Proof rules for purely quantum programs

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Abstract

We apply the notion of quantum predicate proposed by D’Hondt and Panangaden to analyze a purely quantum language fragment which describes the quantum part of a future quantum computer in Knill’s architecture. The denotational semantics, weakest precondition semantics, and weakest liberal precondition semantics of this language fragment are introduced. To help reasoning about quantum programs involving quantum loops, we extend proof rules for classical probabilistic programs to our purely quantum programs.

1 Introduction

The theory of quantum computing has attracted considerable research efforts in the past twenty years. Benefiting from the possibility of superposition of different states and the linearity of quantum operations, quantum computing may provide considerable speedup over its classical analogue [15, 6, 7]. The existing quantum algorithms, however, are described at a very low level: they are usually represented as quantum circuits. A few works have been done in developing quantum programming languages which identify and promote high-level abstractions. Knill [8] moved the first step by outlining a set of basic principles for writing quantum pseudo-code; while the first actual quantum programming language is due to ¨Omer [12]. After that, Sanders and Zuliani [13], Bettelli et al. [1], and Selinger [14] also proposed various quantum languages each having different features.

The standard weakest precondition calculus [4] and its probabilistic extension [11] have been successful in reasoning about the correctness and even the rigorous derivation of classical programs. This success motivates us to develop analogous tools for quantum programs. Sanders and Zuliani [13] have provided for their qGCL a stepwise refinement mechanics. The approach, however, is classical in the sense that they treated quantum programs as special cases of probabilistic programs. As a consequence, known results about probabilistic weakest precondition calculus can be applied directly to quantum programs. Indeed, Butler and Hartel [2] have used it to reason about Grover’s algorithm.

The first step towards really quantum weakest precondition calculus was made by D’Hondt and Panangaden [3]. They proposed the brilliant idea that we can treat an observable, mathematically described by a Hermitian matrix, as the quantum analogue of ‘predicate’. The elegant duality between state-transformer semantics and the weakest precondition semantics of quantum programs was then proven to hold in a more direct way.

In this paper, we apply the ideas in [3] to analyze a purely quantum language fragment describing the quantum part of a potential quantum computer in Knill’s architecture [8]. The syntax follows Selinger’s style but we consider only purely quantum data. We introduce the denotational semantics...
for this purely quantum language fragment, which are represented by super-operators. The weakest precondition semantics corresponding to total correctness and weakest liberal precondition semantics corresponding to partial correctness are also introduced. To help reasoning about quantum loops, we also extend proof rules for classical probabilistic programs to our purely quantum programs.

2 Preliminaries

In this section, we review some notions and results from [3] which are the basis of our work.

Let $\mathcal{H}$ be the associated Hilbert space of the quantum system we are concerned with, and $L(\mathcal{H})$ the set of linear operators (or complex matrices, we do not distinguish between these two notions) on $\mathcal{H}$. Let $D\mathcal{H}$ be the set of all density operators on $\mathcal{H}$, that is,

$$D\mathcal{H} := \{ \rho \in L(\mathcal{H}) | \mathbf{0} \sqsubseteq \rho, \text{Tr}(\rho) \leq 1 \},$$

where $\mathbf{0}$ denotes the zero operator. The convention of allowing the trace of a density matrix to be less than 1 makes it possible to represent both the actual state (by the normalized density matrix) and the probability with which the state is reached (by the trace of the density matrix) [14]. The partial order $\sqsubseteq$ is defined on the set of all matrices with the same dimension by letting $M \sqsubseteq N$ if $N - M$ is positive. Then the set of quantum programs over $\mathcal{H}$ is defined as

$$Q\mathcal{H} := \{ \mathcal{E} \in D\mathcal{H} \rightarrow D\mathcal{H} | \mathcal{E} \text{ is a super-operator} \}.$$ 

We lift the partial order in $D\mathcal{H}$ to the one in $Q\mathcal{H}$ by letting $\mathcal{E} \sqsubseteq \mathcal{F}$ if $\mathcal{E}(\rho) \sqsubseteq \mathcal{F}(\rho)$ for any $\rho \in D\mathcal{H}$. It is proved in [3] that the two sets $D\mathcal{H}$ and $Q\mathcal{H}$ are both CPOs.

