Formal Semantics of a Quantum Imperative Language

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Abstract

We introduce a simple quantum imperative language that has both classical and quantum constructs. We investigate its formal semantics by providing an operational semantics, a denotational semantics and two Hoare-style proof systems: an abstract one and a concrete one. The two proof systems are sound and relatively complete.

Programming is the core of software development, but it is also an inherently error-prone activity. The likelihood of errors will even be significantly higher when programming with a quantum computer, as the techniques used for classical programming are, unfortunately, hard to apply to quantum computers because quantum systems are essentially different from classical ones. Thus, there is a pressing need to provide verification and analysis techniques for reasoning about the correctness of quantum programs. Furthermore, these techniques would also be very useful for compiling and optimising quantum programs.

Among other techniques, Hoare logic [11] provides a syntax-oriented proof system to reason about program correctness. After decades of development, Hoare logic has been successfully applied in analysis of programs with non-determinism, recursion, parallel execution, etc [2, 1]. It was also extended to programming languages with probabilistic features. Remarkably, as the program states for probabilistic languages are (sub)distributions over evaluations of program variables, the extension naturally follows two different approaches, depending on how assertions of probabilistic states are defined. The first one takes subsets of distributions as (qualitative) assertions, similar to the non-probabilistic case, and the *satisfaction* relation between distributions and assertions is then just the ordinary membership [20, 8, 6, 4]. In contrast, the other approach takes non-negative functions on evaluations as (quantitative) assertions. Consequently, one is concerned with the *expectation* of a distribution satisfying an assertion [17, 16, 19, 13, 14].

In the past two decades, several Hoare-type logic systems for quantum programs (QHL) have been proposed, also following the two approaches as in the probabilistic setting.

Expectation-based QHLs. In the logic systems proposed in [24, 26, 27, 15] for purely quantum programs, the assertions P and Q in a Hoare triple $\{P\}S\{Q\}$ are both positive operators with the eigenvalues lying in $[0, 1]$, and such a triple is valid in the sense of total correctness if for any initial quantum state ρ, $\text{tr}(P\rho) \leq \text{tr}(Q\rho')$ where ρ' is the final state obtained by executing S on ρ, and $\text{tr}(P\rho)$ denotes the expectation/degree of ρ satisfying P (or physically, the average outcome when measuring ρ according to the projective measurement determined by P). This definition captures the idea that the precondition P (on the initial state) provides a lower bound on the degree of satisfaction of the postcondition Q (on the finial state). More recently, this type of expectation-based QHL has been extended to quantum programs with classical variables [10] as well as distributed quantum programs with classical communication [9]. These logic systems have proven to be useful in describing and verifying correctness of a wide range of quantum algorithms such as Grover's algorithm, Shor's algorithm, etc. Moreover, they are theoretically elegant: all of these system are (relatively) complete in the sense that every semantically valid Hoare triple can be deduced from the corresponding proof system.

Limit of the expectation-based approach. However, the expectation-based quantum Hoare logic systems proposed in the literature all suffer from the following *expressiveness* problems.

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- Unlike the classical boolean-valued assertions, the positive operator assertions cannot exclude undesirable quantum inputs. Note that the correctness of many algorithms such as quantum teleportation (an EPR pair is assumed as part of the input) and phase estimation (the corresponding eigenstate is given) all have some restriction on the input. The expressiveness of expectation-based QHL might be limited, as the following artificial example suggests. Let

$$S \equiv x := M_\pm[q]$$

where $M_\pm$ is the measurement according to the $|\pm\rangle$ basis. Obviously, starting with $|0\rangle$, the program ends at $|+\rangle$ with probability 0.5. However, expectation-based QHL cannot describe this property: the natural candidate

$$\{0.5|0\rangle\langle 0|\} \; S \; \{|+\rangle\langle +|\} \tag{1}$$

is actually not valid. The reason is, it somehow *over-specifies* the correctness: in addition to the above desirable property, it also puts certain requirement for *all other* possible input states. To see this, take $\rho = |-\rangle\langle -|$. Then $[\![S]\!](\rho) = |-\rangle\langle -|$. Thus

$$\mathrm{tr}(0.5|0\rangle\langle 0|\rho) = 0.25 > \mathrm{tr}(|+\rangle\langle +|[\![S]\!](\rho)) = 0,$$

making the Hoare triple in Eq. (1) invalid.

- As logic operations such as conjunction and disjunction are difficult, if at all possible, to define for positive operators, complicated properties can only be analysed separately, making the verification process cumbersome. This has been pointed out in [3] for expectation-based probabilistic Hoare logics. The same is obviously true for expectation-based QHLs as well.

Satisfaction-based QHLs. An Ensemble Exogenous Quantum Propositional Logic (EEQPL) was proposed in [7] for a simple quantum language with bounded iteration. The assertions in EEQPL can access amplitudes of quantum states, which makes it very strong in expressiveness but also hinders its use in applications such as debugging, as amplitudes are not physically accessible through measurements. The completeness of EEQPL is only proven in a special case where all real and complex values involved range over a finite set. In contrast, the QHL proposed in [12] takes as the assertion language an extended first-order logic with the primitives of applying a matrix on a set of qubits and computing the probability that a classical predicate is satisfied by the outcome of a quantum measurement. The proof system is shown to be sound, but no completeness result was established.

Another way of defining satisfaction-based QHLs proposed in [28, 21] regard subspaces of the Hilbert space as assertions, and a quantum state ρ satisfies an assertion P iff the support (the image space of linear operators) of ρ is included in P. The subspace assertion makes it easy to describe and determine properties of quantum programs, but the expressive power of the assertions is limited: they only assert if a given quantum state lies completely within a subspace. Consequently, quantum algorithms which succeed with certain probability cannot be verified in their logic systems.

Contribution of the current paper. In this paper, motivated by [3], we propose two Hoare-style proof systems: an abstract one and a concrete one, and prove that they are both sound and relatively complete. It is worth noting that the imperative language we consider here involves both classical and quantum constructs. Our work distinguishes itself from the works on QHLs mentioned above in the following aspects:

- *Assertion language.* The assertions used in our logic systems are boolean-typed, so that they can be easily combined using logic operations such as disjunction and conjunction. On the other hand, all information used in the assertions are physically accessible: they can be obtained through quantum measurement applying on the program states.

- *Satisfaction-based complete QHL.* The existing satisfaction-based QHLs proposed in the literature all lack of completeness; the only exception is [28] but as mention above, the assertions there are not expressive enough to verify probabilistic correctness.

1 Preliminaries

We briefly recall some basic notations from linear algebra and quantum mechanics which are needed in this paper. For more details, we refer to [18].

A *Hilbert space* $\mathcal{H}$ is a complete vector space with an inner product $\langle \cdot | \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbf{C}$ such that

1. $\langle \psi | \psi \rangle \geq 0$ for any $|\psi\rangle \in \mathcal{H}$, with equality if and only if $|\psi\rangle = 0$;

2. $\langle \varphi | \psi \rangle = \langle \psi | \varphi \rangle^*$;

3. $\langle \varphi | \sum_i c_i | \psi_i \rangle = \sum_i c_i \langle \varphi | \psi_i \rangle$,

where $\mathbf{C}$ is the set of complex numbers, and for each $c \in \mathbf{C}$, c^* stands for the complex conjugate of c. For any vector $|\psi\rangle \in \mathcal{H}$, its length $|||\psi\rangle||$ is defined to be $\sqrt{\langle \psi | \psi \rangle}$, and it is said to be *normalised* if $|||\psi\rangle|| = 1$. Two vectors $|\psi\rangle$ and $|\varphi\rangle$ are *orthogonal* if $\langle \psi | \varphi \rangle = 0$. An *orthonormal basis* of a Hilbert space $\mathcal{H}$ is a basis $\{|i\rangle\}$ where each $|i\rangle$ is normalised and any pair of them are orthogonal.

Let $\mathcal{L}(\mathcal{H})$ be the set of linear operators on $\mathcal{H}$. For any $A \in \mathcal{L}(\mathcal{H})$, A is *Hermitian* if $A^\dagger = A$ where $A^\dagger$ is the adjoint operator of A such that $\langle \psi | A^\dagger | \varphi \rangle = \langle \varphi | A | \psi \rangle^*$ for any $|\psi\rangle, |\varphi\rangle \in \mathcal{H}$. A linear operator $A \in \mathcal{L}(\mathcal{H})$ is *unitary* if $A^\dagger A = A A^\dagger = I_{\mathcal{H}}$ where $I_{\mathcal{H}}$ is the identity operator on $\mathcal{H}$. The *trace* of A is defined as $\mathrm{tr}(A) = \sum_i \langle i | A | i \rangle$ for some given orthonormal basis $\{|i\rangle\}$ of $\mathcal{H}$. A linear operator $A \in \mathcal{L}(\mathcal{H})$ is *positive* if $\langle \varphi | A | \varphi \rangle \geq 0$ for any state $|\varphi\rangle \in \mathcal{H}$. The *Löwner order* $\sqsubseteq$ on the set of Hermitian operators on $\mathcal{H}$ is defined by letting $A \sqsubseteq B$ iff $B - A$ is positive.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces. Their *tensor product* $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined as a vector space consisting of linear combinations of the vectors $|\psi_1 \psi_2\rangle = |\psi_1\rangle|\psi_2\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ with $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$. Here the tensor product of two vectors is defined by a new vector such that

$$\left(\sum_i \lambda_i |\psi_i\rangle \right) \otimes \left(\sum_j \mu_j |\varphi_j\rangle \right) = \sum_{i,j} \lambda_i \mu_j |\psi_i\rangle \otimes |\varphi_j\rangle.$$

Then $\mathcal{H}_1 \otimes \mathcal{H}_2$ is also a Hilbert space where the inner product is defined as the following: for any $|\psi_1\rangle, |\varphi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle, |\varphi_2\rangle \in \mathcal{H}_2$,

$$\langle \psi_1 \otimes \psi_2 | \varphi_1 \otimes \varphi_2 \rangle = \langle \psi_1 | \varphi_1 \rangle_{\mathcal{H}_1} \langle \psi_2 | \varphi_2 \rangle_{\mathcal{H}_2}$$

where $\langle \cdot | \cdot \rangle_{\mathcal{H}_i}$ is the inner product of $\mathcal{H}_i$.

By applying quantum gates to qubits, we can change their states. For example, the Hadamard gate (H gate) can be applied on a single qubit, while the CNOT gate can be applied on two qubits. Some commonly used gates and their representation in terms of matrices are as follows.

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

According to von Neumann's formalism of quantum mechanics [22], an isolated physical system is associated with a Hilbert space which is called the *state space* of the system. A *pure state* of a quantum system is a normalised vector in its state space, and a *mixed state* is represented by a density operator on the state space. Here a *density operator* ρ on Hilbert space $\mathcal{H}$ is a positive linear operator such that $\mathrm{tr}(\rho) = 1$. A *partial density operator* ρ is a positive linear operator with $\mathrm{tr}(\rho) \leq 1$.

The evolution of a closed quantum system is described by a unitary operator on its state space: if the states of the system at times t_1 and t_2 are ρ_1 and ρ_2, respectively, then $\rho_2 = U \rho_1 U^\dagger$ for some unitary operator U which depends only on t_1 and t_2.

A quantum *measurement* is described by a collection $\{M_m\}$ of measurement operators, where the indices m refer to the measurement outcomes. It is required that the measurement operators satisfy the completeness equation $\sum_m M_m^\dagger M_m = I_\mathcal{H}$. If the system is in state ρ, then the probability that measurement result m occurs is given by

$$p(m) = \text{tr}(M_m^\dagger M_m \rho),$$

and the state of the post-measurement system is $M_m \rho M_m^\dagger / p(m)$.

2 QIMP

We define the syntax and operational semantics of a simple quantum imperative language called **QIMP**. The language is essentially extended from **IMP** [23] by adding quantum data and a few operations for manipulating quantum data.

2.1 Syntax

We assume three types of data in our language: `Bool` for booleans, `Int` for integers, and qubits `Qbt` for quantum data. Let $\mathbb{Z}$ be the set of constant integer numbers, ranged over by n. Let **Cvar**, ranged over by $x, y, ...$, be the set of classical variables, and **Qvar**, ranged over by $q, q', ...$, the set of quantum variables. It is assumed that both **Cvar** and **Qvar** are countably infinite. We assume a set **Aexp** of arithmetic expressions over `Int`, which includes **Cvar** as a subset and is ranged over by $a, a', ...$, and a set of boolean-valued expressions **Bexp**, ranged over by $b, b', ...$, with the usual boolean constants **true**, **false** and boolean operators $\neg, \wedge, \vee$. In particular, we let $a = a'$ and $a \leq a'$ be boolean expressions for any $a, a' \in$ **Aexp**. We further assume that only classical variables can occur free in both arithmetic and boolean expressions.

We let U range over unitary operators, which can be user-defined matrices or built in if the language is implemented. For example, we often denote by H the 1-qubit Hadamard operator, $CNOT$ the controlled-NOT 2-qubit operator, etc. Similarly, we write M for the measurement described by a collection $\{M_i\}$ of measurement operators, with each index i representing a measurement outcome. For example, to describe the measurement of the qubit referred to by variable q in the computational basis, we can write $M := \{M_0, M_1\}$, where $M_0 = |0\rangle_q\langle 0|$ and $M_1 = |1\rangle_q\langle 1|$.

Sometimes we use metavariables which are primed or subscripted, e.g. x', x_0 for classical variables. We abbreviate a tuple of quantum variables $\langle q_1, ..., q_n \rangle$ as $\bar{q}$ if the length n of the tuple is not important. The formation rules for arithmetic and boolean expressions as well as commands are defined by the following grammar.

