Quantum Hoare Logic with Ghost Variables

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Abstract
Quantum Hoare logic allows us to reason about quantum programs. We present an extension of quantum Hoare logic that introduces “ghost variables” to extend the expressive power of pre-/postconditions. Ghost variables are variables that do not actually occur in the program and are allowed to have arbitrary quantum states (in a sense, they are existentially quantified), and be entangled with program variables. Ghost variables allow us to express properties such as the distribution of a program variable or the fact that a variable has classical content. And as a case study, we show how quantum Hoare logic with ghost variables can be used to prove the security of the quantum one-time pad.

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1 Introduction

Designing algorithms is an inherently error-prone process. This is especially true for quantum algorithms. Quantum algorithms can solve certain computational problems much faster than classical computers (e.g., [18, 10, 11]), and most likely will be of great impact once quantum computers are available. And already now, analyzing quantum algorithms is of practical relevance when proving the security of cryptosystems against future quantum attackers (post-quantum cryptography). But quantum algorithms are difficult to get right: Quantum mechanics has many properties that go against human intuition, and quantum programs are difficult to test and debug since we cannot directly observe their state (except in small-scale simulations). A solution to this problem is formal verification where we prove the behavior of the algorithm. In the classical realm, Hoare logic [12] (and its close relative, the predicate transformers [8], which we treat as the same for the sake of this introduction) has proven to be an invaluable tool for the analysis of imperative programs. In Hoare logics, we analyze the behavior of a program by investigating what “postcondition” the final state of a program satisfies if the initial state satisfies a certain “precondition”. This allows us to formally prove the behavior of a complex program by first deriving the behavior of individual lines of code and then modularly plugging these together to get a description of the behavior of the whole program. Hoare logics have been developed also for probabilistic programs [14, 15] and quantum programs [7, 20, 5, 9, 13].

However, existing Hoare logics still have limitations as to what can be expressed within a pre-/postcondition. For example, we cannot express that the value of a certain variable is uniformly distributed.\(\frac{1}{2}\) (E.g., to state that inside a while-loop, we have the invariant that \(x\) is a uniformly random bit.) Or, specific to the quantum case, that a quantum variable has a certain distribution (e.g., is in the “completely mixed state”, the quantum analogue to a uniform distribution). Or that a quantum variable is not entangled with other variables. Or that a quantum variable contains classical data at a certain point in the program. (Some logics distinguish classical and quantum variables, e.g., [19], at the costs of more complex semantics. But this does not allow us to reason about dynamic properties, e.g., that a variable becomes classical after a measurement.)

In this article, we present an extension of quantum Hoare logic that removes these limitations. We introduce “ghost variables” and show that using ghost variables, we can encode properties such as “\(x\) has distribution \(D\)” or “\(x\) is separable (unentangled)” or “\(x\) is classical”. (That is, all of these are emerging properties, not hardcoded into our logic.) A ghost variable is a variable that does not actually occur in the program but is introduced merely in a predicate (pre-/postcondition). The ghost variable is then allowed to take any value that makes the predicate true (effectively existentially quantified). E.g., the classical predicate \(x = g^2\) (where \(g\) is a ghost variable) would express that \(x\) is a square. Classical ghost variables, however, do not yield any new expressive power since existential quantifiers are already allowed in most Hoare logics (so we could state the predicate as \(\exists g. x = g^2\)). In the quantum setting, however, a ghost variable can have a quantum state, and possibly be entangled with other variables! For example, if \(\psi\) is a maximally entangled state between two variables, then looking at only one of those variables, we would see a uniformly distributed variable. And a uniformly distributed variable can always be seen as part of a system with two variables in state \(\psi\). Thus the predicate “\(xe\) together are in state \(\psi\)” (where \(e\) is a ghost variable) models the fact that \(x\) is uniformly distributed. Similarly we can encode classicality and separability. Thus, using ghost variables, we can continue reasoning about quantum programs using Hoare logic, but additionally have program invariants that state

\(\frac{1}{2}\)Classical/quantum calculi that use “expectations” (predicates that do not just hold/not hold, but hold to a certain degree, [14, 15, 7, 20]) allow us to reason about probabilistic behavior. But they only allow us to reason about the probability of a certain event (or the expectation value of a quantity), but not about the distribution of value. (I.e., we can express “\(x\) has value \(0\) with probability at least \(\alpha\)” but not “\(x\) is uniform”.)
that variables are distributed in certain ways, are classical, are separable, and more. (We stress that this even is an advance over the state of the art for classical programs. Our logic could be used in the analysis of classical programs to express the fact that certain variables have certain distributions. This is quite unexpected since we would be using a quantum phenomenon to analyze purely classical programs.)

Additionally the introduction of ghost variables makes the foundations of the investigated programming language simpler. Many operations that one thinks of as elementary (such as random sampling, measurements) can actually be built from more elementary operations (such as applying a unitary operation, initializing a quantum register). Using ghost variables we can then derive the properties of the derived operations from the properties of the elementary one. (E.g., show that after random sampling the assigned variable has a certain distribution and is classical.) This means that the language is simpler (and thus arguably more foundationally elegant), and the core set of rules of our logic is quite small (eleven rules).