In D’Hondt and Panangaden’s approach, a quantum predicate is described by a Hermitian positive matrix with the maximum eigenvalue bounded by 1. To be specific, the set of quantum predicates on Hilbert space $\mathcal{H}$ is defined by

$$P\mathcal{H} := \{ M \in L(\mathcal{H}) | M^\dagger = M, \mathbf{0} \sqsubseteq M \sqsubseteq \mathbf{I} \}.$$ 

For any $\rho \in D\mathcal{H}$ and $M \in P\mathcal{H}$, the degree of $\rho$ satisfying $M$ is denoted by the expression $\text{Tr} M \rho$. It is exactly the expectation of the outcomes when performing a measurement represented by $M$ on the state $\rho$.

The ‘healthy’ predicate transformers which exactly characterize all valid quantum programs are proved to be those who are linear and completely positive [3]. That is, there exists an isomorphic map between the set of healthy quantum predicate transformers

$$T\mathcal{H} := \{ T \in P\mathcal{H} \rightarrow P\mathcal{H} | T \text{ is linear and completely positive} \}$$

and the set of quantum programs $Q\mathcal{H}$ defined above, just as the cases for classical standard [4] and probabilistic programs [11].

3 The purely quantum language fragment and its semantics

In this section, we concentrate our attention on the purely quantum fragment of a general programming language. That is, only quantum data but no classical data are considered. Following Knill’s QRAM model [8], a quantum computer in the future possibly consists of a general-purpose classical computer which controls a special quantum hardware device. The quantum device contains a large, but finite number of individually addressable quantum bits. The classical controller communicates with the quantum device by sending a sequence of control instructions and receiving the results of the measurements on quantum bits. Our purely quantum language considered here then aims at
describing the action of the special quantum device, rather than the behavior of the whole computer including the classical controller.

Suppose \( S, S_0 \) and \( S_1 \) denote purely quantum programs, \( q_1, \ldots, q_n \) and \( q \) denote qubit-typed variables, and \( U \) denotes a unitary transformation which applies on a \( 2^n \)-dimensional Hilbert space.

The syntax of our purely quantum language is defined as follows:

\[
S ::= \text{abort} \mid \text{skip} \mid q := 0 \mid q_1, q_2, \ldots, q_n \ast = U \mid S_0; S_1 \mid \text{measure } q \text{ then } S_0 \text{ else } S_1 \mid \text{while } q \text{ do } S.
\]

Here we borrow the notations from [14] except for the loop statements in which loop conditions are also purely quantum. Intuitively, the statement \( q := 0 \) initializes qubit \( q \) by setting it to the standard state \( |0\rangle \). Note that it is the only assignment in the language. This is also why our language is functional rather than imperative. The statement \( q_1, q_2, \ldots, q_n \ast = U \) applies the unitary transformation \( U \) on \( n \) distinct qubits \( q_1, q_2, \ldots, q_n \). We put the constraint that \( q_1, q_2, \ldots, q_n \) must be distinct to avoid syntactically some no-go operations such as quantum cloning. The statement \( \text{measure } q \text{ then } S_0 \text{ else } S_1 \) first applies a measurement on qubit \( q \), then executes \( S_0 \) or \( S_1 \) depending on whether the measurement result is 0 or 1. The loop statement \( \text{while } q \text{ do } S \) measures qubit \( q \) first. If the result is 1, then it terminates; otherwise it executes \( S \) and the loop repeats.

