an infinite non-decreasing sequence of assertions $\{Q_n\}_{n \geq 0}$ with $Q_0 = 0$, $Q_n \subseteq Q_{n+1}$. If program point $l_2$ is attached currently with assertion $Q_{n+1}$, then, after one iteration, the data flow at $l_2$ should be constrained by a stronger assertion, namely $Q_n$. Finally, when the loop exits, we require the data flow not enter the loop body. Thus, at that time, the assertion at $l_2$ is 0, namely $Q_0$. Putting this idea into a proof rule, we obtain (Total While Rule) for total correctness of while-statement.

\[
Q_0 = 0, Q_n \subseteq Q_{n+1}
\]

\[
\frac{\langle Q_{n+1} \rangle S\langle M_1'PM_0 + M_1'QM_1 \rangle, \text{for all } n \geq 0}{\langle M_0'PM_0 + M_1'(\bigcup_{n=0}^{n} Q_n)M_1 \rangle \text{while} \ M[q] = 1 \text{do} \ S \ \{P\}}
\]

Note that (Total While Rule) is purely syntactic: only formulas of Hoare’s triple and Löwner ordering assertions are allowed. In contrast, its counterpart in $qTD$ of Ying [32] is a mixture of syntax and semantics — (Partial While Rule) together with a semantic condition for guaranteeing termination.

We are now positioned to obtain the axiom system $qTW$, for proving total correctness of quantum while-programs $PL$, from $qPW$, by substituting $\langle P \rangle S\langle Q \rangle$ for $\langle P \rangle S\langle Q \rangle$ and by replacing (Partial While Rule) with (Total While Rule). Combining (Partial REC Rule) with the idea of handling termination, we achieve (Total REC Rule) for total correctness of simple recursive procedure $rec$ with body $S$. (The case of complex recursion is deferred to the end of this section.)

\[
P_0 = 0, P_n \subseteq P_{n+1}, \text{for all } n \geq 0
\]

\[
\frac{\text{Tr}_{\{l\}, \langle P_n \rangle \text{call rec}\langle Q \rangle \text{while} \ P_{n+1} \langle S \rangle \text{do} \ S \ \{P_n\}, \text{call rec}\langle Q \rangle}}{\langle \{l\}M[q] = 1 \text{do} \ S \ \{P_n\}, \text{call rec}\langle Q \rangle}}
\]

Then $qTR$ is obtained by adding (Total REC Rule) to $qTW$.

Since $qTW$ is properly contained in $qTR$, in the sequel, we will only show proofs for soundness and completeness of $qTR$. Let $qTT$ denote the (trivial) axiom system obtained from $qTW$ by removing (Total While Rule). The soundness of $qTR$ will be proved by reducing to that of $qTT$. 
**Theorem 6.1.** $qTR$ is sound. That is, for any quantum program $S \in RPL$ and any quantum predicate terms $P, Q$, we have

$$Tr_I \vdash qTR \langle P \rangle S \langle Q \rangle \implies \models_I \langle P \rangle S \langle Q \rangle.$$  

**Proof.** By induction on the length of proof of theorems of $qTR$. We consider cases of the last step of the proof, where the only nontrivial cases are by using (Total While Rule) or (Total REC Rule).

1. Suppose that $\langle M_0^!PM_0 + M_1^!Q_nM_1^! \rangle$ while $\langle P \rangle$ is deduced by using (Total While Rule) in the last step, where $\{Q_n\}_{n=0}^{\infty}$ is a sequence of quantum predicate terms such that $Q_0 = 0$, $Q_n \equiv Q_{n+1}$. Then we have, for all $n \geq 0$,

$$Tr_I \vdash qTR \langle Q_{n+1} \rangle S \langle M_0^!PM_0 + M_1^!Q_nM_1 \rangle.$$  

By induction hypothesis, it follows that, for all $n \geq 0$,

$$\models_I \langle Q_{n+1} \rangle S \langle M_0^!PM_0 + M_1^!Q_nM_1 \rangle.$$  

Let $D$ denote the union of $\{\langle Q_0 \rangle S; (\text{while})^0\langle P \rangle \}$ and $\{\langle Q_{n+1} \rangle S \langle M_0^!PM_0 + M_1^!Q_nM_1 \rangle : n \geq 0\}$.