Finally, we demonstrate that our logic can be applied to problems that seem out of reach of existing Hoare logics: We analyze quantum one-time pad encryption and show that it is secure, i.e., that an encrypted quantum message indeed “looks random”.

**Related work.** Hoare logic was first introduced by Hoare [12]. A different view was provided by Dijkstra [8] using predicate transformers. Hoare logics/predicate transformers were generalized by Kozen [14] (and [15] for the case of combined probabilism/nondeterminism). Quantum Hoare logics and predicate transformer calculi for quantum programs have been presented by D’Hondt and Panangaden [7], Chadha, Mateus and Sernadas [5], Feng, Duan, Ji, and Ying [9], Ying [20], and Kakutani [13]. Unruh [19] gives a quantum Hoare logic for analyzing pairs of programs (based on the classical pRHL [2]). A different approach is taken by pictorial calculi where quantum processes can be formalized and rewritten as diagrams, starting with Abramsky and Coecke [1]. [6, Example 4.91] applies this approach to the classical one-time pad, but only to its correctness, not its security. The quantum one-time pad was discovered by [3, 16].

**Organisation.** Section 2 introduces some quantum basics as well as important notation and auxiliary concepts. Section 3 introduces syntax and semantics of the simple imperative quantum language we use for our calculus. (And explains how random sampling, measurements, etc. are encoded using more basic language features.) Section 4 introduces our Hoare logic with ghosts. (The concept of ghost variables and the semantics of Hoare judgments.) Section 5 shows how important properties such as distributions of variables, classicality, separability can be encoded in pre-/postconditions using ghost variables. Section 6 presents and explains the eleven core rules of the logic from which all other rules can be derived. Section 7 derives a number of additional rules from the core rules. (For reasoning about derived language features, and for convenient reasoning about programs with classical variables.) Section 8 analyses the quantum one-time pad.

## 2 Preliminaries: Variables, Memories, and Predicates

In this section, we introduce some fundamental concepts and notations needed for this paper, and recap some of the needed quantum background as we go along. When introducing some notation $X$, the place of definition is marked like this: $X$. All symbols are listed in the symbol index.
**Variables.** Before we introduce the syntax and semantics of programs, we first need to introduce some basic concepts. A *variable* is described by a variable name $x$ that identifies the variable, and a type $T$. The *type* of $x$ is simply the set of all (classical) values the variable can take. E.g., a variable might have type $\{0, 1\}$, or $\mathbb{N}^2$. We will assume that there is always some distinguished value in $T$ that we denote $\emptyset$.

We distinguish between three kinds of variables: program variables $x, y, z$ (that can occur in programs), entangled ghost variables $\mathfrak{e}$, and unentangled ghost variables $\mathfrak{u}$. We write $\mathfrak{g}$ for variables that are entangled ghosts or unentangled ghosts. (The meaning of these kinds will become clear later, for now they simply form a partition of the set of all variables.) We use $v, w$ when we do not wish to specify the kind of variable.

Lists or sets of variables will be denoted $V, W$ or $X, Y, Z$ or $E$ or $U$ or $G$ (depending on the kind of variable they contain). Given a list $V = v_1 \ldots v_n$ of variables, we say its *type* is $T_1 \times \cdots \times T_n$ if $T_i$ is the type of $v_i$. We write $\text{provars}(V)$ for the program variables in $V$.

**Memoires and quantum states.** An assignment assigns to each variable a classical value. Formally, for a set $V$, the assignments over $V$ are all functions $m$ with domain $V$ such that: for all $x \in V$ with type $T_x$, $m(x) \in T_x$. That is, assignments can represent the content of classical memories.

To model quantum memories, we simply consider superpositions of assignments: A (pure) quantum memory is a superposition of assignments. Formally, $\ell^2[V]$, the set of all quantum memories over $V$, is the Hilbert space with basis\(^3\) $\{ |m \rangle \}_m$ where $m$ ranges over all assignments over $V$. Here $|m \rangle$ simply denotes the basis vector labeled $m$, we often write $|m\rangle_V$ to stress which space we are talking about. Intuitively, a quantum memory $\psi$ over $V$ with $\|\psi\| = 1$ represents a state a quantum computer with variables $V$ could be in. (We do not require $\|\psi\| = 1$ for a quantum memories unless this is explicitly mentioned.)

We also consider quantum states over arbitrary sets $X$ (as opposed to sets of assignments). Namely, $\ell^2(X)$ denotes the Hilbert space with orthonormal basis $\{ |x \rangle \}_x$. (In that notation, $\ell^2[V]$ is simply $\ell^2(A)$ where $A$ is the set of all assignments on $V$. ) Elements $\psi \in \ell^2(X)$ with $\|\psi\| = 1$ represent quantum states.

We often treat elements of $\ell^2(T)$ and $\ell^2[V]$ interchangeably if $T$ is the type of $V$ since there is a natural isomorphism between those spaces.