Formally, we have the following denotational semantics:

**Definition 3.1** For any purely quantum program \( S \), the denotational semantics of \( S \) is a map \([S]\) from \( \mathcal{DH} \) to \( \mathcal{DH} \) defined inductively in Figure 1, where \((\text{while } q \text{ do } S) \downarrow = \text{abort} \) and

\[
(\text{while } q \text{ do } S)^{i+1} := \text{measure } q \text{ then } S; (\text{while } q \text{ do } S)^i \text{ else skip}.
\]

In Definition 3.1, \( \bar{q} \) denotes the abbreviation of \( q_1, \ldots, q_n \), \( U_{\bar{q}} \) means applying \( U \) on the Hilbert space spanned by qubits \( \bar{q} \), and \( |0\rangle_q (0)_{\bar{q}} |0\rangle_q (0) \) denotes the application \( |0\rangle_q (0) \bullet |0\rangle_q (0) \) on qubit \( q \) when the initial state is \( \rho \), leaving other qubits unchanged. That is,

\[
|0\rangle_q (0)_{\bar{q}} |0\rangle_q (0) = (I_{\mathcal{H}_1} \otimes |0\rangle_q (0) \otimes I_{\mathcal{H}_2}) \rho (I_{\mathcal{H}_1} \otimes |0\rangle_q (0) \otimes I_{\mathcal{H}_2})
\]

for some appropriate Hilbert spaces \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \). In Section 4, we often omit the subscript \( q \) for simplicity when no confusion arises.

The following lemma shows that the denotational semantics of our purely quantum programs are all super-operators. So they can be physically implemented in a future quantum computer.
Lemma 3.2 For any purely quantum program $S$, the denotational semantics of $S$ is a super-operator on $\mathcal{D}H$, i.e., $[S] \in QH$.

Proof. We prove the theorem by induction on the structure of $S$. When $S$ has the form other than quantum loop, the proof is straightforward. So in what follows, we assume $S \equiv \text{while } q \text{ do } S'$ and $[S'] \in QH$ for induction hypothesis.

To prove $[S] \in QH$, we need only to show that for any $i \geq 0$,

$$\llbracket (\text{while } q \text{ do } S)^i \rrbracket \in QH \tag{1}$$

and

$$\llbracket (\text{while } q \text{ do } S)^i \rrbracket \subseteq \llbracket (\text{while } q \text{ do } S)^{i+1} \rrbracket. \tag{2}$$

Eq.(1) is easy to prove by induction on $i$. To prove Eq.(2), notice first that for any $\rho \in \mathcal{D}H$, $[\text{abort}]_\rho = 0$ is the bottom element of $\mathcal{D}H$. So $[\text{abort}]_\rho$ is the bottom element of $QH$ and then Eq.(2) holds trivially for the case $i = 0$. Suppose further Eq.(2) holds for $i = k$. Then we calculate that for any $\rho \in \mathcal{D}H$,

$$\llbracket (\text{while } q \text{ do } S)^{k+1} \rrbracket_\rho = \llbracket (\text{while } q \text{ do } S)^k \rrbracket_\rho ([S]([0](0)(0),|0\rangle\langle 0)\rho,|0\rangle\langle 0]) + |1\rangle_q\langle 1|_q|1\rangle_1\langle 1|_1$$

by definition

$$\subseteq \llbracket (\text{while } q \text{ do } S)^{k-1} \rrbracket_\rho ([S]([0](0)(0),|0\rangle\langle 0)\rho,|0\rangle\langle 0]) + |1\rangle_q\langle 1|_q|1\rangle_1\langle 1|_1$$

induction hypothesis

$$= \llbracket (\text{while } q \text{ do } S)^k \rrbracket_\rho.$$

by definition

Finally, from the fact that $QH$ is a CPO we have $[S] \in QH$. \hfill \Box

Note that the syntax of the language we consider does not provide the power to create new qubits. So by our purely quantum programs we cannot implement all super-operators on $\mathcal{D}H$ since in general to realize a super-operator we need to introduce some auxiliary qubits. It seems to be a bad news. In practice, however, the number of qubits a quantum program can use is restricted by the maximum a real quantum computer can provide. The domain of the semantics of our purely quantum programs is the Hilbert space associated with the quantum device as a whole, so they indeed include all real operations we can perform on a quantum computer.