- For **Aexp**: $a ::= n \mid x \mid a_0 + a_1 \mid a_0 - a_1 \mid a_0 \times a_1$

- For **Bexp**: $b ::= \textbf{true} \mid \textbf{false} \mid a_0 = a_1 \mid a_0 \leq a_1 \mid \neg b \mid b_0 \wedge b_1 \mid b_0 \vee b_1$

- For **Com**:
$$c ::= \quad \textbf{skip} \mid x := a \mid c_0; c_1 \mid \textbf{if } b \textbf{ then } c_0 \textbf{ else } c_1 \mid \textbf{while } b \textbf{ do } c$$
$$\mid q := |0\rangle \mid U[\bar{q}] \mid x := M[\bar{q}]$$

An arithmetic expression can be an integer, a variable, or built from other arithmetic expressions by addition, substraction, or multiplication. A boolean expression can be formed by comparing arithmetic expressions or by using the usual boolean operators. A command can be a skip statement, a classical assignment, a conditional statement, or a while-loop, as in many classical imperative languages. In addition, there are three commands that involve quantum data. The command $q := |0\rangle$ initialises the qubit referrred to by variable q to be the basis state $|0\rangle$. The command $U[\bar{q}]$ applies the unitary operator U to the quantum system referred to by $\bar{q}$. The command $x := M[\bar{q}]$ performs a measurement M on $\bar{q}$ and assigns the measurement outcome to x. It differs from a classical assignment because the measurement M may change the quantum state of $\bar{q}$, besides the fact that the value of x is updated.

$$\langle x, \sigma \rangle \hookrightarrow \langle \sigma(x), \sigma \rangle$$

$$\frac{\langle a_0, \sigma \rangle \hookrightarrow \langle a_0', \sigma \rangle}{\langle a_0 + a_1, \sigma \rangle \hookrightarrow \langle a_0' + a_1, \sigma \rangle} \qquad \frac{\langle a_1, \sigma \rangle \hookrightarrow \langle a_1', \sigma \rangle}{\langle n + a_1, \sigma \rangle \hookrightarrow \langle n + a_1', \sigma \rangle}$$

$$\langle n + m, \sigma \rangle \hookrightarrow \langle p, \sigma \rangle \qquad \text{if } p \text{ is the sum of } n \text{ and } m$$

$$\frac{\langle a_0, \sigma \rangle \hookrightarrow \langle a_0', \sigma \rangle}{\langle a_0 \leq a_1, \sigma \rangle \hookrightarrow \langle a_0' \leq a_1, \sigma \rangle} \qquad \frac{\langle a_1, \sigma \rangle \hookrightarrow \langle a_1', \sigma \rangle}{\langle n \leq a_1, \sigma \rangle \hookrightarrow \langle n \leq a_1', \sigma \rangle}$$

$$\langle n \leq m, \sigma \rangle \hookrightarrow \langle \mathbf{true}, \sigma \rangle \qquad \text{if } n \text{ is less than or equal to } m.$$

$$\langle n \leq m, \sigma \rangle \hookrightarrow \langle \mathbf{false}, \sigma \rangle \qquad \text{if } n \text{ is greater than } m.$$

Figure 1: Evaluation of arithmetic and boolean expressions (selected rules)

2.2 Operational Semantics

Since the execution of a **QIMP** program may involve both classical and quantum data, we consider the setting where the CPU that processes the program has two registers: one stores classical data and the other quantum data. Therefore, we will model a machine state as a pair composed of a classical state and a quantum state.

The notion of classical state is standard. Formally, a *classical state* is a function $\sigma : \mathbf{Cvar} \to \mathbb{Z}$ from classical variables to integers. Thus $\sigma(x)$ is the value of varible x in state σ. The notion of quantum state is slightly more complicated. For each quantum variable $q \in \mathbf{Qvar}$, we assume a 2-dimensional Hilbert space $\mathcal{H}_q$ to be the state space of the q-system. For any nonempty set $V \subseteq \mathbf{Qvar}$, we denote

$$\mathcal{H}_V = \bigotimes_{q \in V} \mathcal{H}_q.$$

That is, $\mathcal{H}_V$ is the tensor product of the individual state spaces of all the quantum variables in V. In particular, $\mathcal{H} = \mathcal{H}_{\mathbf{Qvar}}$ is the state space of the whole environment consisting of all the quantum variables. The set of *quantum states* consists of all partial density operators in the space $\mathcal{H}$, denoted by $\mathcal{D}^-(\mathcal{H})$. A *machine state* is a pair $\langle \sigma, \rho \rangle$ where σ is a classical state and ρ a quantum state. In the presence of measurements, we often need to consider an ensemble of states. For that purpose, we introduce a notion of distribution.

Definition 2.1 Let Σ be the set of classical states, i.e., the set of functions of type $\mathbf{Cvar} \to \mathbb{Z}$. A *partial density operator valued distribution (POVD)* is a function $\mu : \Sigma \to \mathcal{D}^-(\mathcal{H})$ with $\sum_{\sigma \in \Sigma} \mathrm{tr}(\mu(\sigma)) \leq 1$.

Intuitively, a POVD μ represents a collection of machine states where each classical state σ is associated with a quantum state $\mu(\sigma)$. If the collection has only one element σ, we explicitly write $(\sigma, \mu(\sigma))$ for μ. The support of μ, written $\lceil \mu \rceil$, is the set $\{\sigma \in \Sigma \mid \mu(\sigma) \neq 0\}$. We can also define the addition of two distributions by letting $(\mu_1 + \mu_2)(\sigma) = \mu_1(\sigma) + \mu_2(\sigma)$.

A *configuration* is a pair $\langle e, \sigma, \rho \rangle$, where e is an expression and (σ, ρ) is a POVD. We define the small-step operational semantics of arithmetic and boolean expressions as well as commands in a syntax-directed way by using an evaluation relation $\hookrightarrow$ between configurations. In Figure 1 we list the rules for evaluating integer variables, sums, and expressions of the form $a_0 \leq a_1$; the rules for other arithmetic and boolean expressions are similar. When evaluating an arithmetic or boolean expression, we only rely on the information from the given classical state, therefore we omit the quantum state in the configuration. This is not the case when we execute commands.

Let σ be a classical state and $n \in \mathbb{Z}$. We write $\sigma[n/x]$ for the updated state satisfying

$$\sigma[n/x](y) = \begin{cases} n & \text{if } y = x, \\ \sigma(y) & \text{if } y \neq x. \end{cases}$$

$$\langle \mathbf{skip}, \sigma, \rho \rangle \rightarrow \langle \mathbf{nil}, \sigma, \rho \rangle$$

$$\frac{\langle a, \sigma \rangle \hookrightarrow \langle a', \sigma' \rangle}{\langle x := a, \sigma, \rho \rangle \rightarrow \langle x := a', \sigma', \rho \rangle} \qquad \langle x := n, \sigma, \rho \rangle \rightarrow \langle \mathbf{nil}, \sigma[n/x], \rho \rangle$$

$$\frac{\langle c_0, \sigma, \rho \rangle \rightarrow \langle c'_0, \sigma', \rho' \rangle}{\langle c_0; c_1, \sigma, \rho \rangle \rightarrow \langle c'_0; c_1, \sigma', \rho' \rangle} \qquad \frac{\langle c_1, \sigma, \rho \rangle \rightarrow \langle c'_1, \sigma', \rho' \rangle}{\langle \mathbf{nil}; c_1, \sigma, \rho \rangle \rightarrow \langle c'_1, \sigma', \rho' \rangle}$$

$$\frac{\langle b, \sigma \rangle \hookrightarrow \langle b', \sigma' \rangle}{\langle \mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1, \sigma, \rho \rangle \rightarrow \langle \mathbf{if}\ b'\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1, \sigma', \rho' \rangle}$$

$$\langle \mathbf{if\ true\ then}\ c_0\ \mathbf{else}\ c_1, \sigma, \rho \rangle \rightarrow \langle c_0, \sigma, \rho \rangle \qquad \langle \mathbf{if\ false\ then}\ c_0\ \mathbf{else}\ c_1, \sigma, \rho \rangle \rightarrow \langle c_1, \sigma, \rho \rangle$$

$$\langle \mathbf{while}\ b\ \mathbf{do}\ c, \sigma, \rho \rangle \rightarrow \langle \mathbf{if}\ b\ \mathbf{then}\ (c; \mathbf{while}\ b\ \mathbf{do}\ c)\ \mathbf{else\ skip}, \sigma, \rho \rangle$$

$$\langle q := |0\rangle, \sigma, \rho \rangle \rightarrow \langle \mathbf{nil}, \sigma, \rho' \rangle \qquad \text{with } \rho' = |0\rangle_q \langle 0|\rho|0\rangle_q \langle 0| + |0\rangle_q \langle 1|\rho|1\rangle_q \langle 0|$$

$$\langle U[\bar{q}], \sigma, \rho \rangle \rightarrow \langle \mathbf{nil}, \sigma, U\rho U^\dagger \rangle$$

$$\frac{M := \{M_i\}_{i \in I}}{\langle x := M[\bar{q}], \sigma, \rho \rangle \rightarrow \langle \mathbf{nil}, \sigma[i/x], M_i \rho M_i^\dagger \rangle}$$

Figure 2: Execution of commands

We are going to write $\rightarrow$ for the execution of commands. The transition rules are given in Figure 2. For convenience of presentation, we introduce a special command **nil** that stands for a successful termination of programs. We follow [25] to define the operational semantics of quantum measurements in a nondeterministic way, and the probabilities of different branches are encoded in the quantum part of the configurations. For that reason we need to take partial density operators instead of the normalised density operators to represent quantum states. After the measurement M defined by some measurement operators M_i, the original state (σ, ρ) may evolve into a new state whose classical part is the updated state $\sigma[i/x]$ and the quantum part is the new quantum state $M_i \rho M_i^\dagger$. In all other rules, the execution of a command changes a configuration to another one. Among them, the rules for initialising qubits and unitary transformations only affect the quantum part of the original machine state. On the contrary, the commands for manipulating classical data only update the classical part of a state.

2.3 Denotational Semantics

For convenience of presenting the denotational semantics, we add an **abort** command that halts the computation with no result. We interpret programs as POVD transformers. We write **State** for the set of machine states and **SDist(State)** for the set of POVDs called distribution states.

Lemma 2.2 We impose an order between POVDs by letting $\mu_1 \leq \mu_2$ if for any classical state σ we have $\mu_1(\sigma) \sqsubseteq \mu_2(\sigma)$, where $\sqsubseteq$ is the Löwner order. Let $(\mu_n)_{n \in \mathbb{N}} \in \mathbf{SDist(State)}$ be an increasing sequence of POVDs. This sequence converges to some POVD μ_∞ and $\mu_n \leq \mu_\infty$ for any $n \in \mathbb{N}$.

Given an expression e, we denote its interpretation with respect to machine state (σ, ρ) by $[\![e]\!]_{(\sigma, \rho)}$. The denotational semantics of commands is displayed in Figure 3, where we omit the denotational semantics of arithmetic and boolean expressions such as $[\![a]\!]_\sigma$ and $[\![b]\!]_\sigma$, which is almost the same as in the classical setting because the quantum part plays no role for those expressions. This is an extension of the semantics for probabilistic programs presented in [3]. Instead of probabilistic assignments are measurements of quantum systems. A state evolves into a POVD after some quantum qubits are measured, with the measurement outcomes assigned to a classical variable. Two other quantum commands, initialisation of qubits and unitary operations, are deterministic and only affect the quantum part of a state. As usual,

$$\begin{aligned}
[\![\mathbf{skip}]\!]_{(\sigma,\rho)} &= (\sigma,\rho) \\
[\![\mathbf{abort}]\!]_{(\sigma,\rho)} &= \varepsilon \\
[\![x := a]\!]_{(\sigma,\rho)} &= (\sigma[[\![a]\!]_\sigma/x],\rho) \\
[\![c_0; c_1]\!]_{(\sigma,\rho)} &= [\![c_1]\!]_{[\![c_0]\!]_{(\sigma,\rho)}} \\
[\![\mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1]\!]_{(\sigma,\rho)} &= \begin{cases} [\![c_0]\!]_{(\sigma,\rho)} & \text{if } [\![b]\!]_\sigma = \mathbf{true} \\ [\![c_1]\!]_{(\sigma,\rho)} & \text{if } [\![b]\!]_\sigma = \mathbf{false} \end{cases} \\
[\![\mathbf{while}\ b\ \mathbf{do}\ c]\!]_{(\sigma,\rho)} &= \lim_{n\to\infty}[\![(\mathbf{if}\ b\ \mathbf{then}\ c)^n; \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_{(\sigma,\rho)} \\
[\![q := |0\rangle]\!]_{(\sigma,\rho)} &= \langle\sigma,\rho'\rangle \\
& \quad \text{where } \rho' := |0\rangle_q\langle0|\rho|0\rangle_q\langle0| + |0\rangle_q\langle1|\rho|1\rangle_q\langle0| \\
[\![U[\bar q]]\!]_{(\sigma,\rho)} &= \langle\sigma, U\rho U^\dagger\rangle \\
[\![x := M[\bar q]]\!]_{(\sigma,\rho)} &= \mu \\
& \quad \text{where } M = \{M_i\}_{i\in I} \text{ and } \mu(\sigma') = \sum_i\{M_i\rho M_i^\dagger \mid \sigma[i/x] = \sigma'\} \\
[\![c]\!]_\mu &= \sum_{\sigma\in\lceil\mu\rceil}[\![c]\!]_{(\sigma,\mu(\sigma))}.
\end{aligned}$$

Figure 3: Denotational semantics of commands

we define the semantics of a loop ($\mathbf{while}\ b\ \mathbf{do}\ c$) as the limit of its lower approximations, where the n-th lower approximation of $[\![\mathbf{while}\ b\ \mathbf{do}\ c]\!]_{(\sigma,\rho)}$ is $[\![(\mathbf{if}\ b\ \mathbf{then}\ c)^n; \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_{(\sigma,\rho)}$, where ($\mathbf{if}\ b\ \mathbf{then}\ c$) is shorthand for ($\mathbf{if}\ b\ \mathbf{then}\ c\ \mathbf{else}\ \mathbf{skip}$) and c^n is the command c iterated n times with $c^0 \equiv \mathbf{skip}$. The limit exists because the sequence $([\![(\mathbf{if}\ b\ \mathbf{then}\ c)^n; \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_{(\sigma,\rho)})_{n\in\mathbb{N}}$ is increasing and bounded. We write ε for the special POVD whose support is the empty set.

Proposition 2.3 The semantics $[\![c]\!]_{(\sigma,\rho)}$ of a command c in initial state (σ,ρ) is a POVD. The lifted semantics $[\![c]\!]_\mu$ of a command c in initial POVD μ is a POVD.

The operational and denotational semantics are related by the following theorem.

Theorem 2.4 For any command c and state (σ,ρ), we have

$$[\![c]\!]_{(\sigma,\rho)} = \sum_i \{(\sigma_i,\rho_i) \mid \langle c,\sigma,\rho\rangle \to^* \langle\mathbf{nil},\sigma_i,\rho_i\rangle\}\ .$$

Proof: We proceed by induction on the structure of c. The most difficult case is when $c \equiv \mathbf{while}\ b\ \mathbf{do}\ c'$ for some command c'. Below we consider this case.

Let $\mathbf{While}^n = (\mathbf{if}\ b\ \mathbf{then}\ c')^n; \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}$ and $\langle c,\sigma,\rho\rangle \to^n \langle\mathbf{nil},\sigma',\rho'\rangle$ be the sequence of maximal transitions from $\langle c,\sigma,\rho\rangle$ such that the unfolding rule

$$\langle\mathbf{while}\ b\ \mathbf{do}\ c',\sigma'',\rho''\rangle \to \langle\mathbf{if}\ b\ \mathbf{then}\ (c'; \mathbf{while}\ b\ \mathbf{do}\ c')\ \mathbf{else}\ \mathbf{skip},\sigma'',\rho''\rangle\ ,$$

for any σ'' and ρ'', has been applied at most n times.

Claim:
$$[\![\mathbf{While}^n]\!]_{(\sigma,\rho)} = \sum_i\{(\sigma_i,\rho_i) \mid \langle c,\sigma,\rho\rangle \to^{n+1} \langle\mathbf{nil},\sigma_i,\rho_i\rangle\}\ .$$

We prove the above claim by induction on n.