The tensor product $\otimes$ combines two quantum states $\psi \in \ell^2(X), \phi \in \ell^2(Y)$ into a joint system $\psi \otimes \phi \in \ell^2(X \times Y)$. In the case of quantum memories $\psi, \phi$ over $V, W$, respectively, $\psi \otimes \phi \in \ell^2[VW]$. (And $\psi \otimes \phi = \phi \otimes \psi$ since we are composing “named” systems.)

For a vector (or operator) $a$, we write $a^*$ for its adjoint. (In the finite dimensional case, the adjoint is simply the conjugate transpose of a vector/matrix. The literature also knows the notation $a^\dagger$. ) The adjoint of $|x\rangle$ is written $\langle x |$. We abbreviate $\text{proj}(\psi) := \psi \psi^*$. This is the projector onto $\psi$ when $\|\psi\| = 1$.

**Mixed quantum memories.** In many situations, we need to model probabilistic quantum states (e.g., a quantum state that is $|0\rangle$ with probability $\frac{1}{2}$ and $|1\rangle$ with probability $\frac{1}{2}$). This is modeled using mixed states (a.k.a. density operators). Having state $\psi_i$ with probability $p_i$ is

\[^{2}\text{We stress that we do not assume that the type is a finite or even a countable set. Consequently, the Hilbert spaces considered in this paper are not necessarily finite dimensional or even separable. However, all results can be informally understood by thinking of all sets as finite and hence of all Hilbert spaces as $\mathbb{C}^N$ for suitable $N \in \mathbb{N}$.)\]

\[^{3}\text{When we say “basis”, we always mean orthonormal basis.}\]
represented by the operator $\rho := \sum_i p_i \proj{\psi_i}$. Then $\rho$ encodes all observable information about the distribution of the quantum state (that is, two distributions of quantum states have the same $\rho$ if they cannot be distinguished by any physical process). And $\tr \rho$ is the total probability $\sum_i p_i$. (That is, $\tr \rho = 1$ unless we wish to represent the outcome of a non-terminating program.) We will often need to consider mixed states of quantum memories (i.e., mixed states with underlying Hilbert space $\mathbb{H}$). We call them mixed (quantum) memories over $\mathbb{H}$.

For a mixed memory $\rho$ over $\mathbb{H}$ the partial trace $\tr_\mathbb{W} \rho$ is the result of throwing away variables $\mathbb{W}$ (i.e., it is a mixed memory over $\mathbb{H} \setminus \mathbb{W}$). Formally, $\tr_\mathbb{W} \rho$ is defined as the continuous linear function satisfying $\tr_\mathbb{W} (\sigma \otimes \tau) := \sigma \cdot \tr \tau$ where $\tau$ is an operator over $\mathbb{W}$.

A mixed memory $\rho$ is $(\mathbb{V}, \mathbb{W})$-separable (i.e., not entangled between $\mathbb{V}$ and $\mathbb{W}$) iff it can be written as $\rho = \sum_i p_i \otimes \rho_i$ for mixed memories $\rho_i$ over $\mathbb{V}, \mathbb{W}$, respectively.

**Operations on quantum states.** An operation on a quantum state is modeled by an isometry $U$ on $\ell^2(\mathcal{X})$. If we apply such an operation on a mixed state $\rho$, the result is $U \rho U^*$. Most often, isometries will occur in the context of operations that are performed on a single variable or list of variables, i.e., an isometry $U$ on $\ell^2(\mathbb{V})$. Then $U$ can also be applied to $\ell^2(\mathbb{W})$ with $\mathbb{W} \supseteq \mathbb{V}$: we identify $U$ with $U \otimes \id_{\mathbb{W}\setminus\mathbb{V}}$. Furthermore, if $\mathbb{V}$ has type $T$, then an isometry $U$ on $\ell^2(\mathcal{T})$ can be seen as an isometry on $\ell^2(\mathbb{V})$ since we identify $\ell^2(\mathcal{T})$ and $\ell^2(\mathbb{V})$. If we want to make $\mathbb{W}$ explicit, we write $U_{\mathbb{V}}$ for the isometry $U$ on $\ell^2(\mathbb{V})$. For example, if $U$ is a $2 \times 2$-matrix and $\mathbf{x}$ has type bit, then $U_{\mathbb{X}}$ can be applied to quantum memories over $\mathbf{x}$, acting on $\mathbf{x}$ only. This notation is not limited to isometries, of course, but applies to other operators, too. (By “operator” we always mean a bounded linear operator in this paper.)

An important operation is CNOT on $\mathbb{V} \mathbb{W}$ (where $\mathbb{V}, \mathbb{W}$ both have type $\{0, 1\}^n$), defined by $\text{CNOT}(|x\rangle_\mathbb{V} \otimes |y\rangle_\mathbb{W}) := |x\rangle_\mathbb{V} \otimes |x \oplus y\rangle_\mathbb{W}$. (That is, we allow CNOT not only on single bits but bitstrings.)