Following the idea of quantum predicate presented in [3], we define the weakest precondition semantics of our purely quantum programs as follows:

Definition 3.3 For any purely quantum program $S$, the weakest precondition semantics of $S$ is defined by a map $wp.S$ from $PH$ to $\mathcal{P}H$ defined inductively in Figure 2, where $(\text{while } q \text{ do } S)^i$ is defined in Definition 3.1.

An alternative definition of $wp.(\text{while } q \text{ do } S).M$ is the least fixed point $\mu X.(|0\rangle_q(0)wp.S.X|0\rangle_q(0) + |1\rangle_q(1)M|1\rangle_q(1))$. It is easy to check that these two definitions are equivalent.

The following theorem shows a quantitative relation between denotational semantics and weakest precondition semantics. Intuitively, the expectation of observing any quantum predicate on the output of a quantum program is equal to the expectation of observing the weakest precondition of this predicate on the input state.

Theorem 3.4 For any purely quantum program $S$, quantum predicate $M \in PH$, and $\rho \in DH$, we have

$$\text{Tr}(wp.S.M)_\rho = \text{Tr}M[S]_\rho \tag{3}$$

Proof. We need only to consider the case that $S \equiv \text{while } q \text{ do } S'$ is a quantum loop. Other cases are easy to check.
Suppose Eq. (3) holds for the program $S'$, i.e.,

$$
\forall M \in \mathcal{PH}; \rho \in \mathcal{DH} \cdot \text{Tr}(wp.S'.M)\rho = \text{Tr}M[S']\rho.
$$

(4)

We first prove by induction that for any $i \geq 0$

$$
\forall M \in \mathcal{PH}; \rho \in \mathcal{DH} \cdot \text{Tr}(wp.S'.M)\rho = \text{Tr}M[S^i]\rho.
$$

(5)

When $i = 0$, Eq. (5) holds because both sides equal to 0. Suppose now that Eq. (5) holds for $i = k$. Then when $i = k + 1$, we calculate that for any $M \in \mathcal{PH}$ and $\rho \in \mathcal{DH}$,

$$
\text{Tr}(wp.S^{k+1}.M)\rho
= \text{Tr}([0]_q \langle 0|wp.S'.(wp.S^k.M)|0\rangle_q\langle 0| + [1]_q\langle 1|M|1\rangle_q\langle 1|)\rho
= \text{Tr}(wp.S'.(wp.S^k.M)|0\rangle_q\langle 0|\rho) + \text{Tr}M[1]_q\langle 1|\rho\rangle_q\langle 1| + \text{Tr}M[1]_q\langle 1|\rho\rangle_q\langle 1|)
= \text{Tr}M[S^k][S^k]\rho + \text{Tr}M[1]_q\langle 1|\rho\rangle_q\langle 1|)\rho
= \text{Tr}M[S^{k+1}]\rho.
$$

So we deduce that Eq. (5) holds for any $i \geq 0$. And then

$$
\text{Tr}(wp.S.M)\rho = \text{Tr}(\sqcup_i wp.S^i.M)\rho
= \sqcup_i \text{Tr}(wp.S^i.M)\rho
= \sqcup_i \text{Tr}M[S^i]\rho
= \text{Tr}M\sqcup_i [S]\rho
= \text{Tr}M[S]\rho.
$$

That completes our proof.

Taking $M = I$ in Eq. (3), we have

$$
\text{Tr}(wp.S.I)\rho = \text{Tr}[S]\rho.
$$

Notice that the righthand side of the above equation denotes the probability the (un-normalized) output state $[S]\rho$ is reached. So intuitively, for any purely quantum program $S$, the quantum
We have so far defined the weakest precondition semantics, which is useful when we consider the total correctness of quantum programs. That is, what we care is not only the correctness of the final state when the program terminates, but also the condition and the probability a quantum program can terminate. To deal with partial correctness of quantum programs, we introduce the notion of weakest liberal precondition semantics as follows:

**Definition 3.5** For any purely quantum program $S$, the weakest liberal precondition semantics of $S$ is defined by a map $wlp.S$ from $\mathcal{PH}$ to $\mathcal{PH}$ defined inductively in Figure 3, where $(\text{while } q \text{ do } S)_i$ is defined in Definition 3.1.