**Claim 2.** For every $n \geq 0$, $Tr_I, D \vdash qTR \langle M_0^!PM_0 + M_1^!Q_nM_1 \rangle$ while $\langle \text{while} \rangle^{n+1}\langle P \rangle$.

**Proof.** By induction on $n$.

Consider the base $n = 0$. By (Skip Axiom), it follows that

$$Tr_I, D \vdash qTR \langle P \rangle \text{skip} \langle P \rangle.$$  

(4)

By definition of $D$, it’s trivial that

$$Tr_I, D \vdash qTR \langle Q_0 \rangle S; (\text{while})^0\langle P \rangle.$$  

By (If Rule), together with definition of (while)$^1$, it follows that

$$Tr_I, D \vdash qTR \langle M_0^!PM_0 + M_1^!Q_0M_1 \rangle (\text{while})^1\langle P \rangle.$$  

As the inductive step, suppose that Claim 2 holds for $n = k$. That is,

$$Tr_I, D \vdash qTR \langle M_0^!PM_0 + M_1^!Q_kM_1 \rangle (\text{while})^{k+1}\langle P \rangle.$$  

(5)

Then we have to prove that Claim 2 holds for $n = k + 1$. By definition of $D$, it follows that

$$Tr_I, D \vdash qTR \langle Q_{k+1} \rangle S \langle M_0^!PM_0 + M_1^!Q_kM_1 \rangle.$$  

By (Composition Rule), together with (5), it follows that

$$Tr_I, D \vdash qTR \langle Q_{k+1} \rangle S; (\text{while})^{k+1}\langle P \rangle.$$  

By (4) and (If Rule), together with definition of (while)$^{k+2}$, it follows that

$$Tr_I, D \vdash qTR \langle M_0^!PM_0 + M_1^!Q_{k+1}M_1 \rangle (\text{while})^{k+2}\langle P \rangle.$$  

This completes the proof for the inductive step.  

\[\square\]
Since $\models I D$, by Claim 2 jointly with soundness of $\vdash_{qTR}$, it follows that

$$\models I \langle M_0^1 P M_0 + M_1^1 Q_n M_1 \rangle \langle \text{while} \rangle^{n+1} \langle P \rangle,$$

for every $n \geq 0$. Fix $n \geq 0$. By definition of total correctness, it follows that

$$tr((M_0^1 P M_0 + M_1^1 Q_n M_1)\rho) \leq tr(P[\langle \text{while} \rangle^{n+1}]\rho),$$

for all $\rho \in \mathcal{D}(\mathcal{H})$. Let $n \to \infty$. By semantics of iteration, it follows that

$$tr((M_0^1 P M_0 + M_1^1 (\bigcup_{n=0}^{\infty} Q_n) M_1)\rho) \leq tr(P[\langle \text{while} \rangle(\rho)],$$

for all $\rho \in \mathcal{D}(\mathcal{H})$. By definition of total correctness, it follows that

$$\models I \langle M_0^1 P M_0 + M_1^1 (\bigcup_{n=0}^{\infty} Q_n) M_1 \rangle \langle \text{while} \rangle \langle P \rangle.$$

(ii) Suppose that $\langle \bigcup_{n=0}^{\infty} P_n \rangle \langle \text{call rec} \rangle$ is deduced by (Total REC Rule) in the last step, where $\{P_n\}_{n=0}^{\infty}$ is a sequence of quantum predicate terms such that $P_0 = 0$, $P_n \subseteq P_{n+1}$. Let $S$ be the body of $\text{rec}$. Then we have, for all $n \geq 0$,

$$\text{Tr}_{1}, \langle P_n \rangle \text{call rec} \langle Q \rangle \vdash_{qTR} \langle P_{n+1} \rangle \langle S \rangle \langle Q \rangle.$$