**Predicates.** In Hoare judgments, we need to express properties of the state of a quantum memory. In this paper, we only consider properties that are closed under superpositions of quantum states. That is, a predicate $\mathbf{A}, \mathbf{B}, \mathbf{C}$ on $\mathbb{V}$ is a subspace of $\ell^2(\mathbb{V})$. The syntax of predicates will not be fixed to a specific language, i.e., any mathematically expressible subspace is a valid predicate. But we fix some syntactic sugar for expressing predicates succinctly:

- $\top, \bot$: The predicate that is always satisfied is denoted $\top := \ell^2(\mathbb{V})$. The predicate that is never satisfied is $\bot := \{0\}$.
- $\mathbf{A} \land \mathbf{B}$, $\mathbf{A}, \mathbf{B}$, $\mathbf{A} \lor \mathbf{B}$: To model that both $\mathbf{A}$ and $\mathbf{B}$ hold (conjunction), we simply use the intersection of $\mathbf{A}$ and $\mathbf{B}$ (as sets). That is, we write $\mathbf{A} \land \mathbf{B}$ to denote $\mathbf{A} \cap \mathbf{B}$. We will often also write this as “$\mathbf{A}, \mathbf{B}$” instead of “$\mathbf{A} \land \mathbf{B}$” where “,$,” is understood to bind less closely than “,$,”. To model that $\mathbf{A}$ or $\mathbf{B}$ holds (disjunction), we use the sum $\mathbf{A} + \mathbf{B}$ (the space of all linear combinations from $\mathbf{A}$ and $\mathbf{B}$). That is, we write $\mathbf{A} \lor \mathbf{B}$ to denote $\mathbf{A} + \mathbf{B}$. This choice of connectives corresponds to Birkhoff-von Neumann quantum logic. But we stress that we

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4Mathematically, these are the set of all positive Hermitian trace-class operators on $\ell^2(\mathcal{X})$. The requirement “trace-class” ensures that the trace exists and can be ignored in the finite-dimensional case.

5Sums without index set are always assumed to have an arbitrary (not necessarily finite or even countable) index set. In the case of sums of vectors in a Hilbert space, convergence is with respect to the Hilbert space norm, and in the case of sums of positive operators, the convergence is with respect to the Loewner order.

6That is, a norm-preserving linear operation. Often, one models quantum operations as unitaries instead because in the finite-dimensional case an isometry is automatically unitary. However, in the infinite-dimensional case, unitaries are unnecessarily restrictive. Consider, e.g., the isometry $|i\rangle \mapsto |i + 1\rangle$ with $i \in \mathbb{N}$ which is a perfectly valid quantum operation but not a unitary.

7By subspace, we always mean closed subspaces. In the finite-dimensional case, all subspaces are closed anyway.
are not restricted to using only these connectives, we may use any well-defined operations on subspaces. These are just the ones that will turn out useful in the remainder of the paper.

- $M \cdot A$: For an operator $M$ (typically an isometry or a projector) and a predicate $A$, we write $M \cdot A$ for the subspace $\{M \psi : \psi \in A\}$. Thus, $M \cdot A$ is satisfied if we apply $M$ to a quantum memory in $A$.

- $X \in_q S$: For some variable list $X$ of type $T$, we may wish to express the fact that the value of $X$ lies in a certain subspace $S \subseteq \ell^2(T)$. Notice that $S$ can be naturally seen as a subspace of $\ell^2[V]$. Then $V$ being in a state in $S$ means that the state of the whole quantum memory is in $S \otimes \ell^2[V \setminus X]$. We introduce the syntactic sugar $X \in_q S$ to denote $S \otimes \ell^2[V \setminus X]$. Note that even though it looks like a Boolean expression, it actually is a subspace of $\ell^2[V]$ and thus a predicate in our sense.

- $W =_q \psi$. Often, we will also want to express that the variables $W$ are in a specific state $\psi$. This means the variables lie in span{$\psi$}, using the previous syntactic sugar we can write this as $W \in_q \text{span}\{\psi\}$. We introduce the abbreviation $W =_q \psi$ for this common case.

- $A(W/W')$. Renaming variables $W$ to $W'$ in predicate $A$. This assumes $A$ is a predicate over $V \supseteq W$, that $W \cap (V \setminus W) = \emptyset$, and that $W$ and $W'$ have the same type. Then $A(W/W')$ is the predicate over $(V \setminus W) \cup W'$ defined by $U_{W \rightarrow W'} \cdot A$ where $U_{W \rightarrow W'}$ is the natural isomorphism between $\ell^2[W]$ and $\ell^2[W']$, i.e., $U_{W \rightarrow W'} i \cdot W := i \cdot W'$ for all $i$. ($U_{W \rightarrow W'}$ renames $W$ to $W'$ when applied to a quantum memory.)