Analogous with weakest precondition semantics, an alternative definition of $\text{wlp. (while } q \text{ do } S)_i.M$ is the greatest fixed point $\nu X \cdot (|0\rangle_q\langle 0| wlp.S.X |0\rangle_q\langle 0| + |1\rangle_q\langle 0| M |0\rangle_q\langle 1|)$. The following theorem shows a quantitative connection between denotational semantics and weakest liberal precondition semantics.

**Theorem 3.6** For any purely quantum program $S$, quantum predicate $M \in \mathcal{PH}$, and $\rho \in \mathcal{DH}$, we have

$$\text{Tr}(wlp.S.M)\rho = \text{Tr}M[S]\rho + \text{Tr}\rho - \text{Tr}[S]\rho.$$  \hfill (6)

**Proof.** Similar to Theorem 3.4. \hfill $\Box$

Taking $M = 0$ in Eq.(6), we have

$$\text{Tr}(wlp.S.0)\rho = \text{Tr}\rho - \text{Tr}[S]\rho.$$  

Notice that the righthand side of the above equation denotes the probability the program $S$ does not terminate when the input state is $\rho$. So intuitively the quantum predicate $wlp.S.0$ denotes the condition the program $S$ diverges.

**Corollary 3.7** For any purely quantum program $S$ and quantum predicate $M \in \mathcal{PH}$,

$$wp.S.M \sqsubseteq wlp.S.M$$

and

$$wlp.S.M + wp.S.(I - M) = I$$
To get a clearer picture of the connection between these two precondition semantics, let us introduce a notion which is the analogue of conjunction $\land$ of classical standard predicates and probabilistic conjunction $\&$ of classical probabilistic predicates (see, for example, [10]).

**Definition 3.8** Suppose $M$ and $N$ are two quantum predicate. We define $M \& N$ as a new predicate $M \& N := (M + N - I)^+$, where for any Hermitian matrix $X$, if $X = \sum \lambda_i P_i$ is the spectrum decomposition of $X$, then $X^+ = \sum \max\{\lambda_i, 0\} P_i$. It is obvious that if $M + N \supseteq I$, then $M \& N = M + N - I$.

**Theorem 3.9** For any quantum predicates $M, N \in \mathcal{PH}$ and any purely quantum program $S$, if $M + N \supseteq I$ then

$$wp.S(M \& N) = wp.S.M \& wlp.S.N \quad (7)$$

and

$$wlp.S(M \& N) = wlp.S.M \& wlp.S.N \quad (8)$$

**Proof.** We only prove Eq.(7); the proof of Eq.(8) is similar. From the assumption that $M + N \supseteq I$, we have $M \& N = M + N - I$. Then for any $\rho : \mathcal{DH}$,

$$Trwp.S.(M \& N)\rho = Trwp.S.(M + N - I)\rho$$
$$= Tr(M + N - I)[S]\rho \quad \text{Theorem 3.4}$$
$$= TrM[S]\rho + TrN[S]\rho - Tr[S]\rho$$
$$= Trwp.S.M\rho + Trwlp.S.N\rho - Tr\rho \quad \text{Theorems 3.4 and 3.6}$$
$$= Tr(wp.S.M + wlp.S.N - I)\rho$$

So we have $wp.S.(M \& N) = wp.S.M + wlp.S.N - I$ and then $wp.S.(M \& N) = wp.S.M \& wlp.S.N$ from the fact that $wp.S.(M \& N) \supseteq 0$. $\square$

When taking $N = I$ in Eq.(7), we have the following direct but useful corollary:

**Corollary 3.10** For any purely quantum program $S$ and quantum predicate $M$,

$$wp.S.M = wp.S.I \& wlp.S.M \quad (9)$$

Recall that $wp.S.I$ denotes the condition the program $S$ terminates. So the intuitive meaning of Eq.(9) is that a program is total correct (represented by weakest precondition semantics) if and only if it is partial correct (represented by weakest liberal precondition semantics) and it terminates. This capture exactly the intuition of total correctness and partial correctness.