Let $D_n$ denote the set of formulas $\langle P' \rangle S' \langle Q' \rangle$ occurring in the above proof of $\langle P_{n+1} \rangle S \langle Q \rangle$, $S'$ containing no occurrence of $\text{call rec}$. Let $D = \{\langle P_0 \rangle S(0) \langle Q \rangle\} \cup (\bigcup_{n=0}^{\infty} D_n)$. By induction hypothesis, it follows that $\models I D_n$. Then $\models I D$ follows. As with Claim 3 we obtain:

**Claim 3.** For every $n \geq 0$, $\text{Tr}_{1}, D \vdash_{qTT} \langle P_n \rangle S^{(n)} \langle Q \rangle$.

Since $\models I D$, by Claim 3 together with soundness of $\vdash_{qTT}$, it follows that

$$\models I \langle P_n \rangle S^{(n)} \langle Q \rangle,$$

for every $n \geq 0$. Fix $n \geq 0$. By definition of total correctness, it follows that

$$tr(P_n \rho) \leq tr(Q[\langle S^{(n)} \rangle](\rho)),$$

for all $\rho \in \mathcal{D}(\mathcal{H})$. Let $n \to \infty$. By semantics of recursion, it follows that

$$tr((\bigcup_{n=0}^{\infty} P_n)\rho) \leq tr(Q[\langle \text{call rec} \rangle](\rho)),$$

for all $\rho \in \mathcal{D}(\mathcal{H})$. By definition of total correctness, it follows that

$$\models I (\bigcup_{n=0}^{\infty} P_n) \langle \text{call rec} \rangle \langle Q \rangle.$$

And we are done.

**Theorem 6.2.** $qTR$ is complete; That is, for any quantum program $S \in \text{RPL}$ and any quantum predicate terms $P, Q$, we have

$$\models I \langle P \rangle S \langle Q \rangle \text{ implies Tr}_{1} \vdash_{qTR} \langle P \rangle S \langle Q \rangle.$$
Proof. We proceed by induction on $S$, where the nontrivial cases are for $S$ equal to $\textbf{while } M[q] = 1 \textbf{ do } S_0 \textbf{ od}$ or $\textbf{call } \text{rec}$. We consider the two cases as follows.

(a) $S = \textbf{while } M[q] = 1 \textbf{ do } S_0 \textbf{ od}$. Suppose that $\models_I \langle P \rangle \textbf{while } \langle Q \rangle$. Then we have to prove that $\text{Tr}_I \vdash_{qTR} \langle P \rangle \textbf{while } \langle Q \rangle$. Let $Q_n = \text{wp} \langle S_0 ; (\textbf{while } )^n \rangle Q$ for $n \geq 0$. It’s easy to see that $Q_0 = 0$. First, we claim that

$$\text{tr}((\text{wp} \langle \textbf{while } \rangle^{n+1} Q) \rho) = \text{tr}((M_0^1 Q M_0 + M_1^1 Q_n M_1) \rho),$$

for any $\rho \in \mathcal{D}(\mathcal{H})$. Fix $\rho \in \mathcal{D}(\mathcal{H})$. Consider $\text{tr}((\text{wp} \langle \textbf{while } \rangle^{n+1} Q) \rho)$ as “it” in the sequel: by Theorem 4.1 it is equal to

$$\text{tr}(Q[[\textbf{while } ]^{n+1}] \rho);$$

by semantics of $(\textbf{while } )^{n+1}$, it is equal to

$$\text{tr}(Q(M_0 \rho M_0^1 + [S_0 ; (\textbf{while } )^n (M_1 \rho M_1^1)]));$$