An example $A_{\text{example}}$ of a predicate would be:

$$(xy = \frac{1}{\sqrt{2}} \langle 00 \rangle + \frac{1}{\sqrt{2}} \langle 11 \rangle) \lor (x = \langle 0 \rangle), \ z = \langle 1 \rangle$$

This means, intuitively, that $xy$ are maximally entangled (in state $\frac{1}{\sqrt{2}} \langle 00 \rangle + \frac{1}{\sqrt{2}} \langle 11 \rangle$ up to a global phase factor) or $x$ has state $\langle 0 \rangle$, and in addition $z$ has state $\langle 1 \rangle$.

Note that our predicates seems to be lacking in expressiveness compared with the predicates, e.g., from [19]: It is not possible to parameterize the predicate using the values of classical variables. E.g., we cannot write $y =_q \langle x \rangle$ where $x$ is a classical variable. This is because our semantics does not hardcode the distinction between classical and quantum variables (all variables are quantum by default). But, in Section 7.2, we will see how to express classical variables as a derived feature, and introduce additional syntactic sugar that allows us to recover full expressiveness of the predicates from [19].

Given a predicate $A$, we will often wish to indicate which variables it talks about, i.e., what are its free variables. Since our definition of predicates is semantic (i.e., we are not limited to predicates expressed using the syntax above) we cannot simply speak about the variables occurring in the expression describing $A$. Instead, we say $A$ contains only variables from $W$ (written: $\text{fv}(A) \subseteq W$) iff there exists a subspace $S$ such that $A = (W \in_q S)$. (That is, if $A$ can be described solely in terms of the content of the variables $W$.) Note that there is a certain abuse of notation here: We formally defined “$\text{fv}(A) \subseteq W$”, but we do not define $\text{fv}(A)$; $\text{fv}(A) \subseteq W$ should formally just be seen as an abbreviation for $\exists S. A = (W \in_q S)$. For example, $\text{fv}(A_{\text{example}}) \subseteq \{x, y, z\}$. Similarly, we treat $\text{fv}(A) \cap W = \emptyset$.

\footnote{In fact, defining $\text{fv}(A)$ is possible only if there is a smallest set $W$ such that $\exists S. A = (W \in_q S)$. This is not necessarily the case. For example, assume that $V$ is infinite, let $A$ be the space spanned by all $|m\rangle$ where $m(v) \neq 0$ for only finitely many $v \in V$. Then $A = (W \in_q S)$ for any cofinite $W$ (by defining $S$ as the span of all $|m\rangle$ with only finitely many $m(v) \neq 0$), but $A \neq (W \in_q S)$ whenever $W$ is not cofinite. Since there is no smallest cofinite $W$, $\text{fv}(A)$ cannot be defined, but we can still meaningfully use the notation $\text{fv}(A) \subseteq W$.}
If two predicates \( A \) and \( A' \) on variables \( V \) and \( W \), respectively, satisfy \( A \otimes \ell^2[\overline{W \setminus V}] = A' \otimes \ell^2[\overline{V \setminus W}] \), then \( A \) and \( A' \) intuitively describe the same property on the shared variables \( V \cap W \) (and say nothing about the remaining variables). Therefore we will identify such \( A \) and \( A' \) throughout this paper. In particular, any predicate \( A \) can be seen as a predicate \( A' \) on \( \text{fv}(A) \).

### 3 Quantum programs

**Syntax.** We will now define a small imperative quantum language. The set of all programs is described by the following syntax:

\[
\begin{align*}
\ell_d & ::= \text{apply } U \text{ to } X | \text{init } x | \text{if } y \text{ then } \ell \text{ else } \ell | \text{while } y \text{ do } \ell | \ell; \ell | \ell \\
\end{align*}
\]

Here \( X \) is a list of program variables, \( x \) a program variable, \( y \) a program variable of type \( \{0, 1\} \), and \( U \) an isometry on \( \ell^2[X] \) (there is no fixed set of allowed isometries, any isometry that we can describe can be used here).\(^9\)

Intuitively, \( \text{apply } U \text{ to } X \) means that the operation \( U \) is applied to the quantum variables \( X \). E.g., \( \text{apply } H \text{ to } x \) would apply the Hadamard gate to the variable \( x \) (we assume that \( H \) denote the Hadamard matrix). It is important that we can apply \( U \) to several variables \( X \) simultaneously, otherwise no entanglement between variables can ever be produced.

The program \( \text{init } x \) initializes \( x \) with the quantum state \( |0\rangle \). (Remember that we assumed that every variable type contains a distinguished element \( 0 \).)

The program \( \text{if } y \text{ then } \ell \text{ else } \ell \) will measure the qubit \( y \), and, if the outcome is 1, execute \( \ell \), otherwise execute \( \ell \).

The program \( \text{while } y \text{ do } \ell \) will measure the qubit \( y \), and if the outcome is 1, it executes \( \ell \). This is repeated until the outcome is 0.

Finally, \( \ell; \ell \) executes \( \ell \) and then \( \ell \). And \( \text{skip} \) does nothing. We will always implicitly treat \\
\( \cdot; \) as associative and \( \text{skip} \) as its neutral element.