- $n = 0$. On the left hand side, we have

$$[\![\mathbf{While}^0]\!]_{(\sigma,\rho)} = [\![\mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_{(\sigma,\rho)} = \begin{cases} \varepsilon & \text{if } [\![b]\!]_\sigma = \mathbf{true} \\ (\sigma,\rho) & \text{if } [\![b]\!]_\sigma = \mathbf{false} \end{cases}\ .$$

On the right hand side, we observe that

$$
\begin{aligned}
\langle \textbf{while } b \textbf{ do } c', \sigma, \rho \rangle \quad &\rightarrow \quad \langle \textbf{if } b \textbf{ then } (c'; \textbf{while } b \textbf{ do } c') \textbf{ else skip}, \sigma, \rho \rangle \\
&\rightarrow^* \begin{cases} \langle (c'; \textbf{while } b \textbf{ do } c'), \sigma, \rho \rangle & \text{if } \llbracket b \rrbracket_\sigma = \textbf{true} \\ \langle \textbf{skip}, \sigma, \rho \rangle & \text{if } \llbracket b \rrbracket_\sigma = \textbf{false} \end{cases}
\end{aligned}
\tag{2}
$$

The unfolding rule has been used in the first reduction step in (2). If $\llbracket b \rrbracket_\sigma = \textbf{false}$ then the claim clearly holds. If $\llbracket b \rrbracket_\sigma = \textbf{true}$ then the configuration $\langle (c'; \textbf{while } b \textbf{ do } c'), \sigma, \rho \rangle$ cannot reduce to any $\langle \textbf{nil}, \sigma'', \rho'' \rangle$ without using the unfolding rule again, which means that there is no maximal transition from $\langle c, \sigma, \rho \rangle$ that uses the unfolding rule at most once. It follows that the claim also holds in this case.

- Suppose $n = k + 1$ and the claim holds for some k. On the left hand side, we have

$$
\begin{aligned}
\llbracket \textbf{While}^{k+1} \rrbracket_{(\sigma, \rho)} \quad &= \quad \llbracket \textbf{if } b \textbf{ then } c'; \textbf{While}^{k} \rrbracket_{(\sigma, \rho)} \\
&= \begin{cases} \llbracket \textbf{While}^{k} \rrbracket_{\llbracket c' \rrbracket_{(\sigma, \rho)}} & \text{if } \llbracket b \rrbracket_\sigma = \textbf{true} \\ (\sigma, \rho) & \text{if } \llbracket b \rrbracket_\sigma = \textbf{false} \end{cases}
\end{aligned}
\tag{3}
$$

On the right hand side, we have the same transitions as in (2). If $\llbracket b \rrbracket_\sigma = \textbf{false}$ then the claim clearly holds. If $\llbracket b \rrbracket_\sigma = \textbf{true}$ then we infer as follows. Since c' is a subterm of c, we know from the hypothesis of the structural induction that

$$
\llbracket c' \rrbracket_{(\sigma, \rho)} = \sum_{j \in J} \{ (\sigma_j, \rho_j) \mid \langle c', \sigma, \rho \rangle \rightarrow^* \langle \textbf{nil}, \sigma_j, \rho_j \rangle \}
\tag{4}
$$

for some set J. It follows that

$$
\llbracket \textbf{While}^{k} \rrbracket_{\llbracket c' \rrbracket_{(\sigma, \rho)}} = \sum_{j \in J} \llbracket \textbf{While}^{k} \rrbracket_{(\sigma_j, \rho_j)} .
\tag{5}
$$

By induction hypothesis on k,

$$
\llbracket \textbf{While}^{k} \rrbracket_{(\sigma_j, \rho_j)} = \sum_{i \in I_j} \{ (\sigma_i, \rho_i) \mid \langle c, \sigma_j, \rho_j \rangle \rightarrow^{k+1} \langle \textbf{nil}, \sigma_i, \rho_i \rangle \}
\tag{6}
$$

for some index set I_j. As a result, when $\llbracket b \rrbracket_\sigma = \textbf{true}$, we have

$$
\begin{aligned}
\langle c, \sigma, \rho \rangle \quad &\rightarrow \quad \langle \textbf{if } b \textbf{ then } (c'; c) \textbf{ else skip}, \sigma, \rho \rangle \\
&\rightarrow^* \quad \langle (c'; c), \sigma, \rho \rangle \\
&\rightarrow^* \quad \langle c, \sigma_j, \rho_j \rangle \qquad \text{by (4)} \\
&\rightarrow^{k+1} \quad \langle \textbf{nil}, \sigma_i, \rho_i \rangle \qquad \text{by (6)}
\end{aligned}
\tag{7}
$$

for each $j \in J$ and $i \in I_j$. This means that

$$
\langle c, \sigma, \rho \rangle \rightarrow^{k+2} \langle \textbf{nil}, \sigma_i, \rho_i \rangle
\tag{8}
$$

for each $j \in J$ and $i \in I_j$. Thus, we rewrite (6) as follows.

$$
\llbracket \textbf{While}^{k} \rrbracket_{(\sigma_j, \rho_j)} = \sum_{i \in I_j} \{ (\sigma_i, \rho_i) \mid \langle c, \sigma, \rho \rangle \rightarrow^{k+2} \langle \textbf{nil}, \sigma_i, \rho_i \rangle \}
\tag{9}
$$

Combining (3), (5) and (9), we obtain the desired result that

$$
\llbracket \textbf{While}^{k+1} \rrbracket_{(\sigma, \rho)} = \sum_{j \in J} \sum_{i \in I_j} \{ (\sigma_i, \rho_i) \mid \langle c, \sigma, \rho \rangle \rightarrow^{k+2} \langle \textbf{nil}, \sigma_i, \rho_i \rangle \}
$$

So far we have proved the claim. Then by taking the limit on both sides of the claim, we see that $\llbracket c \rrbracket_{(\sigma, \rho)} = \sum_i \{ (\sigma_i, \rho_i) \mid \langle c, \sigma, \rho \rangle \rightarrow^* \langle \textbf{nil}, \sigma_i, \rho_i \rangle \}$. $\qquad \square$

3 An Abstract Proof System

In this section, we present an abstract proof system, where assertions are arbitrary predicates on POVDs. We show that the proof system is sound and relatively complete.

Definition 3.1 The set **Assn** of assertions is defined as $\mathcal{P}(\mathbf{SDist}(\mathbf{State}))$. Each assertion P can be constructed by the following grammar.

$$P \; := \; \mathbf{1}_\mu \mid S \mid \neg P \mid P_1 \wedge P_2 \mid \square\psi \mid P_1 \oplus P_2 \mid P[f]$$

where $\mu \in \mathbf{SDist}(\mathbf{State})$, $S \subseteq \mathbf{SDist}(\mathbf{State})$, ψ is a predicate over states and f is a function from $\mathbf{SDist}(\mathbf{State})$ to $\mathbf{SDist}(\mathbf{State})$.

Here $\mathbf{1}_\mu$ is also called the characteristic function of the POVD μ, which is a predicate requiring that $\mathbf{1}_\mu$ holds on μ' if and only if $\mu' = \mu$, for any distribution state μ'. The satisfaction relation $\models$ between a POVD and an assertion is defined as follows.

$$
\begin{aligned}
\mu &\models \mathbf{1}_{\mu'} &\text{iff}\quad& \mu = \mu' \\
\mu &\models S &\text{iff}\quad& \mu \in S \\
\mu &\models \neg P &\text{iff}\quad& \text{not } \mu \models P \\
\mu &\models P_1 \wedge P_2 &\text{iff}\quad& \mu \models P_1 \wedge \mu \models P_2 \\
\mu &\models \square\psi &\text{iff}\quad& \forall \sigma.\sigma \in \lceil \mu \rceil \Rightarrow \llbracket \psi \rrbracket_\sigma = \mathbf{true} \\
\mu &\models P_1 \oplus P_2 &\text{iff}\quad& \exists \mu_1, \mu_2.\ \mu = \mu_1 + \mu_2 \wedge \mu_1 \models P_1 \wedge \mu_2 \models P_2 \\
\mu &\models P[f] &\text{iff}\quad& f(\mu) \models P
\end{aligned}
$$

Let $\llbracket P \rrbracket := \{\mu \mid \mu \models P\}$ be the semantic interpretation of assertion P. We see that boolean operations of assertions are represented by set operations. For example, we have $\llbracket \neg P \rrbracket = \mathcal{P}(\mathbf{SDist}(\mathbf{State}))\backslash\llbracket P \rrbracket$ and $\llbracket P_1 \wedge P_2 \rrbracket = \llbracket P_1 \rrbracket \cap \llbracket P_2 \rrbracket$. The predicate $\square\psi$ is lifted from a state predicate by requiring that $\square\psi$ holds on the POVD μ when ψ holds on all the states in the support of μ. For example, a particular predicate over states is a boolean expression b with $\sigma \models b$ iff $\llbracket b \rrbracket_\sigma = \mathbf{true}$. Therefore, the predicate $\square b$ holds on the POVD μ when b evalueates to be true under any state σ in the support of μ. The assertion $P_1 \oplus P_2$ holds on the POVD μ if we can split μ into the sum of two POVDs such that P_1 and P_2 hold on each of them. Lastly, $P[f]$ holds on a POVD μ only when P holds on the image of μ under f.

Definition 3.2 A sequence of assertions $(P_n)_{n\in\mathbb{N}^\infty}$ is *u-closed*, if for each increasing sequence of POVDs $(\mu_n)_{n\in\mathbb{N}}$ such that $\mu_n \models P_n$ for all $n \in \mathbb{N}$, we have $\lim_{n\to\infty}\mu_n \models P_\infty$.

Definition 3.3 A judgement is a triple in the form $\{P\}\, c\, \{P'\}$, where c is a command, P and P' are assertions. It is valid, written $\models \{P\}\, c\, \{P'\}$, if

$$\forall \mu.\ \mu \models P \; \Rightarrow \; \llbracket c \rrbracket_\mu \models P'.$$

In Figure 4 we give the rules for an abstract proof system denoted by $\mathcal{S}_a$. It extends the system in [3] with the last three rules to handle the manipulations of quantum systems. In order to show the soundness of $\mathcal{S}_a$, we need a few technical lemmas.

Lemma 3.4 Let P be an assertion and c a command. Then $\models \{P[\llbracket c \rrbracket]\}\, c\, \{P\}$.

Proof: Suppose μ is a distribution state and $\mu \models P[\llbracket c \rrbracket]$. By the definition of $P[\llbracket c \rrbracket]$, this means that $\llbracket c \rrbracket_\mu \models P$, which is the desired result. $\qquad\qquad\square$

Lemma 3.5 Let σ be a classical state, ρ_1, ρ_2 be two quantum states, and μ_1, μ_2 be two POVDs. For any command c, we have

1. $\llbracket c \rrbracket_{(\sigma, \rho_1+\rho_2)} = \llbracket c \rrbracket_{(\sigma, \rho_1)} + \llbracket c \rrbracket_{(\sigma, \rho_2)}$;

$$\frac{}{\{P\}\ \mathbf{skip}\ \{P\}}\,[\mathsf{Skip}] \qquad \frac{}{\{P\}\ \mathbf{abort}\ \{\Box\bot\}}\,[\mathsf{Abort}] \qquad \frac{}{\{P[\![x:=a]\!]\}\ x:=a\ \{P\}}\,[\mathsf{Assgn}]$$

$$\frac{\{P_0\}\ c_0\ \{P_1\}\quad \{P_1\}\ c_1\ \{P_2\}}{\{P_0\}\ c_0;c_1\ \{P_2\}}\,[\mathsf{Seq}] \qquad \frac{\{P_0\}\ c\ \{P_0'\}\quad \{P_1\}\ c\ \{P_1'\}}{\{P_0\oplus P_1\}\ c\ \{P_0'\oplus P_1'\}}\,[\mathsf{Split}]$$

$$\frac{\{P_0\wedge\Box b\}\ c_0\ \{P_0'\}\quad \{P_1\wedge\Box\neg b\}\ c_1\ \{P_1'\}}{\{(P_0\wedge\Box b)\oplus(P_1\wedge\Box\neg b)\}\ \mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1\ \{P_0'\oplus P_1'\}}\,[\mathsf{Cond}]$$

$$\frac{}{\{\bot\}\ c\ \{P\}}\,[\mathsf{Absurd}] \qquad \frac{P_0\Rightarrow P_1\quad \{P_1\}\ c\ \{P_2\}\quad P_2\Rightarrow P_3}{\{P_0\}\ c\ \{P_3\}}\,[\mathsf{Conseq}] \qquad \frac{\forall\mu.\ \{\mathbf{1}_\mu\wedge P\}\ c\ \{P'\}}{\{P\}\ c\ \{P'\}}\,[\mathsf{All}]$$

$$\frac{\mathsf{uclosed}((P_n')_{n\in\mathbb{N}\infty})\\ \forall n.\ \{P_n\}\ \mathbf{if}\ b\ \mathbf{then}\ c\ \{P_{n+1}\}\quad \forall n.\ \{P_n\}\ \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}\ \{P_n'\}}{\{P_0\}\ \mathbf{while}\ b\ \mathbf{do}\ c\ \{P_\infty'\wedge\Box\neg b\}}\,[\mathsf{While}]$$

$$\frac{}{\{P[\![q:=|0\rangle]\!]\}\ q:=|0\rangle\ \{P\}}\,[\mathsf{QInit}] \qquad \frac{}{\{P[\![U[\bar{q}]]\!]\}\ U[\bar{q}]\ \{P\}}\,[\mathsf{QUnit}]$$

$$\frac{}{\{P[\![x:=M[\bar{q}]]\!]\}\ x:=M[\bar{q}]\ \{P\}}\,[\mathsf{QMeas}]$$

Figure 4: Proof rules for $\mathcal{S}_a$

2. $[\![c]\!]_{(\mu_1+\mu_2)} = [\![c]\!]_{\mu_1} + [\![c]\!]_{\mu_2}$.

Proof: The two clauses can be proved by a simultaneous induction on the structure of command c. $\square$

Lemma 3.6 For any commands c_0, c_1 and distribution state μ, we have $[\![c_0;c_1]\!]_\mu = [\![c_1]\!]_{[\![c_0]\!]_\mu}$.