To conclude this section, we present some properties of weakest liberal precondition semantics which are useful in the next section. The proofs are direct so we omit the details here.

**Lemma 3.11** For any purely quantum program $S$ and quantum predicate $M, N \in \mathcal{PH}$, we have

1) $wlp.S.I = I$;
2) (monotonicity) if $M \subseteq N$ then $wlp.S.M \subseteq wlp.S.N$;
3) if $M + N \subseteq I$ then $wlp.S.(M + N) = wp.S.M + wlp.S.N$;
4) if $M \supseteq N$ then $wlp.S.(M - N) = wp.S.M - wp.S.N$. 

7
4 Proof rules for quantum loops

Proof rules for programs are important on the way to designing more general refinement techniques for programming. In this section, we derive some rules for reasoning about loops in our purely quantum language fragment. We find that almost all loop rules derived in classical probabilistic programming (see, for example, [10] or [9]) can be extended to quantum case.

In classical standard or probabilistic programming languages, an appropriate invariant is the key to reasoning about loops. It is also true in quantum case. So our first theorem is devoted to reasoning about quantum loops within partial correctness setting using $wlp$-invariants. Recall that in classical probabilistic programming, if $Inv$ is a $wlp$-invariant of a loop statement $loop \equiv \text{"while } b \text{ do } S\text{"}$ satisfying

$$[b] * Inv \Rightarrow wlp.S.Inv,$$

then

$$Inv \Rightarrow wlp.loop.([b] * Inv).$$

Here $\Rightarrow$ means “everywhere no more than”, which is the probabilistic analogue of the implication relation “$\Rightarrow$" in standard logic.

**Theorem 4.1** For any quantum predicate $M \in \mathcal{P}H$, if

$$|0\rangle\langle 0| M|0\rangle\langle 0| \sqsubseteq wlp.S.\left(\sum_{i=0}^{1}|i\rangle\langle i|M|i\rangle\langle i|\right)$$

then

$$\sum_{i=0}^{1}|i\rangle\langle i|M|i\rangle\langle i| \sqsubseteq wlp.qloop.(|1\rangle\langle 1|M|1\rangle\langle 1|).$$

Here and in what follows, by $qloop$ we denote the quantum program “while $q$ do $S$”.

**Proof.** By definition, we have

$$wlp.qloop.(|1\rangle\langle 1|M|1\rangle\langle 1|) = \bigcap_{j=0}^{\infty} M_j,$$

where $M_0 = I$ and for $j \geq 1$,

$$M_{j+1} = |0\rangle\langle 0| wlp.S.M_j|0\rangle\langle 0| + |1\rangle\langle 1|M|1\rangle\langle 1|.$$

In what follows, we prove by induction that for any $j \geq 0$,

$$\sum_{i=0}^{1}|i\rangle\langle i|M|i\rangle\langle i| \sqsubseteq M_j.$$

When $j = 0$, Eq.(11) holds trivially. Suppose Eq.(11) holds for $j = k$. Then when $j = k + 1$, we have

$$M_{k+1} = |0\rangle\langle 0| wlp.S.M_k|0\rangle\langle 0| + |1\rangle\langle 1|M|1\rangle\langle 1|$$

$$\sqsubseteq |0\rangle\langle 0| wlp.S.\left(\sum_{i=0}^{1}|i\rangle\langle i|M|i\rangle\langle i|\right)|0\rangle\langle 0| + |1\rangle\langle 1|M|1\rangle\langle 1|$$

induction hypothesis and Lemma 3.11 (2)

$$\sqsubseteq |0\rangle\langle 0| M|0\rangle\langle 0| + |1\rangle\langle 1|M|1\rangle\langle 1|.$$  Eq.(10)

With that we complete the proof of this theorem. □
We say \( \sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| \) is a \textit{wp}-invariant of \textit{qloop} if Eq. (10) holds; similarly, \( \sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| \) is a \textit{wp}-invariant of \textit{qloop} if

\[
|0\rangle \langle 0| M |0\rangle \langle 0| \subseteq \text{wp.S.} \left( \sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| \right).
\]  

We now turn to reasoning about quantum loops in total correctness setting. Following the remark behind Corollary 3.10, we give the total correctness of quantum loops by combining partial correctness with the termination condition. To simplify notations, we define

\[
T := \text{wp.qloop.I}.
\]

Intuitively, \( T \) denotes the termination condition of \textit{qloop}.