**On the minimalism of the language.** This language is intentionally minimalistic. It seems to lack a number of features that are present, e.g., in [19]. Initializing variables with states other than \( |0\rangle \). Performing measurements. Probabilism (i.e., random sampling). Parameterizing operations/states using classical variables (e.g., \( \text{apply } R_x \text{ to } y \) where \( x \) is a variable of type \( \mathbb{R} \), and \( R_\theta \) a rotation by angle \( \theta \)). All these features are very important if we want to model anything but the simplest programs. Yet, as we will see, these features are not actually lacking. Using syntactic sugar (introduced in this section and in Section 7.2), we can recover all those features. Keeping the language minimal and encoding all advanced features allows us to get a much simpler core logic. Rules for working with the advanced features can then be derived from the core features.

**Semantics.** The *denotational semantics* of our programs \( \ell \) are represented as functions \( [\ell] \) on the mixed memories over \( X^{\text{all}} \), defined by recursion on the structure of the programs. Here \( X^{\text{all}} \) is a fixed set of program variables, and we will assume that \( \text{fv}(\ell) \subseteq X^{\text{all}} \) for all programs in this paper.\(^{10}\) The obvious cases are \( [\text{skip}] := \text{id} \) and \( [x] := [0] \circ [x] \). And application of an isometry \( U \) is also fairly straightforward given the syntactic sugar introduced above: \( [\text{apply } U \text{ to } X](\rho) := (U \text{ on } X)\rho(U \text{ on } X)^* \).

\(^9\)We will assume throughout the paper that all programs satisfy those well-typedness constraints. In particular, rules may implicitly impose type constraints on the variables and constants occurring in them by this assumption.

\(^{10}\)We fix some set \( X^{\text{all}} \) in order to avoid a more cumbersome notation \( [\ell]^X \) where we explicitly indicate the set \( X \) of program variables with respect to which the semantics is defined.
Initialization of a quantum variable is slightly more complicated: \texttt{init x} initializes the variable \texttt{x} with \texttt{0}, which is the same as removing \texttt{x}, and then creating a new variable \texttt{x} with content \texttt{0}. Removing \texttt{x} is done by the operation \texttt{tr}_{\text{x}} (partial trace, see page 5). And creating a new variable \texttt{x} is done by the operation \texttt{\otimes proj}|0\rangle_{\text{x}}. Thus we define \texttt{[init x] } (\rho) := \texttt{tr}_{\text{x}} \rho \otimes \texttt{proj}|0\rangle_{\text{x}}.

The if-command first performs a measurement and then branches. A measurement is described by one projector for each outcome. In our case, \texttt{proj}(i)} on \texttt{y} corresponds to outcome \texttt{i} = 0, 1. We then have that the state after measurement (without renormalization) is (\texttt{proj}(i)} on \texttt{y}) \rho (\texttt{proj}(i)} on \texttt{y})^* . Then \texttt{c} or \texttt{d} is applied to that state and the resulting states are added together to get the final mixed state. Altogether:

\[
[ \texttt{if y then c else d} ](\rho) := [c] (\downarrow_1(\rho)) + [d] (\downarrow_0(\rho))
\]

where \(\downarrow_i(\rho) := (\texttt{proj}(i)} on \texttt{y}) \rho (\texttt{proj}(i)} on \texttt{y})^*\)

While-commands are modeled similar: In an execution of a while statement, we have \(n \geq 0\) iterations of "measure with outcome 1 and run \(c\)" (which applies [\(c\) \(\otimes 1_{1}\) to the state), followed by "measure with outcome 0" (which applies \(\downarrow_{0}\) to the state). Adding all those branches up, we get the definition:

\[
[ \texttt{while y do c} ](\rho) := \sum_{n=0}^{\infty} \downarrow_0(([c] \circ \downarrow_1)^n(\rho))
\]

Syntactic sugar. To work productively with the minimal language from above, we introduce some syntactic sugar:

- \(\texttt{X} \triangleleft \psi\) (initialization with quantum state): To assign a quantum state \(\psi \in \ell^2(T)\) to variables \(\texttt{X}\) of type \(T\), we have to do the following: We fix an isometry \(U_\psi\) with \(U\texttt{|0}, \ldots, 0\rangle = \psi\). And then we initialize all \(\texttt{X}\) with \(\texttt{0}\) and apply \(U\). That is, \(\texttt{X} \triangleleft \psi\) abbreviates "\texttt{init x}_1; \ldots; \texttt{init x}_n; \texttt{apply U_\psi to X}" with \(\texttt{x}_1 \ldots \texttt{x}_n := \texttt{X}\) and some arbitrary isometry \(U_\psi\texttt{|0}, \ldots, 0\rangle := \psi\). (Such \(U_\psi\) is not unique but always exists.)

- \(\texttt{X} \leftarrow z\) (classical initialization / assign-statement): This is short for \(\texttt{X} \triangleleft |z\rangle\). (We assume that \(z\) is in the type of \(\texttt{X}\).)