Proof:

$$
\begin{aligned}
[\![c_1]\!]_{[\![c_0]\!]_\mu} &= \sum_\sigma [\![c_1]\!]_{(\sigma,\,[\![c_0]\!]_\mu(\sigma))} \\
&= \sum_\sigma [\![c_1]\!]_{(\sigma,\,\sum_{\sigma'}[\![c_0]\!]_{(\sigma',\mu(\sigma'))}(\sigma))} \\
&= \sum_\sigma \sum_{\sigma'} [\![c_1]\!]_{(\sigma,\,[\![c_0]\!]_{(\sigma',\mu(\sigma'))}(\sigma))} \qquad \text{by Lemma 3.5(1)} \\
&= \sum_{\sigma'} \sum_\sigma [\![c_1]\!]_{(\sigma,\,[\![c_0]\!]_{(\sigma',\mu(\sigma'))}(\sigma))} \\
&= \sum_{\sigma'} [\![c_1]\!]_{[\![c_0]\!]_{(\sigma',\mu(\sigma'))}} \\
&= \sum_{\sigma'} [\![c_0;c_1]\!]_{(\sigma',\mu(\sigma'))} \\
&= [\![c_0;c_1]\!]_\mu
\end{aligned}
$$

$\square$

Theorem 3.7 [Soundness] Every judgement provable using the proof system $\mathcal{S}_a$ is valid.

Proof: We analyze the cases one by one.

- Rule [Skip]. Suppose $\mu \models P$ for some distribution state μ. Then we have $[\![\mathbf{skip}]\!]_\mu = \mu$ and thus $[\![\mathbf{skip}]\!]_\mu \models P$ as required.

- Rule [Abort]. This case is easy by noting that $[\![\mathbf{abort}]\!]_\mu = \varepsilon$ and $\varepsilon \models \Box\bot$ for any μ.

- The cases for rules [Assgn], [QInit], [QUnit], and [QMeas] follow from Lemma 3.4.

- Rule [Seq]. Suppose $\mu \models P_0$ for some distribution state μ. By the premises, both $\{P_0\}\ c_0\ \{P_1\}$ and $\{P_1\}\ c_1\ \{P_2\}$ are valid. It follows that $[\![c_0]\!]_\mu \models P_1$ and then $[\![c_1]\!]_{[\![c_0]\!]_\mu} \models P_2$, which is $[\![c_0;c_1]\!]_\mu \models P_2$ by Lemma 3.6 as required.

- Rule [Split]. Suppose $\mu \models P_0 \oplus P_1$ for some distribution state μ. Then there exist μ_0 and μ_1 such that $\mu = \mu_0 + \mu_1$, $\mu_0 \models P_0$ and $\mu_1 \models P_1$. By the premises, both $\{P_0\}\, c_0\, \{P_0'\}$ and $\{P_1\}\, c_1\, \{P_1'\}$ are valid. Therefore, we have that $[\![c]\!]_{\mu_0} \models P_0'$ and $[\![c]\!]_{\mu_1} \models P_1'$. By Lemma 3.5 we obtain $[\![c]\!]_\mu = [\![c]\!]_{\mu_0} + [\![c]\!]_{\mu_1}$. It follows that $[\![c]\!]_\mu \models P_0' \oplus P_1'$ as required.

- Rule [Cond]. We first claim that $\{P_0 \wedge \Box b\}$ **if** b **then** c_0 **else** c_1 $\{P_0'\}$ is valid. To see this, suppose μ is a POVD with $\mu \models P_0 \wedge \Box b$. Obviously, we have $\mu \models \Box b$ and thus $[\![b]\!]_\sigma = \mathbf{true}$ for each $\sigma \in \lceil \mu \rceil$. It follows that

$$
\begin{aligned}
[\![\mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1]\!]_\mu &= \sum_\sigma [\![\mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1]\!]_{(\sigma,\mu(\sigma))} \\
&= \sum_\sigma [\![c_0]\!]_{(\sigma,\mu(\sigma))} \\
&= [\![c_0]\!]_\mu.
\end{aligned}
$$

By the first premise, $\{P_0 \wedge \Box b\}\, c_0\, \{P_0'\}$ is valid. Therefore, we have $[\![c_0]\!]_\mu \models P_0'$, and thus

$$
[\![\mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1]\!]_\mu \models P_0'
$$

and the above claim is proved. Similarly, we can prove that $\{P_1 \wedge \Box \neg b\}$ **if** b **then** c_0 **else** c_1 $\{P_1'\}$ is valid. By the soundness of [Split], it follows that

$$
\{(P_0 \wedge \Box b) \oplus (P_1 \wedge \Box \neg b)\}\ \mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1\ \{P_0' \oplus P_1'\}
$$

is also valid.

- Rule [Absurd]. There exists no μ with $\mu \models \bot$. Thus, we always have $\forall \mu.\ \mu \models \bot \Rightarrow [\![c]\!]_\mu \models P$.

- Rule [Conseq]. Let μ be a distribution state and $\mu \models P_0$. The first premise gives $\mu \models P_1$. The second premise tells us that $[\![c]\!]_\mu \models P_2$. By the third premise, we derive that $[\![c]\!]_\mu \models P_3$. It follows that $\{P_0\}\, c\, \{P_3\}$ is valid.

- Rule [All]. Let μ be a POVD and $\mu \models P$. It is clear that $\mu \models \mathbf{1}_\mu \wedge P$. By the premise, $\{\mathbf{1}_\mu \wedge P\}\, c\, \{P'\}$ is valid. Therefore, we have $[\![c]\!]_\mu \models P'$, and thus $\{P\}\, c\, \{P'\}$ is valid.

- Rule [While]. We first observe that, for any state (σ, ρ),

$$
[\![\mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_{(\sigma,\rho)} = \begin{cases} \varepsilon & \text{if } [\![b]\!]_{(\sigma,\rho)} = \mathbf{true} \\ (\sigma,\rho) & \text{if } [\![b]\!]_{(\sigma,\rho)} = \mathbf{false}. \end{cases}
$$

Thus, if a state σ' is in the support of $[\![\mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_{(\sigma,\rho)}$, it must be the case that $\sigma' \models \neg b$. Furthermore, for any distribution state μ, if a state σ' is in the support of $[\![\mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_\mu$ then $\sigma' \models \neg b$. It follows that, for any command c' and distribution state μ, we have

$$
[\![c'; \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_\mu \models \Box \neg b.
$$

By definition, $[\![\mathbf{while}\ b\ \mathbf{do}\ c]\!]_\mu$ is the limit of the sequence

$$
([\![(\mathbf{if}\ b\ \mathbf{then}\ c)^n; \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_\mu)_{n \in \mathbb{N}}
$$

and so we have that

$$
[\![\mathbf{while}\ b\ \mathbf{do}\ c]\!]_\mu \models \Box \neg b. \tag{10}
$$

By the first premise and the soundness of [Seq], it is easy to show by induction that

$$
\forall n.\ \{P_0\}\ (\mathbf{if}\ b\ \mathbf{then}\ c)^n\ \{P_n\}
$$

is valid. By the second premise and [Seq] again, the following judgement

$$
\forall n.\ \{P_0\}\ (\mathbf{if}\ b\ \mathbf{then}\ c)^n; \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}\ \{P_n'\}
$$

11

is valid. Let μ be any POVD with $\mu \models P_0$. Then

$$\forall n. \, [\![(\textbf{if } b \textbf{ then } c)^n; \textbf{if } b \textbf{ then abort}]\!]_\mu \models P'_n.$$

By assumption, the sequence of assertions $(P'_n)_{n \in \mathbb{N}^\infty}$ is u-closed. Hence, we can infer that

$$[\![\textbf{while } b \textbf{ do } c]\!]_\mu \models P'_\infty,$$

which means that the jugdement

$$\{P_0\} \textbf{ while } b \textbf{ do } c \, \{P'_\infty\} \tag{11}$$

is valid. Combining (10) and (11), we finally obtain that $\{P_0\}$ **while** b **do** c $\{P'_\infty \wedge \Box \neg b\}$ is valid.

$\square$

Now we turn to the relative completeness of the proof system $\mathcal{S}_a$. Formulas of the form $\mathbf{1}_\mu$ will be helpful for that purpose.

Lemma 3.8 For any distribution state μ and command c,

$$\mathbf{1}_\mu \Rightarrow \mathbf{1}_{[\![c]\!]_\mu}[\![c]\!].$$

Proof: Let μ' be any distribution state.

$$
\begin{aligned}
\mu' \models \mathbf{1}_\mu \quad &\Leftrightarrow \quad \mu' = \mu \\
&\Rightarrow \quad [\![c]\!]_{\mu'} = [\![c]\!]_\mu \\
&\Leftrightarrow \quad [\![c]\!]_{\mu'} \models \mathbf{1}_{[\![c]\!]_\mu} \\
&\Leftrightarrow \quad \mu' \models \mathbf{1}_{[\![c]\!]_\mu}[\![c]\!]
\end{aligned}
$$

$\square$

Definition 3.9 Let μ be a distribution state and b a boolean expression. The restriction $\mu_{|b}$ of μ to b is the distribution state such that $\mu_{|b}(\sigma) = \mu(\sigma)$ if $[\![b]\!]_\sigma = \textbf{true}$ and 0 otherwise.

According to the definition above, it is easy to see that we can split any μ into two parts w.r.t. a boolean expression.

Lemma 3.10 For any distribution state μ and boolean expression b, we have $\mu = \mu_{|b} + \mu_{|\neg b}$.

Proof: This is straightforward because, at each state σ in the support of μ, the boolean expression b evaluates to either **true** or **false**. $\square$

With Lemmas 3.10 and 3.5, it is easy to see that the denotational semantics of conditional commands can be rewritten as follows.

$$[\![\textbf{if } b \textbf{ then } c_0 \textbf{ else } c_1]\!]_\mu \;=\; [\![c_0]\!]_{\mu_{|b}} + [\![c_1]\!]_{\mu_{|\neg b}} \tag{12}$$

The following facts are also easy to show.

$$
\begin{aligned}
\mathbf{1}_{\mu_{|b}} \quad &\Leftrightarrow \quad \mathbf{1}_{\mu_{|b}} \wedge \Box b \\
\mathbf{1}_\mu \quad &\Leftrightarrow \quad \mathbf{1}_\mu \wedge P \qquad \text{if } \mu \models P \\
\mathbf{1}_\mu \quad &\Leftrightarrow \quad \mathbf{1}_{\mu_{|b}} \oplus \mathbf{1}_{\mu_{|\neg b}} \\
\mathbf{1}_{\mu_1 + \mu_2} \quad &\Leftrightarrow \quad \mathbf{1}_{\mu_1} \oplus \mathbf{1}_{\mu_2}
\end{aligned}
\tag{13}
$$

Lemma 3.11 For any POVD μ, the following judgement is provable:

$$\{\mathbf{1}_\mu\} \, c \, \{\mathbf{1}_{[\![c]\!]_\mu}\}.$$

Proof: We proceed by induction on the structure of c.

- $c \equiv \mathbf{skip}$. This case is immediate as $[\![\mathbf{skip}]\!]_\mu = \mu$ and by [Skip] we have $\vdash \{\mathbf{1}_\mu\}\, c\, \{\mathbf{1}_\mu\}$.

- $c \equiv \mathbf{abort}$. Then $[\![c]\!]_\mu = \varepsilon$. For any POVD μ', we note that

$$\mu' \models \Box\bot \;\Leftrightarrow\; \mu' = \varepsilon \;\Leftrightarrow\; \mu' \models \mathbf{1}_\varepsilon.$$

  By rules [Abort] and [Conseq] we can infer $\vdash \{\mathbf{1}_\mu\}\, c\, \{\mathbf{1}_\varepsilon\}$.

- $c \equiv x := a,\ q := |0\rangle,\ U[\bar{q}]$ or $x := M[\bar{q}]$. By the corresponding rules [Assgn], [QInit], [QUnit] or [QMeas], we have

$$\vdash \{\mathbf{1}_{[\![c]\!]_\mu}[[\![c]\!]]\}\, c\, \{\mathbf{1}_{[\![c]\!]_\mu}\}.$$

  By Lemma 3.8 and rule [Conseq], we obtain that $\vdash \{\mathbf{1}_\mu\}\, c\, \{\mathbf{1}_{[\![c]\!]_\mu}\}$.

- $c \equiv c_0; c_1$. By induction, we have $\vdash \{\mathbf{1}_\mu\}\, c_0\, \{\mathbf{1}_{[\![c_0]\!]_\mu}\}$ and $\vdash \{\mathbf{1}_{[\![c_0]\!]_\mu}\}\, c_1\, \{\mathbf{1}_{[\![c_1]\!]_{[\![c_0]\!]_\mu}}\}$. Using the rule [Seq], we obtain that $\vdash \{\mathbf{1}_\mu\}\, c\, \{\mathbf{1}_{[\![c_1]\!]_{[\![c]\!]_\mu}}\}$.

- $c \equiv \mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1$. By induction, we have $\vdash \{\mathbf{1}_{\mu_{|b}}\}\, c_0\, \{\mathbf{1}_{[\![c_0]\!]_{\mu_{|b}}}\}$. By the first clause in (13) and rule [Conseq], we have $\vdash \{\mathbf{1}_{\mu_{|b}} \wedge \Box b\}\, c_0\, \{\mathbf{1}_{[\![c_0]\!]_{\mu_{|b}}}\}$. Similarly, $\vdash \{\mathbf{1}_{\mu_{|\neg b}} \wedge \Box\neg b\}\, c_1\, \{\mathbf{1}_{[\![c_1]\!]_{\mu_{|\neg b}}}\}$. Using rule [Cond], we infer

$$\vdash \{(\mathbf{1}_{\mu_{|b}} \wedge \Box b) \oplus (\mathbf{1}_{\mu_{|\neg b}} \wedge \Box\neg b)\}\ \mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1\ \{\mathbf{1}_{[\![c_0]\!]_{\mu_{|b}}} \oplus \mathbf{1}_{[\![c_1]\!]_{\mu_{|\neg b}}}\}.$$

  Using (12), (13) and rule [Conseq], we finally obtain that

$$\vdash \{\mathbf{1}_\mu\}\ \mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1\ \{\mathbf{1}_{[\![\mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1]\!]_\mu}\}.$$

- $c \equiv \mathbf{while}\ b\ \mathbf{do}\ c'$. For each $n \in \mathbb{N}$, let

$$
\begin{aligned}
P_n &= \mathbf{1}_{[\![(\mathbf{if}\ b\ \mathbf{then}\ c')^n]\!]_\mu} \\
P'_n &= \mathbf{1}_{[\![(\mathbf{if}\ b\ \mathbf{then}\ c')^n;\mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_\mu} \\
P'_\infty &= \mathbf{1}_{\lim_{n\to\infty}[\![(\mathbf{if}\ b\ \mathbf{then}\ c')^n;\mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}]\!]_\mu}
\end{aligned}
$$

  Obviously, the sequence of assertions $(P'_n)_{n\in\mathbb{N}^\infty}$ is u-closed. As in the last case, we can show that $\vdash \{P_n\}\ \mathbf{if}\ b\ \mathbf{then}\ c'\ \{P_{n+1}\}$ by induction hypothesis and rules [Conseq], [Skip] and [Cond]. It is also easy to see that $\vdash \{P_n\}\ \mathbf{if}\ b\ \mathbf{then}\ \mathbf{abort}\ \{P'_n\}$ for each $n \in \mathbb{N}$. Therefore, we can use rule [While] to infer that $\vdash \{P_0\}\ \mathbf{while}\ b\ \mathbf{do}\ c\ \{P'_\infty \wedge \Box\neg b\}$. Using (10), the second clause of (13), and rule [Conseq], we obtain that $\vdash \{P_0\}\ \mathbf{while}\ b\ \mathbf{do}\ c\ \{P'_\infty\}$, which is exactly $\vdash \{\mathbf{1}_\mu\}\ \mathbf{while}\ b\ \mathbf{do}\ c'\ \{\mathbf{1}_{[\![\mathbf{while}\ b\ \mathbf{do}\ c']\!]_\mu}\}$.