For any quantum loop, if a \textit{wp}-invariant implies the termination condition, then its partial correctness is sufficient to guarantee its total correctness, as the following lemma states.

**Lemma 4.2** For any quantum predicate \( M \in \mathcal{PH} \), if \( \sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| \) is a \textit{wp}-invariant of \textit{qloop}, \( \text{wp.S.T} \sqsubseteq T \), and

\[
\sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| \subseteq T,
\]

then

\[
\sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| \sqsubseteq \text{wp.qloop.}(|1\rangle \langle 1| M |1\rangle \langle 1|).
\]

**Proof.** Let

\[
M' := \sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| + I - T.
\]

Noticing that from definition we have \( T = |0\rangle \langle 0| \text{wp.S}.T |0\rangle \langle 0| + |1\rangle \langle 1| \), then

\[
|0\rangle \langle 0| T |0\rangle \langle 0| = |0\rangle \langle 0| \text{wp.S}.T |0\rangle \langle 0|,
\]

\[
|1\rangle \langle 1| T |1\rangle \langle 1| = |1\rangle \langle 1|
\]

and

\[
\sum_{i=0}^{1} |i\rangle \langle i| T |i\rangle \langle i| = T.
\]

Furthermore, we can check that \( M' = \sum_{i=0}^{1} |i\rangle \langle i| M' |i\rangle \langle i| \). From the assumption Eq. (13), we can easily derive \( 0 \sqsubseteq M' \subseteq I \), and \( M' \) is also a quantum predicate on \( \mathcal{H} \). We calculate

\[
\text{wp.S.} \sum_{i=0}^{1} |i\rangle \langle i| M' |i\rangle \langle i| = \text{wp.S.} \left( \sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| + I - T \right)
\]

\[
= \text{wp.S.} \left( \sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| + \text{wp.S.}(I - T) \right) \text{ Lemma 3.11 (3)}
\]

\[
= \text{wp.S.} \sum_{i=0}^{1} |i\rangle \langle i| M |i\rangle \langle i| + \text{wp.S.}(I - T) \text{ Lemma 3.11 (4)}
\]

\[
\sqsubseteq |0\rangle \langle 0| M |0\rangle \langle 0| + I - T \text{ Lemma 3.11 (1) and Eq. (12)}
\]

\[
= |0\rangle \langle 0| M |0\rangle \langle 0| + |0\rangle \langle 0| - |0\rangle \langle 0| T |0\rangle \langle 0| \text{ Eqs. (14) - (16)}
\]

\[
= |0\rangle \langle 0| M' |0\rangle \langle 0|.
\]
So \( \sum_{i=0}^{1} |i\rangle\langle i| M'|i\rangle\langle i| \) is a \(\text{wlp}\)-invariant of \(qloop\). We further calculate

\[
\sum_{i=0}^{1} |i\rangle\langle i| M|i\rangle\langle i|
= M' + T - I \quad \text{definition of } M'
\leq \text{wlp.qloop}.(|1\rangle\langle 1| M'|1\rangle\langle 1|) + T - I \quad \text{Theorem 4.1}
= \text{wlp.qloop}.(|1\rangle\langle 1| M'|1\rangle\langle 1|) \& T \quad \text{Corollary 3.7}
= \text{wp.qloop}.(|1\rangle\langle 1| M|1\rangle\langle 1|) \quad \text{Eq. (9)}
= \text{wp.qloop}.(|1\rangle\langle 1| M|1\rangle\langle 1|) \quad \text{Eq. (15)}.
\]

That completes our proof. \(\square\)

To conclude this section, we generalize the powerful 0-1 law in classical programming to quantum case. Informally, 0-1 law states that if the probability of a loop terminating from a state is at least \(p\) for some fixed \(p > 0\) (no matter how small \(p\) is), then the loop terminates with certainty when started from that state. In other words, the terminating probability is either 0 or 1 and cannot lie properly between 0 and 1.