by linearity of trace function, it is equal to

$$\text{tr}(Q(M_0 \rho M_0^1)) + \text{tr}(Q([S_0 ; (\textbf{while } )^n (M_1 \rho M_1^1)]));$$

by Theorem 4.1 together with definition of $Q_n$, it is equal to

$$\text{tr}(Q(M_0 \rho M_0^1)) + \text{tr}(Q_n (M_1 \rho M_1^1));$$

by commutativity and linearity of trace function, it is equal to

$$\text{tr}((M_0^1 Q M_0 + M_1^1 Q_n M_1) \rho).$$

This proves the claim. By definition of total correctness, together with Theorem 4.1 it follows that

$$\models_I \langle Q_{n+1} \rangle S_0 \langle \text{wp} \langle \textbf{while } \rangle^{n+1} Q \rangle.$$ 

By induction hypothesis, it follows that

$$\text{Tr}_I \vdash_{qTR} \langle Q_{n+1} \rangle S_0 \langle \text{wp} \langle \textbf{while } \rangle^{n+1} Q \rangle.$$ 

By the claim, it follows that

$$\text{wp} \langle \textbf{while } \rangle^{n+1} Q \subseteq M_0^1 Q M_0 + M_1^1 Q_n M_1.$$ 

By (Order Rule), it follows that

$$\text{Tr}_I \vdash_{qTR} \langle Q_{n+1} \rangle S_0 \langle M_0^1 Q M_0 + M_1^1 Q_n M_1 \rangle.$$ 

By (Total While Rule), it follows that

$$\text{Tr}_I \vdash_{qTR} \langle M_0^1 Q M_0 + M_1^1 (\bigsqcup_{n=0}^\infty Q_n) M_1 \rangle \textbf{while } M[q] = 1 \textbf{ do } S \langle Q \rangle.$$ 

Since $\bigsqcup_{n=0}^\infty Q_n = \text{wp} \langle S_0 ; (\textbf{wp} \langle \textbf{while } \rangle) \rangle$, by the fact (cf. Prop. 7.3 in Ying [32])

$$\text{wp} \langle \textbf{while } \rangle Q = M_0^1 Q M_0 + M_1^1 (\text{wp} \langle S_0 ; (\textbf{while } \rangle) M_1),$$

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together with (Order Rule), it follows that

\[ TpI \vdash_{qTR} \langle wp. \textbf{while}.Q \rangle \textbf{while} M[q] = 1 \textbf{do} S(Q). \]

By the supposition, together with Theorem 4.1, it follows that

\[ \models_I P \subseteq wp. \textbf{while}.Q. \]

By (Order Rule), it follows that

\[ TpI \vdash_{qTR} \langle P \rangle \textbf{while} M[q] = 1 \textbf{do} S(Q). \]

(b) \( S = \textbf{call} \textbf{rec} \). Suppose that \( \models_I \langle P \rangle \textbf{call} \textbf{rec}(Q) \). Then we have to prove that \( TpI \vdash_{qTR} \langle P \rangle \textbf{call} \textbf{rec}(Q) \). Let \( S \) be the body of \( \textbf{rec} \). As in the completeness proof for partial correctness, we claim that the most general total correctness formula, namely \( \langle wp.(\textbf{call} \textbf{rec}).X \rangle \textbf{call} \textbf{rec}(X) \), where \( X \) is a fresh quantum predicate variable, satisfy that for any quantum predicate terms \( P' \) and \( Q' \) with \( \models_I \langle P' \rangle \textbf{call} \textbf{rec}(Q') \),

\[ TpI, \langle wp.(\textbf{call} \textbf{rec}).X \rangle \textbf{call} \textbf{rec}(X) \vdash_{qTW} \langle P' \rangle \textbf{call} \textbf{rec}(Q'). \]

(6) Since \( \models_I \langle P \rangle \textbf{call} \textbf{rec}(Q) \), by Assertion (6), it follows that

\[ TpI, \langle wp.(\textbf{call} \textbf{rec}).X \rangle \textbf{call} \textbf{rec}(X) \vdash_{qTW} \langle P \rangle \textbf{call} \textbf{rec}(Q). \]