$\hfill\square$

With the preparations above, we are in the position to show that the proof system $\mathcal{S}_a$ is relatively complete.

Theorem 3.12 (Relative completeness) Every valid judgement is derivable in $\mathcal{S}_a$.

Proof: Let $\{P\}\, c\, \{P'\}$ be a valid judgement. Suppose μ be any POVD. There are two possibilities:

- $\mu \models P$. The validity of the judgement says that $[\![c]\!]_\mu \models P'$. By Lemma 3.11, we have that $\vdash \{\mathbf{1}_\mu\}\, c\, \{\mathbf{1}_{[\![c]\!]_\mu}\}$. By the second clause of (13) and rule [Conseq], we obtain $\vdash \{\mathbf{1}_\mu \wedge P\}\, c\, \{\mathbf{1}_{[\![c]\!]_\mu} \wedge P'\}$. Using [Conseq] again gives $\vdash \{\mathbf{1}_\mu \wedge P\}\, c\, \{P'\}$.

- $\mu \not\models P$. Then it is obvious that $\mathbf{1}_\mu \wedge P \Leftrightarrow \bot$. By rules [Absurd] and [Conseq], we also obtain $\vdash \{\mathbf{1}_\mu \wedge P\}\, c\, \{P'\}$.

Since μ is arbitrarily chosen, the premise of rule [All] is derivable. Therefore, we can use that rule to obtain $\vdash \{P\}\, c\, \{P'\}$. $\hfill\square$

$$
\begin{array}{llll}
e & ::= & x \mid \mathbf{1}_\psi \mid o(\mathbf{e}) & \text{(State expressions)} \\
\psi & ::= & e \bowtie e \mid FO(\psi) & \text{(State assertions)} \\
r & ::= & \mathbb{E}[e] \mid \mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e] \mid o(\mathbf{r}) & \text{(Distribution expressions)} \\
P & ::= & r \bowtie r \mid P \oplus P \mid FO(P) & \text{(Distribution assertions)} \\
\bowtie & \in & \{=, <, \leq\} \qquad o \in Ops & \text{(Operations)}
\end{array}
$$

Figure 5: Syntax of assertions

4 A Concrete Program Logic

In this section, we present a concrete program logic. We first define the concrete syntax of assertions. Following [3], we define a two-level assertion language in Figure 5. Formally, assertions are divided into two categories: *state assertions* are formulas that describe the properties of machine states and *distribution assertions* are used to describe the properties of POVDs. Distribution assertions are based on comparison of distribution expressions, or built with first-order quantifiers and connectives, as well as the connective $\oplus$ mentioned in Section 3. A *distribution expression* is either the expection $\mathbb{E}[e]$ of a state expression e, the expectation $\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]$ of state expression e w.r.t. the measurement M, or an operator applied to state expressions. A *state expression* is either a classical variable, the characteristic function $\mathbf{1}_\psi$ of a state assertion ψ, or an operator applied to state expressions. Finally, a *state assertion* is either a comparison of state expressions, or a first-order formula over state assertions.

For technical reasons, in this section we consider a general form of quantum measurement.

Definition 4.1 A *general measurement* M is a pair $\langle \{M_i\}_{i \in I}, l \rangle$, where each M_i is a measurement operator as usual, and $l : I \mapsto J$ ls a labelling function that maps each measurement outcome i to some some label $l(i)$.

If the state of a quantum system is specified by density operator ρ immediately before the measurement M, then the probability with which those results with label j occur is given by

$$
p(j) = \sum_{i:l(i)=j} \text{tr}(M_i^\dagger M_i \rho),
$$

and the state of the system after the measurement is

$$
\frac{\sum_{i:l(i)=j} M_i \rho M_i^\dagger}{p(j)}.
$$

General measurements are convenient to describe the situation where we would like to group some measurement outcomes. For example, if $i_1, i_2 \in I$ are two different outcomes, but for some reasons we would not like to distinguish them, then we simply give them the same label by letting $l(l_1) = l(l_2)$. In the special case that l is the identity funciton Id, then the labelling function has no effect and we degenerate to the usual notion of measurements.

The interpretation of assertions is given in Figure 6. Comparing the interpretation with that in [3], we see that the main difference is the introduction of a distribution expression related to a quantum measurement. The meaning of $\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]$ is the expected Hermitian operator weighted by the value of e after a measurement entailed by M.

Note that the formula $\Box \psi$, where ψ is a state assertion, can now be viewed as a syntactic sugar in view of the following lemma.

Lemma 4.2   1. $\Box \psi \Leftrightarrow \mathbb{E}[\mathbf{1}_\psi] = \mathbb{E}[\mathbf{1}_{\mathbf{true}}]$

   2. $\Box \psi \Leftrightarrow \mathbb{E}_{\bar{x} \sim M[\bar{q}]}[\mathbf{1}_\psi] = \mathbb{E}_{\bar{x} \sim M[\bar{q}]}[\mathbf{1}_{\mathbf{true}}]$

   3. $\Box \psi \Leftrightarrow \Box(\psi \wedge b) \oplus \Box(\psi \wedge \neg b)$

$$
\begin{aligned}
[\![x]\!]_\sigma &:= \sigma(x) \\
[\![\mathbf{1}_\psi]\!]_\sigma &:= \mathbf{1}_{[\![\psi]\!]_\sigma} \\
[\![o(e)]\!]_\sigma &:= o([\![e]\!]_\sigma)
\end{aligned}
$$

$$
\begin{aligned}
[\![e_1 \bowtie e_2]\!]_\sigma &:= [\![e_1]\!]_\sigma \bowtie [\![e_2]\!]_\sigma \\
[\![FO(\psi)]\!]_\sigma &:= FO([\![\psi]\!]_\sigma)
\end{aligned}
$$

$$
\begin{aligned}
[\![\mathbb{E}[e]]\!]_\mu &:= \sum_\sigma \mu(\sigma) \cdot [\![e]\!]_\sigma \\
[\![\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]]\!]_\mu &:= \sum_\sigma \sum_i M_i \mu(\sigma) M_i^\dagger \cdot [\![e]\!]_{\sigma[l(i)/\bar{x}]} \\
& \quad \text{where } M = \langle \{M_i\}_{i \in I}, l \rangle \\
[\![o(r)]\!]_\mu &:= o([\![r]\!]_\mu)
\end{aligned}
$$

$$
\begin{aligned}
[\![r_1 \bowtie r_2]\!]_\mu &:= [\![r_1]\!]_\mu \bowtie [\![r_2]\!]_\mu \\
[\![P_1 \oplus P_2]\!]_\mu &:= \exists \mu_1, \mu_2. \mu = \mu_1 + \mu_2 \wedge [\![P_1]\!]_{\mu_1} \wedge [\![P_2]\!]_{\mu_2} \\
[\![FO(P)]\!]_\mu &:= FO([\![P]\!]_\mu)
\end{aligned}
$$

Figure 6: Semantics of assertions

$$
\frac{}{\{P[a/x]\}\ x := a\ \{P\}} [\mathsf{Assgn'}] \qquad \frac{}{\{h(P)\}\ q := |0\rangle\ \{P\}} [\mathsf{QInit'}]
$$

$$
\frac{}{\{g^U(P)\}\ U[\bar{q}]\ \{P\}} [\mathsf{QUnit'}] \qquad \frac{}{\{f_{x,\bar{q}}^M(P)\}\ x := M[\bar{q}]\ \{P\}} [\mathsf{QMeas'}]
$$

Figure 7: Selected syntactic proof rules

Proof: Let us consider the first clause; the second one is similar and the third one is easier.

$$
\begin{aligned}
\mu \models \Box\psi \quad & \text{iff} \quad \forall \sigma \in \lceil \mu \rceil. [\![\psi]\!]_\sigma = \mathbf{true} \\
& \text{iff} \quad \sum_\sigma \mu(\sigma) \cdot [\![\mathbf{1}_\psi]\!]_\sigma = \sum_\sigma \mu(\sigma) \cdot [\![\mathbf{1}_{\mathbf{true}}]\!]_\sigma \\
& \text{iff} \quad [\![\mathbb{E}[\mathbf{1}_\psi]]\!]_\mu = [\![\mathbb{E}[\mathbf{1}_{\mathbf{true}}]]\!]_\mu \\
& \text{iff} \quad \mu \models (\mathbb{E}[\mathbf{1}_\psi] = \mathbb{E}[\mathbf{1}_{\mathbf{true}}])
\end{aligned}
$$

$\square$

Using the concrete syntax for assertions, we propose a syntactic version of the existing proof rules by avoiding the semantics of commands. We call the concrete proof system $\mathcal{S}_c$. Specifically, we keep all proof rules in Figure 4 but replace [Assgn], [QInit], [QUnit], and [QMeas] with the four rules in Figure 7.

In rule [QInit'] we use the notation $h(P)$ for a syntactic substitution. It changes all $\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]$ in P into $\mathbb{E}_{\bar{x} \sim M'[\bar{q}]}[e]$ and distributes over most other syntactic constructors of assertions, where M' is obtained from $M = \langle \{M_i\}_i, l \rangle$ by constructing two measurement operators M_{0i}, M_{01} for each M_i in M with the

mapping l' given by $l'(i0) = l'(i1) = l(i)$. A formal definition is given below.

$$
\begin{aligned}
h(x) &:= x \\
h(\mathbf{1}_\psi) &:= \mathbf{1}_{h(\psi)} \\
h(o(e)) &:= o(h(e)) \\
h(e_1 \bowtie e_2) &:= h(e_1) \bowtie h(e_2) \\
h(FO(\psi)) &:= FO(h(\psi)) \\
h(o(r)) &:= o(h(r)) \qquad \text{where } o \in Ops \\
h(\mathbb{E}[e]) &:= \mathbb{E}_{x \sim M[q]}[e] \qquad \text{where } M = \langle\{M_0, M_1\}, Id\rangle \text{ with } M_0 = |0\rangle\langle 0|, \ M_1 = |0\rangle\langle 1|, \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad x \text{ is fresh} \\
h(\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]) &:= \mathbb{E}_{\bar{x} \sim M'[\bar{q}]}[e] \quad \text{where } M' = \langle\{M_{i0}, M_{i1}\}_i, l'\rangle \text{ with } M_{i0} = M_i|0\rangle\langle 0|, \ M_{i1} = M_i|0\rangle\langle 1|, \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad l'(i0) = l'(i1) = l(i) \\[4pt]
h(r_1 \bowtie r_2) &:= h(r_1) \bowtie h(r_2) \\
h(FO(P)) &:= FO(h(P)) \\
h(P_1 \oplus P_2) &:= h(P_1) \oplus h(P_2)
\end{aligned}
$$

In rule [QUnit'] we use the notation $g^U(P)$ for a syntactic substitution. It changes all $\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]$ in P into $\mathbb{E}_{\bar{x} \sim M'[\bar{q}]}[e]$, where $M = \langle\{M_i\}_{i \in I}, l\rangle$, $M' = \langle\{M_i U\}_{i \in I}, l\rangle$, and distributes over most other syntactic constructors of assertions. A formal definition is given below.

$$
\begin{aligned}
g^U(x) &:= x \\
g^U(\mathbf{1}_\psi) &:= \mathbf{1}_{g^U(\psi)} \\
g^U(o(e)) &:= o(g^U(e)) \\
g^U(e_1 \bowtie e_2) &:= g^U(e_1) \bowtie g^U(e_2) \\
g^U(FO(\psi)) &:= FO(g^U(\psi)) \\
g^U(o(r)) &:= o(g^U(r)) \qquad \text{where } o \in Ops \\
g^U(\mathbb{E}[e]) &:= \mathbb{E}_{x \sim M[\bar{q}]}[e] \qquad \text{where } M = \langle\{M_0\}, Id\rangle \text{ with } M_0 = U \text{ and } x \text{ is fresh} \\
g^U(\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]) &:= \mathbb{E}_{\bar{x} \sim M'[\bar{q}]}[e] \qquad \text{where } M' = \langle\{M_i U\}_{i \in I}, l\rangle \\
g^U(r_1 \bowtie r_2) &:= g^U(r_1) \bowtie g^U(r_2) \\
g^U(FO(P)) &:= FO(g^U(P)) \\
g^U(P_1 \oplus P_2) &:= g^U(P_1) \oplus g^U(P_2)
\end{aligned}
$$

In rule [QMeas'] we use the notation $f_{x,\bar{q}}^M(P)$ for a syntactic substitution. It changes all $\mathbb{E}[e]$ in P into $\mathbb{E}_{x \sim M[\bar{q}]}[e]$. For the distribution expression $\mathbb{E}_{\bar{y} \sim N[\bar{q}]}[e]$, it adds an outer layer of measurement to N. A formal definition is given below.

$$
\begin{aligned}
f_{x,\bar{q}}^M(o(r)) &:= o(f_{x,\bar{q}}^M(r)) \qquad \text{where } o \in Ops \\
f_{x,\bar{q}}^M(\mathbb{E}[e]) &:= \mathbb{E}_{x \sim M[\bar{q}]}[e] \\
f_{x,\bar{q}}^M(\mathbb{E}_{\bar{y} \sim N[\bar{q}']}[e]) &:= \begin{cases} \mathbb{E}_{x\bar{y} \sim M'[\bar{q} \cup \bar{q}']}[e] \text{ with } M' = \langle\{N_j M_i\}_{ij}, k'\rangle \text{ and } k'(ij) = (k(i), l(j)) & \text{if } x \notin \bar{y} \\ \mathbb{E}_{\bar{y} \sim M'[\bar{q} \cup \bar{q}']}[e] \text{ with } M' = \langle\{N_j M_i\}_{ij}, k'\rangle \text{ and } k'(ij) = l(j) & \text{if } x \in \bar{y} \end{cases} \\
f_{x,\bar{q}}^M(r_1 \bowtie r_2) &:= f_{x,\bar{q}}^M(r_1) \bowtie f_{x,\bar{q}}^M(r_2) \\
f_{x,\bar{q}}^M(FO(P)) &:= FO(f_{x,\bar{q}}^M(P)) \\
f_{x,\bar{q}}^M(P_1 \oplus P_2) &:= f_{x,\bar{q}}^M(P_1) \oplus f_{x,\bar{q}}^M(P_2)
\end{aligned}
$$

We are going to show that the three functions $h(\cdot)$, $g^U(\cdot)$ and $f_{x,\bar{q}}^M(\cdot)$ behave well as they help to transform postconditions into preconditions for three kinds of commands: initialisation, applications of unitary operations, and measurements of quantum systems.