**Lemma 4.3** For any quantum predicate \(M \in \text{PH}\), if \(\sum_{i=0}^{1} |i\rangle\langle i| M|i\rangle\langle i| \) is a \(\text{wp}\)-invariant of \(qloop\), \(wp.S.T \subseteq T\), and \(\exists 0 < p \leq 1\) such that \(p \ast \sum_{i=0}^{1} |i\rangle\langle i| M|i\rangle\langle i| \subseteq T\) then

\[
\sum_{i=0}^{1} |i\rangle\langle i| M|i\rangle\langle i| \subseteq T.
\]

**Proof.** Let \(M' := p \ast M\). Then \(\sum_{i=0}^{1} |i\rangle\langle i| M'|i\rangle\langle i| \subseteq T\) and furthermore,

\[
|0\rangle\langle 0| M'|0\rangle\langle 0| = p \ast |0\rangle\langle 0| M|0\rangle\langle 0|
\leq p \ast \text{wp.S.}(\sum_{i=0}^{1} |i\rangle\langle i| M|i\rangle\langle i|)
= \text{wp.S.}(\sum_{i=0}^{1} |i\rangle\langle i| M'|i\rangle\langle i|).
\]

So we can derive that

\[
p \ast \sum_{i=0}^{1} |i\rangle\langle i| M|i\rangle\langle i|
= \sum_{i=0}^{1} |i\rangle\langle i| M'|i\rangle\langle i|
\leq \text{wp.qloop}.(|1\rangle\langle 1| M'|1\rangle\langle 1|) \quad \text{Lemma 4.2}
= p \ast \text{wp.qloop}.(|1\rangle\langle 1| M|1\rangle\langle 1|) \quad \text{linearity of wp.qloop}
\leq p \ast \text{wp.qloop}.I \quad \text{monotonicity of wp.qloop}
= p \ast T.
\]

Dividing both sides by the positive number \(p\), we arrive at the desired result. \(\square\)

**Theorem 4.4** (0-1 law for quantum loops) If \(T\) is positive-definite and \(wp.S.T \subseteq T\), then for any quantum predicate \(M \in \text{PH}\) such that

\[
|0\rangle\langle 0| M|0\rangle\langle 0| \subseteq \text{wp.S.}(\sum_{i=0}^{1} |i\rangle\langle i| M|i\rangle\langle i|),
\]

\[
\]
we have
\[ \sum_{i=0}^{1} |i\rangle\langle i| M |i\rangle\langle i| \subseteq wp.qloop.([1|1]\langle 1|1\langle 1|.) \]

Proof. From the assumption that \( T \) is positive-definite, for any \( wp \)-invariant \( \sum_{i=0}^{1} |i\rangle\langle i| M |i\rangle\langle i| \) of \( qloop \) there exists a sufficiently small but positive \( p \) such that \( p \ast \sum_{i=0}^{1} |i\rangle\langle i| M |i\rangle\langle i| \subseteq T \). So \( \sum_{i=0}^{1} |i\rangle\langle i| M |i\rangle\langle i| \subseteq T \) from Lemma 4.3. Then the result of this theorem holds by applying Lemma 4.2.

\[ \square \]

5 Conclusion

In this paper, we applied the notion of quantum predicate proposed by D’Hondt and Panangaden in [3] to analyze a purely quantum language fragment which involves only quantum-typed variables. This language can be treated as the quantum fragment of a general programming language, describing the quantum device of a future quantum computer in Knill’s architecture. The denotational semantics of this language was introduced. We further proposed the weakest precondition semantics and weakest liberal precondition semantics, corresponding respectively to total and partial correctness of quantum programs. The connections between these three semantics were discussed. To help reasoning about quantum loops, we extended all existing proof rules for loops in classical probabilistic programs to the case of our purely quantum programs.

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