- \(\texttt{Y} \leftarrow \texttt{measure X}\) (measurement). We wish to simulate a measurement in the computational basis using the commands from our minimal language. It is a well-known (and easy to check) fact that measuring \(\texttt{X}\) and assigning \(|z\rangle\) to \(\texttt{Y}\) (where \(z\) is the outcome) is equivalent to performing a CNOT from \(\texttt{X}\) to a \(|0\rangle\)-initialized \(\texttt{Y}\) and to a \(|0\rangle\)-initialized auxiliary register and discarding the auxiliary register. This can be expressed using our language: We define \(\texttt{Y} \leftarrow \texttt{measure X}\) to denote "\(\texttt{Y} \triangleleft |0\rangle; z \triangleleft |0\rangle; \texttt{apply CNOT to XY}; \texttt{apply CNOT to Xz}; z \triangleleft |0\rangle)\" where \(z\) is a fresh variable of the same type as \(\texttt{Y}\) and \(\texttt{X}\). (I.e., \(z\) is a variable that is used nowhere else.)

Similarly, we can also define a measurement of \(\texttt{X}\) that does not remember the outcome. (That is, its effect is merely to change the measured variables.) We write \texttt{measure X} to denote "\(z \triangleleft |0\rangle; \texttt{apply CNOT to Xz}; z \triangleleft |0\rangle)\" where \(z\) is a fresh variable of the same type as \(\texttt{X}\).

(Of course, it is also possible to model measurements other than computational basis measurements. To implement a projective measurement described by projectors \(\{P_i\}_i\), we simply replace CNOT by the unitary \(\sum_i P_i \otimes U_{\oplus i}\) where \(U_{\oplus i} : |z\rangle \mapsto |z \oplus i\rangle\). We do not fix a specific syntax for this construction.)
• $X \triangleleft D$ (random sampling). Here $D$ is a discrete probability distribution over $T$, the type of $X$. Sampling for $D$ is easily done by initializing $X$ in the state $\psi_D := \sum_{i \in T} \sqrt{D(i)}|i\rangle$ and then measuring that state in the computational basis (leaving $X$ in state $|i\rangle$ with probability $D(i)$). That is, $X \triangleleft D$ is shorthand for “$X \triangleleft \psi_D; \text{measure } X$.”

4 Hoare Logic with Ghosts

Recap Hoare logic. Before we introduce our Hoare logic with ghost variables, we quickly recap regular quantum Hoare logic.\textsuperscript{11} Intuitively, a Hoare triple $\{A\} \text{c} \{B\}$ means: If the initial state $\rho$ of the program $\text{c}$ satisfies $A$, and we run the program $B$, then the final state $[c](\rho)$ satisfies $B$. Since the states of programs in our semantics are mixed memories $\rho$ (i.e., density operators), we need to first define what it means for a mixed memory to satisfy a predicate. For this, the notion of support of a density operator comes in handy: A density operator can always be represented as $\rho = \sum_i \text{proj}(\psi_i)$, and intuitively this means that $\rho$ is a mixture of states $\psi_i$. (But note that this decomposition is not unique!) Then $\text{supp}\: \rho := \text{span}\{\psi_i\}$ is simply the subspace spanned by all the vectors that constitute $\rho$.\textsuperscript{12} (Fortunately, this definition turns out to be independent of the choice of $\psi_i$.) Now, if $A$ is a predicate over the program variables $X^{\text{all}}$ (formally: a subspace of $\ell^2(\mathbb{X}^{\text{all}})$), and $\rho$ is a mixed memory over $X^{\text{all}}$, then $\rho$ satisfies $A$ (written $\rho \vDash A$) iff $\text{supp}\: \rho \subseteq A$. (I.e., iff $\rho$ is a mixture of quantum memories in $A$.) With this notation (that will be changed somewhat later to accommodate ghost variables), we can formally define $\{A\} \text{c} \{B\}$ as: for all $\rho \vDash A$ we have $[c](\rho) \vDash B$. (We call $A$ the precondition and $B$ the postcondition.) For this logic, we can then prove a number of rules that allow us to derive the behavior of a complex quantum program from the behavior of its elementary building blocks. For example, the (easy to prove) $\text{SEQ}$ rule shows that $\{A\} \text{c} \{B\}$ and $\{B\} \text{d} \{C\}$ implies $\{A\} \text{c} \text{d} \{C\}$. This allows us to break down the analysis of a sequence of commands into an analysis of the individual commands. (And similar rules exist for quantum operations, while-loops, etc.)

However, this Hoare logic is somewhat limited in its expressivity. For example, we cannot express the fact that the variable $x$ is uniformly randomly distributed. Say $\text{c}$ samples $x \triangleleft \mathcal{D}$ where $\mathcal{D}$ is the uniform distribution. Then the final state is $\rho = \sum_{i \in T} \frac{1}{|T|} \text{proj}(|i\rangle)$ where $T$ is the type of $x$, and $\text{supp}\: \rho = \text{span}\{|i\rangle\}_{i \in T} = \ell^2[x] = \mathcal{T}$. So the only postcondition for this $c$ is $\mathcal{T}$, the trivial postcondition. So the above quantum Hoare logic forgets about the distribution of $x$ and remembers only what values have non-zero probability. (I.e., probabilism is treated as possibilistic nondeterminism.) For similar reasons, we cannot express, say, that $x$ is classical (e.g., after the program $\text{measure } x$).