Lemma 4.3 The following two clauses hold.

(i) $[\![h(r)]\!]_\mu = [\![r]\!]_{[\![q := |0\rangle]\!]_\mu}$.

(ii) $[\![h(P)]\!]_\mu \Rightarrow [\![P]\!]_{[\![q := |0\rangle]\!]_\mu}$.

Proof: We prove the two statements by structural induction.

(i) There are three cases for the structure of r.

- $r \equiv \mathbb{E}[e]$. We note that $[\![e]\!]_\sigma = [\![e]\!]_{\sigma[n/x]}$ for any number n and fresh variable x in the sense that x does not appear in e. Then we reason as follows.

$$
\begin{aligned}
[\![h(r)]\!]_\mu &= [\![\mathbb{E}_{x \sim M}[e]]\!]_\mu && \text{where } M = \langle \{M_0, M_1\}, Id \rangle \text{ with } M_0 = |0\rangle\langle 0|, \ M_1 = |0\rangle\langle 1|, \\
& && x \text{ is fresh} \\
&= \sum_\sigma (|0\rangle\langle 0|\mu(\sigma)|0\rangle\langle 0| \cdot [\![e]\!]_{\sigma[0/x]} + |0\rangle\langle 1|\mu(\sigma)|1\rangle\langle 0| \cdot [\![e]\!]_{\sigma[1/x]}) \\
&= \sum_\sigma (|0\rangle\langle 0|\mu(\sigma)|0\rangle\langle 0| \cdot [\![e]\!]_\sigma + |0\rangle\langle 1|\mu(\sigma)|1\rangle\langle 0| \cdot [\![e]\!]_\sigma) && x \text{ is fresh} \\
&= \sum_\sigma (|0\rangle\langle 0|\mu(\sigma)|0\rangle\langle 0| + |0\rangle\langle 1|\mu(\sigma)|1\rangle\langle 0|) \cdot [\![e]\!]_\sigma \\
&= \sum_\sigma [\![q := |0\rangle]\!]_\mu(\sigma) \cdot [\![e]\!]_\sigma \\
&= [\![\mathbb{E}[e]]\!]_{[\![q:=|0\rangle]\!]_\mu} \\
&= [\![r]\!]_{[\![q:=|0\rangle]\!]_\mu}
\end{aligned}
$$

- $r \equiv \mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]$ for some $M = \langle \{M_i\}_i, l \rangle$. Then

$$
\begin{aligned}
[\![h(r)]\!]_\mu &= [\![\mathbb{E}_{\bar{x} \sim M'[\bar{q}]}[e]]\!]_\mu && \text{where } M' = \langle \{M_{i0}, M_{i1}\}_i, l' \rangle \text{ with } M_{i0} = M_i|0\rangle\langle 0|, \ M_{i1} = M_i|0\rangle\langle 1|, \\
& && l'(i0) = l'(i1) = l(i) \\
&= \sum_\sigma \sum_i (M_i|0\rangle\langle 0|\mu(\sigma)|0\rangle\langle 0|M_i^\dagger + M_i|0\rangle\langle 1|\mu(\sigma)|1\rangle\langle 0|M_i^\dagger) \cdot [\![e]\!]_{\sigma[l(i)/\bar{x}]} \\
&= \sum_\sigma \sum_i (M_i(|0\rangle\langle 0|\mu(\sigma)|0\rangle\langle 0| + |0\rangle\langle 1|\mu(\sigma)|1\rangle\langle 0|)M_i^\dagger \cdot [\![e]\!]_{\sigma[l(i)/\bar{x}]} \\
&= \sum_\sigma \sum_i M_i [\![q := |0\rangle]\!]_\mu(\sigma)M_i^\dagger \cdot [\![e]\!]_{\sigma[l(i)/\bar{x}]} \\
&= [\![\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]]\!]_{[\![q:=|0\rangle]\!]_\mu} \\
&= [\![r]\!]_{[\![q:=|0\rangle]\!]_\mu}
\end{aligned}
$$

- $r \equiv o(r_1, ..., r_k)$. The case can be proved by induction.

$$
\begin{aligned}
[\![h(r)]\!]_\mu &= [\![o(h(r_1), ..., h(r_k))]\!]_\mu \\
&= o([\![h(r_1)]\!]_\mu, ..., [\![h(r_k)]\!]_\mu) \\
&= o([\![r_1]\!]_{[\![q:=|0\rangle]\!]_\mu}, ..., [\![r_k]\!]_{[\![q:=|0\rangle]\!]_\mu}) \\
&= [\![o(r_1, ..., r_k)]\!]_{[\![q:=|0\rangle]\!]_\mu} \\
&= [\![r]\!]_{[\![q:=|0\rangle]\!]_\mu}
\end{aligned}
$$

(ii) There are three cases for the structure of P.

- $P \equiv r_1 \bowtie r_2$. In this case, we need to use statement (iii).

$$
\begin{aligned}
[\![h(P)]\!]_\mu &= [\![h(r_1) \bowtie h(r_2)]\!]_\mu \\
&= [\![h(r_1)]\!]_\mu \bowtie [\![h(r_2)]\!]_\mu \\
&= [\![r_1]\!]_{[\![q:=|0\rangle]\!]_\mu} \bowtie [\![r_2]\!]_{[\![q:=|0\rangle]\!]_\mu}) \\
&= [\![r_1 \bowtie r_2]\!]_{[\![q:=|0\rangle]\!]_\mu} \\
&= [\![r]\!]_{[\![q:=|0\rangle]\!]_\mu}
\end{aligned}
$$

- $P \equiv P_1 \oplus P_2$. This case is proved by induction.

$$
\begin{aligned}
[\![h(P)]\!]_\mu &= [\![h(P_1) \oplus h(P_2)]\!]_\mu \\
&= \exists \mu_1, \mu_2. \ \mu = \mu_1 + \mu_2 \wedge [\![h(P_1)]\!]_{\mu_1} \wedge [\![h(P_2)]\!]_{\mu_2} \\
&\Rightarrow \exists \mu_1, \mu_2. \ [\![q := |0\rangle]\!]_\mu = [\![q := |0\rangle]\!]_{\mu_1} + [\![q := |0\rangle]\!]_{\mu_2} \\
&\quad \wedge [\![P_1]\!]_{[\![q:=|0\rangle]\!]_{\mu_1}} \wedge [\![P_2]\!]_{[\![q:=|0\rangle]\!]_{\mu_2}} && \text{by Lemma 3.5} \\
&= [\![P_1 \oplus P_2]\!]_{[\![q:=|0\rangle]\!]_\mu} \\
&= [\![r]\!]_{[\![q:=|0\rangle]\!]_\mu}
\end{aligned}
$$

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- $P \equiv FO(P_1, ..., P_k)$. Again, this case is proved by induction.

$$
\begin{aligned}
[\![h(P)]\!]_\mu &= [\![FO(h(P_1), ..., h(P_k))]\!]_\mu \\
&= FO([\![h(P_1)]\!]_\mu, ..., [\![h(P_k)]\!]_\mu) \\
&= FO([\![P_1]\!]_{[\![q:=|0\rangle]\!]_\mu}, ..., [\![P_k]\!]_{[\![q:=|0\rangle]\!]_\mu}) \\
&= [\![FO(P_1, ..., P_k)]\!]_{[\![q:=|0\rangle]\!]_\mu} \\
&= [\![P]\!]_{[\![q:=|0\rangle]\!]_\mu}
\end{aligned}
$$

$\square$

Lemma 4.4 The following two clauses hold.

(i) $[\![g^U(r)]\!]_\mu = [\![r]\!]_{[\![U[\bar{q}]]\!]_\mu}$.

(ii) $[\![g^U(P)]\!]_\mu \Rightarrow [\![P]\!]_{[\![U[\bar{q}]]\!]_\mu}$.

Proof: The proof is similar to that of Lemma 4.3 except for the treatement of two cases for statement (i).

- $r \equiv \mathbb{E}[e]$. We infer that

$$
\begin{aligned}
[\![g^U(r)]\!]_\mu &= [\![\mathbb{E}_{x \sim M[\bar{q}]}[e]]\!]_\mu \quad \text{where } M = \langle \{M_0\}, Id \rangle \text{ with } M_0 = U \text{ and } x \text{ is fresh} \\
&= \sum_\sigma U\mu(\sigma)U^\dagger \cdot [\![e]\!]_{\sigma[0/x]} \\
&= \sum_\sigma U\mu(\sigma)U^\dagger \cdot [\![e]\!]_\sigma \\
&= \sum_\sigma [\![U[\bar{q}]]\!]_\mu(\sigma) \cdot [\![e]\!]_\sigma \\
&= [\![\mathbb{E}[e]]\!]_{[\![U[\bar{q}]]\!]_\mu} \\
&= [\![r]\!]_{[\![U[\bar{q}]]\!]_\mu}
\end{aligned}
$$

- $r \equiv \mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]$. Suppose $M = \langle \{M_i\}_{i \in I}, l \rangle$. We reason as follows.

$$
\begin{aligned}
[\![g^U(r)]\!]_\mu &= [\![\mathbb{E}_{\bar{x} \sim M'[\bar{q}]}[e]]\!]_\mu \quad \text{where } M' = \langle \{M_i U\}_{i \in I}, l \rangle \\
&= \sum_\sigma \sum_i M_i U\mu(\sigma)U^\dagger M_i^\dagger \cdot [\![e]\!]_{\sigma[l(i)/\bar{x}]} \\
&= \sum_\sigma \sum_i M_i [\![U[\bar{q}]]\!]_\mu(\sigma) M_i^\dagger \cdot [\![e]\!]_{\sigma[l(i)/\bar{x}]} \\
&= [\![\mathbb{E}_{\bar{x} \sim M[\bar{q}]}[e]]\!]_{[\![U[\bar{q}]]\!]_\mu} \\
&= [\![r]\!]_{[\![U[\bar{q}]]\!]_\mu}
\end{aligned}
$$

$\square$

Lemma 4.5 Let a be an arithmetic expression, σ be any state and $\sigma' := \sigma[[\![a]\!]_\sigma/x]$. The following four clauses hold, where x is not a bound variable in e, ψ, r and P.

(i) $[\![e[a/x]]\!]_\sigma = [\![e]\!]_{\sigma'}$

(ii) $[\![\psi[a/x]]\!]_\sigma = [\![\psi]\!]_{\sigma'}$

(iii) $[\![r[a/x]]\!]_\mu = [\![r]\!]_{[\![x:=a]\!]_\mu}$.

(iv) $[\![P[a/x]]\!]_\mu \Rightarrow [\![P]\!]_{[\![x:=a]\!]_\mu}$.

Proof: The proof is similar to that of Lemma 4.3. As an example, we only consider one case for statement (iii).

Suppose $r \equiv \mathbb{E}_{\bar{y} \sim M[\bar{q}]}[e]$ with $M = \langle \{M_i\}_i, l \rangle$. There are two possibilities.

- $x \in \bar{y}$. In this case, x is a bound variable in r, which contradicts our assumption.

- $x \notin \bar{y}$. Notice that

$$[\![x := a]\!]_\mu(\sigma') \;=\; \sum_\sigma \{\mu(\sigma) \mid \sigma[[\![a]\!]_\sigma/x] = \sigma'\} \tag{14}$$

holds for any μ and σ'. We reason as follows.

$$
\begin{aligned}
[\![r[a/x]]\!]_\mu &= [\![\mathbb{E}_{\bar{y} \sim M[\bar{q}]}[e[a/x]]]\!]_\mu \\
&= \sum_\sigma \sum_i M_i \mu(\sigma) M_i^\dagger [\![e[a/x]]\!]_{\sigma[l(i)/\bar{y}]} \\
&= \sum_\sigma \sum_i M_i \mu(\sigma) M_i^\dagger [\![e]\!]_{\sigma[l(i)/\bar{y}][[\![a]\!]_{\sigma[l(i)/\bar{y}]}/x]} \qquad \text{by statement (i)} \\
&= \sum_i M_i \sum_\sigma \mu(\sigma) M_i^\dagger [\![e]\!]_{\sigma[[\![a]\!]_\sigma/x][l(i)/\bar{y}]} \\
&= \sum_i M_i \sum_{\sigma'} \sum_\sigma \{\mu(\sigma) \mid \sigma[[\![a]\!]_\sigma/x] = \sigma'\} M_i^\dagger [\![e]\!]_{\sigma'[l(i)/\bar{y}]} \\
&= \sum_i M_i \sum_{\sigma'} [\![x := a]\!]_\mu(\sigma') M_i^\dagger [\![e]\!]_{\sigma'[l(i)/\bar{y}]} \qquad \text{by (14)} \\
&= \sum_{\sigma'} \sum_i M_i [\![x := a]\!]_\mu(\sigma') M_i^\dagger [\![e]\!]_{\sigma'[l(i)/\bar{y}]} \\
&= [\![\mathbb{E}_{\bar{y} \sim M[\bar{q}]}[e]]\!]_{[\![x:=a]\!]_\mu} \\
&= [\![r]\!]_{[\![x:=a]\!]_\mu}
\end{aligned}
$$

$\square$

Lemma 4.6   (i) $[\![f^M_{x,\bar{q}}(r)]\!]_\mu = [\![r]\!]_{[\![x:=M[\bar{q}]]\!]_\mu}$.

(ii) $[\![f^M_{x,\bar{q}}(P)]\!]_\mu \Rightarrow [\![P]\!]_{[\![x:=M[\bar{q}]]\!]_\mu}$.

Proof: We consider two cases for statement (i); the other cases are easier. Assume that $M = \langle \{M_i\}_i, k \rangle$.

- $r \equiv \mathbb{E}[e]$. We reason as follows.

$$
\begin{aligned}
[\![f^M_{x,\bar{q}}(r)]\!]_\mu &= [\![\mathbb{E}_{x \sim M[\bar{q}]}[e]]\!]_\mu \\
&= \sum_\sigma \sum_i M_i \mu(\sigma) M_i^\dagger \cdot [\![e]\!]_{\sigma[l(i)/x]} \\
&= \sum_{\sigma'} \sum_\sigma \sum_i \{M_i \mu(\sigma) M_i^\dagger \mid \sigma[l(i)/x] = \sigma'\} \cdot [\![e]\!]_{\sigma'} \\
&= \sum_{\sigma'} \sum_\sigma \mu_\sigma(\sigma') \cdot [\![e]\!]_{\sigma'} \qquad \text{where } \mu_\sigma(\sigma') = \sum_i \{M_i \mu(\sigma) M_i^\dagger \mid \sigma[l(i)/x] = \sigma'\} \\
&= [\![\mathbb{E}[e]]\!]_{\sum_\sigma \mu_\sigma} \\
&= [\![\mathbb{E}[e]]\!]_{[\![x:=M[\bar{q}]]\!]_\mu} \\
&= [\![r]\!]_{[\![x:=M[\bar{q}]]\!]_\mu}
\end{aligned}
$$

The second last equality holds because $[\![x := M[\bar{q}]]\!]_{(\sigma,\mu(\sigma))} = \mu_\sigma$.