To close the proof, it suffices to show that

\[ TpI \vdash_{qTR} \langle wp.(\textbf{call} \textbf{rec}).X \rangle \textbf{call} \textbf{rec}(X). \]

Since \( wp.(\textbf{call} \textbf{rec}).X = \bigcup_{n=0}^{\infty} wp.S^{(n)}.X \), together with facts \( wp.S^{(0)}.X = 0 \) and \( wp.S^{(n)}.X \subseteq wp.S^{(n+1)}.X \), by (Total REC Rule), it suffices to show that

\[ TpI, \langle wp.S^{(n)}.X \rangle \textbf{call} \textbf{rec}(X) \vdash_{qTW} \langle wp.S^{(n+1)}.X \rangle S(X), \]

for all \( n \geq 0 \).

As with Assertion (6), we claim that for any quantum predicate terms \( P' \) and \( Q' \) with \( \models_I \langle P' \rangle S^{(n)}(Q') \),

\[ TpI, \langle wp.S^{(n)}.X \rangle S^{(n)}(X) \vdash_{qTW} \langle P' \rangle S^{(n)}(Q'). \]

(7) Since \( \models_I \langle wp.S^{(n+1)}.X \rangle S^{(n+1)}(X) \), by induction hypothesis on sub-statements of \( S^{(n+1)} \) except for \( S^{(n)} \) and applying Assertion (7) to each occurrence of \( S^{(n)} \) in \( S^{(n+1)} \), it follows that

\[ TpI, \langle wp.S^{(n)}.X \rangle S^{(n)}(X) \vdash_{qTW} \langle wp.S^{(n+1)}.X \rangle S^{(n+1)}(X). \]

Observe that in the proof of \( \langle wp.S^{(n+1)}.X \rangle S^{(n+1)}(X) \), each Hoare’s triple of the form \( \langle P' \rangle S^{(n)}(Q') \) should satisfy that \( P' = wp.S^{(n)}.Q' \), and, by Assertion (7), we have

\[ TpI, \langle wp.S^{(n)}.X \rangle S^{(n)}(X) \vdash_{qTW} \langle P' \rangle S^{(n)}(Q'). \]

Replacing each occurrence of \( S^{(n)} \) by \( \textbf{call} \textbf{rec} \) in the program section of all Hoare’s triples of the above proof, it follows that

\[ TpI, \langle wp.S^{(n)}.X \rangle \textbf{call} \textbf{rec}(X) \vdash_{qTW} \langle wp.S^{(n+1)}.X \rangle S(X). \]

This closes the proof. □
We now extend the (Total REC Rule) for simple recursion to the general case. For arbitrary (simple or complex) recursive procedures `rec`, with body `S_i`, `1 ≤ i ≤ n`, the proof rule — generalized (Total REC Rule) — for their total correctness can be given, in a uniform way, by

\[
\text{for } 1 ≤ i ≤ n \text{ and } j ≥ 0, P_i^0 = 0, P_i^j ⊆ P_i^{j+1},
\]

\[
\text{Tr}_I, \{\langle P_i^j \text{call } rec_i(Q_i) : 1 ≤ i ≤ n \rangle \} ⊢_{qTR} \langle \{P_i^{j+1}S_i(Q_i) : 1 ≤ i ≤ n \} \}
\]

\[
\{\bigwedge_{i=0}^n P_i^j \text{call } rec_i(Q_i) : 1 ≤ i ≤ n \}
\]

To achieve more flexibility of finding intermediate assertions when proving total correctness of recursion, the generalized (Total REC Rule) can be released to the following version:

\[
\text{for } 1 ≤ i ≤ n \text{ and } j ≥ 0, P_i^0 = 0, P_i^j ⊆ P_i^{j+1}, Q_i^j ⊆ Q_i^{j+1},
\]

\[
\text{Tr}_I, \{\langle P_i^j \text{call } rec_i(Q_i^j) : 1 ≤ i ≤ n \rangle \} ⊢_{qTR} \langle \{P_i^{j+1}S_i(Q_i^{j+1}) : 1 ≤ i ≤ n \} \}
\]

\[
\{\bigwedge_{i=0}^n P_i^j \text{call } rec_i(Q_i^j) : 1 ≤ i ≤ n \}
\]

Soundness and completeness of the (released) generalized (Total REC Rule) can be proved similarly to the case of simple recursion.