- $r \equiv \mathbb{E}_{\bar{y} \sim N[\bar{q'}]}[e]$. There are two possibilities. Let us first assume that $x \notin \bar{y}$ and $N = \langle \{N_j\}_j, l \rangle$.

$$
\begin{aligned}
[\![f^M_{x,\bar{q}}(r)]\!]_\mu &= [\![\mathbb{E}_{x\bar{y} \sim M'[\bar{q} \cup \bar{q'}]}[e]]\!]_\mu \text{ with } M' = \langle \{N_j M_i\}_{ij}, k' \rangle \text{ and } k'(ij) = (k(i), l(j)) \\
&= \sum_\sigma \sum_{ij} N_j M_i \mu(\sigma) M_i^\dagger N_j^\dagger \cdot [\![e]\!]_{\sigma[k(i),l(j)/x\bar{y}]} \\
&= \sum_\sigma \sum_j N_j (\sum_i M_i \mu(\sigma) M_i^\dagger) N_j^\dagger \cdot [\![e]\!]_{\sigma[k(i)/x][l(j)/\bar{y}]} \\
&= \sum_{\sigma'} \sum_\sigma \sum_j N_j (\sum_i \{M_i \mu(\sigma) M_i^\dagger \mid \sigma[k(i)/x] = \sigma'\}) N_j^\dagger \cdot [\![e]\!]_{\sigma'[l(j)/\bar{y}]} \\
&= \sum_{\sigma'} \sum_\sigma \sum_j N_j \mu_\sigma(\sigma') N_j^\dagger \cdot [\![e]\!]_{\sigma'[l(j)/\bar{y}]} \\
&\qquad \text{where } \mu_\sigma(\sigma') = \sum_i \{M_i \mu(\sigma) M_i^\dagger \mid \sigma[k(i)/x] = \sigma'\} \\
&= \sum_{\sigma'} \sum_j N_j \sum_\sigma \mu_\sigma(\sigma') N_j^\dagger \cdot [\![e]\!]_{\sigma'[l(j)/\bar{y}]} \\
&= [\![\mathbb{E}_{\bar{y} \sim N[\bar{q'}]}[e]]\!]_{\sum_\sigma \mu_\sigma} \\
&= [\![\mathbb{E}_{\bar{y} \sim N[\bar{q'}]}[e]]\!]_{[\![x:=M[\bar{q}]]\!]_\mu} \\
&= [\![r]\!]_{[\![x:=M[\bar{q}]]\!]_\mu}
\end{aligned}
$$

If $x \in \bar{y}$, the proof is similar by noting that $\sigma[k(i)/x][l(j)/\bar{y}] = \sigma[l(j)/\bar{y}]$.

$\square$

The next theorem states that the concrete proof system is sound.

$$
\begin{aligned}
pc(\mathbf{skip}, P) &:= P \\
pc(x := a, P) &:= P[a/x] \\
pc(c_0; c_1, P) &:= pc(c_0, pc(c_1, P)) \\
pc(\mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1, P) &:= \begin{cases} (pc(c_0, P_0) \wedge \Box b) \oplus (pc(c_1, P_1) \wedge \Box \neg b) & \text{if } P = P_0 \oplus P_1 \\ \text{undefined} & \text{otherwise} \end{cases} \\
pc(\mathbf{abort}, P) &:= \begin{cases} \top & \text{if } P = \Box \bot \\ \text{undefined} & \text{otherwise} \end{cases} \\
pc(q := |0\rangle, P) &:= h(P) \\
pc(U[\bar{q}], P) &:= g^U(P) \\
pc(x := M[\bar{q}], P) &:= f_{x,\bar{q}}^M(P)
\end{aligned}
$$

Figure 8: Precondition calculus

Theorem 4.7 Every judgement provable in $\mathcal{S}_c$ is valid.

Proof: We only need to prove that the four new rules [Assgn'], [QInit'], [QUnit'] and [QMeas'] are sound, which follows from Lemmas 4.3 - 4.6; the soundness of all other rules are already shown in Theorem 3.7. $\square$

Note that $\mathcal{S}_c$ is also relatively complete, which follows from the relative completeness of $\mathcal{S}_a$.

Theorem 4.8 Every valid judgement is derivable in $\mathcal{S}_c$.

Proof: The proof system $\mathcal{S}_c$ is the same as $\mathcal{S}_a$ except for the concretisation of four rules. $\square$

We can define a precondition calculus to help with syntactic reasoning. Given an assertion P as a postcondition and a loop-free command c, we construct an assertion as a precondition for c, written as $pc(c, P)$. The computation rules for preconditions are given in Figure 8.

Theorem 4.9 Let c be a non-looping command. The following rule is derivable.

$$
\frac{}{\{pc(c, P)\}\ c\ \{P\}}\ [\mathsf{PC}]
$$

Proof: We proceed by induction on the structure of c.

- $c \equiv \mathbf{skip}$. Then $pc(c, P) = P$ and we have $\vdash \{P\}\ c\ \{P\}$ by rule [Skip].

- $c \equiv \mathbf{abort}$. Then $pc(c, P)$ is only defined for $P = \Box \bot$. In this case, we have $\vdash \{\top\}\ \mathbf{abort}\ \{\Box \bot\}$ by rule [Abort].

- $c \equiv x := a$. Then $pc(c, P) = P[a/x]$ and we have $\vdash \{P[a/x]\}\ c\ \{P\}$ by rule [Assgn'].

- $c \equiv c_0; c_1$. Then $pc(c, P) = pc(c_0, pc(c_1, P))$. By induction, we have $\vdash \{pc(c_1, P)\}\ c_1\ \{P\}$ and $\vdash \{pc(c_0, pc(c_1, P))\}\ c_0\ \{pc(c_1, P)\}$. By using rule [Seq], we obtain $\vdash \{pc(c_0, pc(c_1, P))\}\ c\ \{P\}$.

- $c \equiv \mathbf{if}\ b\ \mathbf{then}\ c_0\ \mathbf{else}\ c_1$. Then $pc(c, P)$ is only defined for $P = P_0 \oplus P_1$ and

$$
pc(c, P_0 \oplus P_1) = (pc(c_0, P_0) \wedge \Box b) \oplus (pc(c_1, P_1) \wedge \Box \neg b).
$$

  By induction, we have that $\vdash \{pc(c_0, P_0)\}\ c_0\ \{P_0\}$ and $\vdash \{pc(c_1, P_1)\}\ c_1\ \{P_1\}$. It is obvious that $pc(c_0, P_0) \wedge \Box b \Rightarrow pc(c_0, P_0)$. We can use rule [Conseq] to infer that $\vdash \{pc(c_0, P_0) \wedge \Box b\}\ c_0\ \{P_0\}$. Similarly, we have $\vdash \{pc(c_1, P_1) \wedge \Box \neg b\}\ c_1\ \{P_1\}$. By applying rule [Cond], we can obtain that $\vdash \{pc(c, P_0 \oplus P_1)\}\ c\ \{P_0 \oplus P_1\}$.

- $c \equiv q := |0\rangle$. A direct consequence of rule [QInit'].

- $c \equiv U[\bar{q}]$. By using rule [QUnit'].

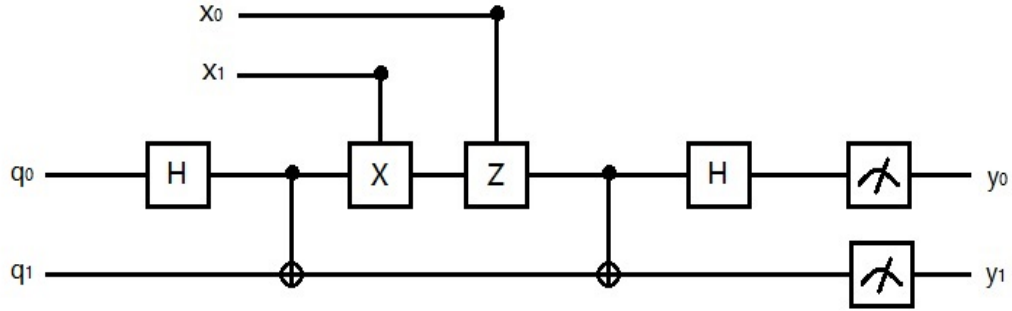- $c \equiv M[\bar{q}]$. By using rule [QMeas'].

$\square$

Figure 9: Superdense coding

5   Example: superdense coding

In this section, we illustrate the use of the proof system $\mathcal{S}_c$ via the example of superdense coding.

Superdense coding was proposed by Bennett and Wiesner in 1992 [5]. It is a quantum communication protocol allowing two classical bits to be encoded in one qubit during a transmission, so it needs only one quantum channel. Such advantage is based on the use of a maximally entangled state, EPR state. An EPR state can be transformed into all the four kinds of EPR states through 1-qubit operations, and these EPR states are mutually orthogonal.

Protocol.   We suppose the sender and the receiver of the communication are Alice and Bob, then the protocol goes as follows:

1. Alice and Bob prepare an EPR state $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$ together. Then they share the qubits, Alice holding q_0 and Bob holding q_1.

2. Depending on the message Alice wants to send, she applies a gate to her qubit. If Alice wants to send 00, she does nothing. If Alice wants to send 01, she applies the X gate. To send 10, she applies the Z gate. To send 11, she applies both X and Z.

3. Then Alice sends the qubit q_0 to Bob.

4. Bob applies a CNOT operation on q_0, q_1 and a Hadamard operation on q_0 to remove the entanglement.

5. Bob measures q_0 and q_1 to get the message.

After the execution of the protocol above, Bob gets the value that Alice wants to send. The protocol exactly transmits two classical bits of information by sending one qubit from Alice to Bob. A quantum circuit implementing the protocol is illustrated in Figure 9.

The protocol can also be described by the quantum program SC given in Figure 10, where for any pure state $|\varphi\rangle$, we write $[|\varphi\rangle]$ for its density operator $|\varphi\rangle\langle\varphi|$.

According to the operational rules in Figure 2, we can derive the following sequence of transitions, where the initial values of the four classical variables in the first configuration can be arbitrary and we

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$$SC \equiv$$

$1:\quad q_0 := |0\rangle;$

$2:\quad q_1 := |0\rangle;$

$3:\quad H[q_0];$

$4:\quad CNOT[q_0 q_1];$

$5:\quad \textbf{if } x_1 = 1 \textbf{ then } X[q_0];$

$6:\quad \textbf{if } x_0 = 1 \textbf{ then } Z[q_0];$

$7:\quad CNOT[q_0 q_1];$

$8:\quad H[q_0];$

$9:\quad y_0 := M[q_0];$

$10:\quad y_1 := M[q_1]$

$$\text{where } M = \langle \{M_0, M_1\}, Id \rangle, M_0 = [|0\rangle], M_1 = [|1\rangle]$$

Figure 10: The quantum program of implementing superdense coding

use $*$ to stand for unimportant commands or the values of variables.

$$(SC, x_0 x_1 y_0 y_1, [|00\rangle])$$

$$\rightarrow \quad (*, *, [\tfrac{|0\rangle + |1\rangle}{\sqrt{2}} |0\rangle])$$

$$\rightarrow \quad (*, *, [\tfrac{|00\rangle + |11\rangle}{\sqrt{2}}])$$

$$\rightarrow \quad (*, *, [X_0^{x_1} \tfrac{|00\rangle + |11\rangle}{\sqrt{2}}])$$

$$\rightarrow \quad (*, *, [Z_0^{x_0} X_0^{x_1} \tfrac{|00\rangle + |11\rangle}{\sqrt{2}}])$$

$$\equiv \begin{cases} (*, 00 y_0 y_1, [\tfrac{|00\rangle + |11\rangle}{\sqrt{2}}]) & \text{if } x_0 = x_1 = 0 \\ (*, 01 y_0 y_1, [\tfrac{|10\rangle + |01\rangle}{\sqrt{2}}]) & \text{if } x_0 = 0, x_1 = 1 \\ (*, 10 y_0 y_1, [\tfrac{|00\rangle - |11\rangle}{\sqrt{2}}]) & \text{if } x_0 = 1, x_1 = 0 \\ (*, 11 y_0 y_1, [\tfrac{|10\rangle - |01\rangle}{\sqrt{2}}]) & \text{if } x_0 = x_1 = 1 \end{cases}$$

$$\rightarrow \begin{cases} (*, 00 y_0 y_1, [\tfrac{|00\rangle + |10\rangle}{\sqrt{2}}]) \\ (*, 01 y_0 y_1, [\tfrac{|11\rangle + |01\rangle}{\sqrt{2}}]) \\ (*, 10 y_0 y_1, [\tfrac{|00\rangle - |10\rangle}{\sqrt{2}}]) \\ (*, 11 y_0 y_1, [\tfrac{|11\rangle - |01\rangle}{\sqrt{2}}]) \end{cases}$$

$$\rightarrow \begin{cases} (*, 00 y_0 y_1, [|00\rangle]) \\ (*, 01 y_0 y_1, [|01\rangle]) \\ (*, 10 y_0 y_1, [|10\rangle]) \\ (*, 11 y_0 y_1, [|11\rangle]) \end{cases}$$

$$\rightarrow \begin{cases} (*, 000 y_1, [|00\rangle]) \\ (*, 010 y_1, [|01\rangle]) \\ (*, 101 y_1, [|10\rangle]) \\ (*, 111 y_1, [|11\rangle]) \end{cases}$$

$$\rightarrow \begin{cases} (\textbf{nil}, 0000, [|00\rangle]) \\ (\textbf{nil}, 0101, [|01\rangle]) \\ (\textbf{nil}, 1010, [|10\rangle]) \\ (\textbf{nil}, 1111, [|11\rangle]) \end{cases}$$

We observe that in each case of the four last configurations, we always have the value of $x_0 x_1$ coincide

with $y_0 y_1$ as expected. Indeed, we would like to show that the judgement

$$\{\top\}\ SC\ \{\Box(x_0 = y_0 \land x_1 = y_1)\} \tag{15}$$

is provable in our concrete proof system. This can be accomplished by a sequence of derivations because for every line of command in Figure 10 we need to prove a Hoare triple. We start from line 10 and proceed backwards. The first six steps can be derived by using the rules [QMeas'], [QUnit'], [Cond] and [Split], as shown in Figure 11. Continue the reasoning until line 1, we obtain the following precondition for SC.

$$\{(\mathbb{E}_{y_0 y_1 \sim M_{10}[q_0 q_1]}[\mathbf{1}_{\psi \land x_0 = 1 \land x_1 = 1}] = \mathbb{E}_{y_0 y_1 \sim M_{10}[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}])$$
$$\oplus (\mathbb{E}_{y_0 y_1 \sim M_9[q_0 q_1]}[\mathbf{1}_{\psi \land x_0 = 1 \land x_1 = 0}] = \mathbb{E}_{y_0 y_1 \sim M_9[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}]) \qquad (\dagger)$$
$$\oplus (\mathbb{E}_{y_0 y_1 \sim M_8[q_0 q_1]}[\mathbf{1}_{\psi \land x_0 = 0 \land x_1 = 1}] = \mathbb{E}_{y_0 y_1 \sim M_8[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}])$$
$$\oplus (\mathbb{E}_{y_0 y_1 \sim M_7[q_0 q_1]}[\mathbf{1}_{\psi \land x_0 = 0 \land x_1 = 0}] = \mathbb{E}_{y_0 y_1 \sim M_7[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}])\},$$

where $M_{10} \equiv \langle \{E_{0000}, E_{0001}, ..., E_{1111}\}, f \rangle$ with

$$E_{0000} \equiv E_{00} H_{q_0} CNOT_{q_0 q_1} Z_{q_0} X_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 0| \cdot |0\rangle_{q_0} \langle 0|,$$
$$E_{0001} \equiv E_{00} H_{q_0} CNOT_{q_0 q_1} Z_{q_0} X_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 0| \cdot |0\rangle_{q_0} \langle 1|,$$
$$E_{0010} \equiv E_{00} H_{q_0} CNOT_{q_0 q_1} Z_{q_0} X_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 1| \cdot |0\rangle_{q_0} \langle 0|,$$
$$E_{0011} \equiv E_{00} H_{q_0} CNOT_{q_0 q_1} Z_{q_0} X_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 1| \cdot |0\rangle_{q_0} \langle 1|,$$
$$E_{0100} \equiv E_{01} H_{q_0} CNOT_{q_0 q_1} Z_{q_0} X_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 0| \cdot |0\rangle_{q_0} \langle 0|,$$
$$\vdots$$
$$E_{1111} \equiv E_{11} H_{q_0} CNOT_{q_0 q_1} Z_{q_0} X_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 1| \cdot |0\rangle_{q_0} \langle 1|,$$
$$f(00**) = 00,\ f(01**) = 01,\ f(10**) = 10,\ f(11**) = 11$$

$$M_9 \equiv \langle \{E'_{0000}, E'_{0001}, ..., E'_{1111}\}, f \rangle \text{ with}$$
$$E'_{0000} \equiv E_{00} H_{q_0} CNOT_{q_0 q_1} Z_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 0| \cdot |0\rangle_{q_0} \langle 0|,$$
$$\vdots$$
$$E'_{1111} \equiv E_{11} H_{q_0} CNOT_{q_0 q_1} Z_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 1| \cdot |0\rangle_{q_0} \langle 1|$$

$$M_8 \equiv \langle \{E''_{0000}, E''_{0001}, ..., E''_{1111}\}, f \rangle \text{ with}$$
$$E''_{0000} \equiv E_{00} H_{q_0} CNOT_{q_0 q_1} X_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 0| \cdot |0\rangle_{q_0} \langle 0|,$$
$$\vdots$$
$$E''_{1111} \equiv E_{11} H_{q_0} CNOT_{q_0 q_1} X_{q_0} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 1| \cdot |0\rangle_{q_0} \langle 1|$$

$$M_7 \equiv \langle \{E'''_{0000}, E'''_{0001}, ..., E'''_{1111}\}, f \rangle \text{ with}$$
$$E'''_{0000} \equiv E_{00} H_{q_0} CNOT_{q_0 q_1} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 0| \cdot |0\rangle_{q_0} \langle 0|,$$
$$\vdots$$
$$E'''_{1111} \equiv E_{11} H_{q_0} CNOT_{q_0 q_1} CNOT_{q_0 q_1} H_{q_0} |0\rangle_{q_1} \langle 1| \cdot |0\rangle_{q_0} \langle 1|$$

The measurement operators in M_{10} look complicated. However, a simple calculation shows that among the 16 operators only four of them are non-zero. Indeed, the simplied form of M_{10} is

$$M_{10} = \langle \{E_{1100}, E_{1101}, E_{1110}, E_{1111}\}, f \rangle$$

where

$$E_{1100} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \quad E_{1101} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad E_{1110} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \quad E_{1111} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Similarly, the simplied form of M_9 is $M_9 = \langle \{E'_{1000}, E'_{1001}, E'_{1010}, E'_{1011}\}, f \rangle$, where

$$E'_{1000} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E'_{1001} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E'_{1010} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E'_{1011} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

The simplied form of M_8 is $M_8 = \langle \{E''_{0100}, E''_{0101}, E''_{0110}, E''_{0111}\}, f\rangle$, where

$$E''_{0100} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E''_{0101} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E''_{0110} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E''_{0111} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Finally, the simplied form of M_7 is $M_7 = \langle \{E'''_{0000}, E'''_{0001}, E'''_{0010}, E'''_{0011}\}, f\rangle$, where

$$E'''_{0000} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E'''_{0001} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E'''_{0010} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad E'''_{0011} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Write P for the assertion in (†). We have seen that

$$\{P\} \; SC \; \{\Box\psi\}. \tag{16}$$

We observe that $\top \Leftrightarrow P$. This can be seen as follows. Let

$$
\begin{aligned}
P_{11} &\equiv (\mathbb{E}_{y_0 y_1 \sim M_{10}[q_0 q_1]}[\mathbf{1}_{\psi \wedge x_0=1 \wedge x_1=1}] = \mathbb{E}_{y_0 y_1 \sim M_{10}[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}]) \\
P_{10} &\equiv (\mathbb{E}_{y_0 y_1 \sim M_9[q_0 q_1]}[\mathbf{1}_{\psi \wedge x_0=1 \wedge x_1=0}] = \mathbb{E}_{y_0 y_1 \sim M_9[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}]) \\
P_{01} &\equiv (\mathbb{E}_{y_0 y_1 \sim M_8[q_0 q_1]}[\mathbf{1}_{\psi \wedge x_0=0 \wedge x_1=1}] = \mathbb{E}_{y_0 y_1 \sim M_8[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}]) \\
P_{00} &\equiv (\mathbb{E}_{y_0 y_1 \sim M_7[q_0 q_1]}[\mathbf{1}_{\psi \wedge x_0=0 \wedge x_1=0}] = \mathbb{E}_{y_0 y_1 \sim M_7[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}]) \\
b_{11} &\equiv x_0 = 1 \wedge x_1 = 1 \\
b_{10} &\equiv x_0 = 1 \wedge x_1 = 0 \\
b_{01} &\equiv x_0 = 0 \wedge x_1 = 1 \\
b_{00} &\equiv x_0 = 0 \wedge x_1 = 0
\end{aligned}
$$

We have $P = P_{11} \oplus P_{10} \oplus P_{10\oplus 00}$. For any POVD μ, it is easy to see that

$$\mu = \mu_{|b_{11}} + \mu_{|b_{10}} + \mu_{|b_{01}} + \mu_{|b_{00}}$$

We have that $\mu_{|b_{11}} \models P_{11}$ because

$$
\begin{aligned}
& \llbracket \mathbb{E}_{y_0 y_1 \sim M_{10}[q_0 q_1]}[\mathbf{1}_{\psi \wedge x_0=1 \wedge x_1=1}] \rrbracket_{\mu_{|b_{11}}} \\
=\;& \textstyle\sum_\sigma \sum_i E_i \mu_{|b_{11}}(\sigma) M_i^\dagger \cdot \mathbf{1}_{\llbracket\psi \wedge x_0=1 \wedge x_1=1\rrbracket_{\sigma[f(i)/y_0 y_1]}} \\
& \text{where } i \in \{1100, 1101, 1110, 1100\} \\
=\;& \textstyle\sum_\sigma \sum_i E_i \mu_{|b_{11}}(\sigma) M_i^\dagger \cdot \mathbf{1}_{\llbracket\psi \wedge x_0=1 \wedge x_1=1\rrbracket_{\sigma[11/y_0 y_1]}} \\
=\;& \textstyle\sum_\sigma \sum_i E_i \mu_{|b_{11}}(\sigma) M_i^\dagger \cdot 1 \\
=\;& \textstyle\sum_\sigma \sum_i E_i \mu_{|b_{11}}(\sigma) M_i^\dagger \cdot \mathbf{1}_{\llbracket\mathbf{true}\rrbracket_{\sigma[11/y_0 y_1]}} \\
=\;& \llbracket \mathbb{E}_{y_0 y_1 \sim M_{10}[q_0 q_1]}[\mathbf{1}_{\mathbf{true}}] \rrbracket_{\mu_{|b_{11}}}
\end{aligned}
$$

which implies $\llbracket P_{11} \rrbracket_{\mu_{|b_{11}}} = \mathbf{true}$. Similarly, we can check that $\mu_{|b_{10}} \models P_{10}$, etc. Therefore, we obtain that $\mu \models P$. As μ is arbitrarily chosen, we have verified that $\top \Leftrightarrow P$. By (16) and rule [Conseq], we finally see that the triple $\{\top\} \; SC \; \{\Box\psi\}$ is provable.

References

[1] K. Apt, F. S. De Boer, and E.-R. Olderog. *Verification of sequential and concurrent programs.* Springer Science & Business Media, 2010.

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$\{\top\}$

$SC \equiv$

1 : $q_0 := |0\rangle;$

2 : $q_1 := |0\rangle;$

3 : $H[q_0];$

4 : $CNOT[q_0q_1];$

$\{(\mathbb{E}_{y_0y_1 \sim M_6[q_0q_1]}[\mathbf{1}_{\psi \wedge x_0=1 \wedge x_1=1}] = \mathbb{E}_{y_0y_1 \sim M_6[q_0q_1]}[\mathbf{1}_{\mathbf{true}}])$

$\oplus(\mathbb{E}_{y_0y_1 \sim M_4[q_0q_1]}[\mathbf{1}_{\psi \wedge x_0=1 \wedge x_1=0}] = \mathbb{E}_{y_0y_1 \sim M_4[q_0q_1]}[\mathbf{1}_{\mathbf{true}}])$

$\oplus(\mathbb{E}_{y_0y_1 \sim M_5[q_0q_1]}[\mathbf{1}_{\psi \wedge x_0=0 \wedge x_1=1}] = \mathbb{E}_{y_0y_1 \sim M_5[q_0q_1]}[\mathbf{1}_{\mathbf{true}}])$

$\oplus(\mathbb{E}_{y_0y_1 \sim M_3[q_0q_1]}[\mathbf{1}_{\psi \wedge x_0=0 \wedge x_1=0}] = \mathbb{E}_{y_0y_1 \sim M_3[q_0q_1]}[\mathbf{1}_{\mathbf{true}}])\},$

where $M_6 \equiv \langle\{E_{00}H_{q_0}CNOT_{q_0q_1}Z_{q_0}X_{q_0},\ E_{01}H_{q_0}CNOT_{q_0q_1}Z_{q_0}X_{q_0},$

$\qquad\qquad E_{10}H_{q_0}CNOT_{q_0q_1}Z_{q_0}X_{q_0},\ E_{11}H_{q_0}CNOT_{q_0q_1}Z_{q_0}X_{q_0}\}, Id\rangle,$

$M_5 \equiv \langle\{E_{00}H_{q_0}CNOT_{q_0q_1}X_{q_0},\ E_{01}H_{q_0}CNOT_{q_0q_1}X_{q_0},$

$\qquad\qquad E_{10}H_{q_0}CNOT_{q_0q_1}X_{q_0},\ E_{11}H_{q_0}CNOT_{q_0q_1}X_{q_0}\}, Id\rangle$

5 :   **if** $x_1 = 1$ **then** $X[q_0];$

$\{(\mathbb{E}_{y_0y_1 \sim M_4[q_0q_1]}[\mathbf{1}_{\psi \wedge x_0=1}] = \mathbb{E}_{y_0y_1 \sim M_4[q_0q_1]}[\mathbf{1}_{\mathbf{true}}])$

$\oplus(\mathbb{E}_{y_0y_1 \sim M_3[q_0q_1]}[\mathbf{1}_{\psi \wedge x_0=0}] = \mathbb{E}_{y_0y_1 \sim M_3[q_0q_1]}[\mathbf{1}_{\mathbf{true}}])\},$

where $M_4 \equiv \langle\{E_{00}H_{q_0}CNOT_{q_0q_1}Z_{q_0},\ E_{01}H_{q_0}CNOT_{q_0q_1}Z_{q_0},$

$\qquad\qquad E_{10}H_{q_0}CNOT_{q_0q_1}Z_{q_0},\ E_{11}H_{q_0}CNOT_{q_0q_1}Z_{q_0}\}, Id\rangle$

6 :   **if** $x_0 = 1$ **then** $Z[q_0];$

$\{\mathbb{E}_{y_0y_1 \sim M_3[q_0q_1]}[\mathbf{1}_\psi] = \mathbb{E}_{y_0y_1 \sim M_3[q_0q_1]}[\mathbf{1}_{\mathbf{true}}]\},$

where $M_3 \equiv \langle\{E_{00}H_{q_0}CNOT_{q_0q_1}, E_{01}H_{q_0}CNOT_{q_0q_1}, E_{10}H_{q_0}CNOT_{q_0q_1}, E_{11}H_{q_0}CNOT_{q_0q_1}\}, Id\rangle$

7 : $CNOT[q_0q_1];$

$\{\mathbb{E}_{y_0y_1 \sim M_2[q_0q_1]}[\mathbf{1}_\psi] = \mathbb{E}_{y_0y_1 \sim M_2[q_0q_1]}[\mathbf{1}_{\mathbf{true}}]\},$

where $M_2 \equiv \langle\{E_{00}H_{q_0}, E_{01}H_{q_0}, E_{10}H_{q_0}, E_{11}H_{q_0}\}, Id\rangle$

8 : $H[q_0];$

$\{\mathbb{E}_{y_0y_1 \sim M_1[q_0q_1]}[\mathbf{1}_\psi] = \mathbb{E}_{y_0y_1 \sim M_1[q_0q_1]}[\mathbf{1}_{\mathbf{true}}]\}$

where $M_1 \equiv \langle\{E_{00}, E_{01}, E_{10}, E_{11}\}, Id\rangle,$

$E_{00} \equiv [|0\rangle]_{q_1} \cdot [|0\rangle]_{q_0},\ E_{01} \equiv [|1\rangle]_{q_1} \cdot [|0\rangle]_{q_0},\ E_{10} \equiv [|0\rangle]_{q_1} \cdot [|1\rangle]_{q_0},\ E_{11} \equiv [|1\rangle]_{q_1} \cdot [|1\rangle]_{q_0}$

9 : $y_0 := M[q_0];$

$\{\mathbb{E}_{y_1 \sim M[q_1]}[\mathbf{1}_\psi] = \mathbb{E}_{y_1 \sim M[q_1]}[\mathbf{1}_{\mathbf{true}}]\}$

10 : $y_1 := M[q_1]$

     where $M = \langle\{E_0, E_1\}, Id\rangle, E_0 = [|0\rangle], E_1 = [|1\rangle]$

$\{\Box\psi\},$ where $\psi \equiv x_0 = y_0 \wedge x_1 = y_1$

Figure 11: The quantum program with pre- and postconditions

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