**Example 6.1** (Total correctness of fixed-point Grover’s search). Recall from Example 5.1 that `P_i[x] ≠ |i⟩_q, i⟩ ⊗ X`. We claim that the quantum program `FGS`, on any input, always terminates with output `V_n|s⟩⟨s|V_n = (1−e^n)|t⟩⟨t|+ e^n|t⟩⟨t|`. In a formal way, the claim can be expressed as the total correctness of a Hoare’s triple:

\[
\vdash_I \langle I_{q_1} ⊗ I_{q_2}⟩ FGS \langle \sum_{i=0}^∞ P_i[V_i|s⟩⟨s|V_i']⟩.
\]

By soundness and completeness of `qTR`, it is equivalent to

\[
\text{Tr}_I ⊢_{qTR} \langle I_{q_1} ⊗ I_{q_2}⟩ FGS \langle \sum_{i=0}^∞ P_i[V_i|s⟩⟨s|V_i']⟩.
\]

The proof of this assertion is almost the same as in Example 5.1 except for proof of the following assertion

\[
\text{Tr}_I ⊢_{qTR} \langle \sum_{i=0}^∞ P_i[X] \text{call } qSearch (\sum_{i=0}^∞ P_i[V_i X V_i'])⟩.
\]

By the released version of generalized (Total REC Rule), it suffices to show, for all `j ≥ 0`, that

\[
\text{Tr}_I, \{ \text{Prem}^1_j \text{Prem}^2_j \}
\]

\[
\vdash_{qTW} \langle \sum_{i=0}^{j+1} P_i[X]S_i^j \sum_{i=0}^{j+1} P_i[V_i X V_i']⟩,
\]

illustrated in Table 1 and

\[
\text{Tr}_I, \{ \text{Prem}^1_j \text{Prem}^2_j \}
\]

\[
\vdash_{qTW} \langle \sum_{i=0}^{j+1} P_i[X]S_i^j \sum_{i=0}^{j+1} P_i[V_i X V_i']⟩,
\]

left as an exercise, where

\[
\text{Prem}^1_j \equiv \langle \sum_{i=0}^j P_i[X] \text{call } qSearch (\sum_{i=0}^j P_i[V_i X V_i'])⟩
\]

\[
\text{Prem}^2_j \equiv \langle \sum_{i=0}^j P_i[X] \text{call } qSearch_{-dag} (\sum_{i=0}^j P_i[V_i X V_i'])⟩
\]

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7 Conclusion

In this paper, we have introduced the mechanism of recursion into Ying’s Floyd-Hoare logic qPD \cite{10,11}, and proposed proof rules for total correctness of while-statement, partial and total correctness of recursive procedures. Such proof rules, together with Ying’s proof rule for partial correctness of while-statement, form the cornerstone of our proof systems for partial and total correctness of recursive quantum programs. In addition, soundness and completeness of these proof systems have been proved. Note that these proof systems are purely syntactic: only formulas of Hoare’s triple and Löwner ordering formulas are allowed. The separation of syntax from semantics is achieved by introducing quantum predicate terms as pre- and post-conditions of quantum Hoare’s triple, and by using Löwner ordering formulas to deal with issues of termination. We have also shown Grover’s fixed-point search algorithm as a running example. This example illustrates usefulness of our programming language and proof rules.

Table 9: Part proof for Example 5.1
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