Extensions of this basic quantum Hoare logic can make some statements about probabilities: Quantum Hoare logic whose pre-/postconditions are expectations\textsuperscript{7, 20} can, e.g., express that a certain predicate will hold with a certain probability. And\textsuperscript{19} can express that the outputs of two programs are identical, even taking into account their distributions. But both still lack the possibility of stating, as part of a pre-/postcondition, e.g., that a variable has a particular distribution. See also discussion in Section 8.2 for further discussion on the limitations of

\textsuperscript{11}Strictly speaking, “recap” is not the right word since as far as we know this variant of quantum Hoare logic has not explicitly been spelled out in the literature. However, we still consider it folklore because it is a relatively simple generalization of [4] (allowing for more general programs, density operator based semantics, and changing the presentation from weakest precondition transformers to Hoare triples), it is a simplification of [19] (which considers pairs of programs instead of single programs), and it is a special case of [20] (by considering only “strict” predicates there, i.e., predicates that are projectors, we get a logic that is roughly the same).

\textsuperscript{12}The usual formal definition of $\text{supp}\: \rho$ is $\text{supp}\: \rho := \text{im}\: P$ where $P$ is the smallest projector such that $P \rho P^* = \rho$. (This definition has the advantage of not requiring a specific choice of decomposition of $\rho$.) But it is easy to verify that this definition coincides with $\text{span}\{\psi_i\}$.}
Ghost variables. Our solution to this problem is the introduction of “ghost variables” (which will will often simply call “ghosts” for brevity). In our context, a ghost variable is a variable that cannot occur in the program (nor in the memory of the program) but only in predicates. The intuitive meaning of a ghost variable is that it can take any value that makes a predicate true. To illustrate the idea, let us forget about quantum programs for a moment and consider the classical case: For example, the classical postcondition $x = g^2$ would mean that after the execution of the program, the variable $x$ contains the square of $g$, if $x$ and $g$ are both program variables of type $\mathbb{N}$. But if $g$ is a ghost, then $x = g^2$ is true whenever there is some way to assign an integer to $g$ that makes $x = g^2$ true. In other words, the postcondition $x = g^2$ is equivalent to just saying that $x$ is a square. Now, in the classical case this is not very impressive: $x = g^2$ is just equivalent to $\exists z. x = z^2$. And any other predicate involving ghosts can also be rewritten into a regular predicate by using existential quantifiers. So, at least if we allow existential quantifiers in predicates (and there is no reason why we should not), ghost variables are useless for classical Hoare logic.\[13\] However, this argument does not apply in the quantum case. A quantum ghost variable cannot just be simulated using an existential quantifier (e.g., because ghost variables might be entangled with quantum variables).

So, how can we formalize ghost variables in the quantum setting? A classical memory $m$ (containing only program variables) satisfies a predicate $A$ involving ghosts iff there exists a larger memory $m^\circ$ containing both program and ghost variables such that $m^\circ$ satisfies $A$, and $m$ is the result of removing all ghosts from $m^\circ$. The quantum analogue of removing variables is the partial trace. That is, if we have a mixed memory $\rho$ on $XG$, then $\rho_X := \text{tr}_G \rho$ is the result of removing all ghosts $G$ from $\rho$. Thus, we are ready for our first tentative definition: $\rho \models A$ iff there exists a density operator $\rho^\circ$ on $XG$ such that $\text{tr}_G \rho^\circ = \rho$ and $\text{supp} \rho^\circ \subseteq A$.

Note that in the previous definition, the program variables $X$ and the ghost variables $G$ can be entangled in arbitrary ways (since we put no restriction on $\rho^\circ$). However, there is a different possibility of defining ghost variables: We could additionally require that $\rho^\circ$ is $(X, G)$-separable. That would mean that ghost and program variables may not be entangled. This will lead to a very different behavior of ghost variables. It will turn out that both variants have their uses, so in our logic we will simply consider both variants: We consider two kinds of ghost variables, entangled ghost variables $E$ and unentangled ghost variables $U$. That is, $A$ may contain both entangled and unentangled ghosts, and $\rho^\circ$ is required to be $(XE, U)$-separable. This means that the variables $U$ cannot be entangled with the program variables $X$, but the variable $E$ can be!

Formal definitions. We can now mold all these ideas into a formal definition:

**Definition 1 (Satisfying a predicate with ghosts)** Let $\rho$ be a mixed memory over $X$. Let $A$ be a predicate over $XEU$. Then a density operator $\rho$ over $X$ satisfies $A$ (written $\rho \models A$) iff there exists a $(XE, U)$-separable mixed memory $\rho^\circ$ over $XEU$ such that $\text{supp} \rho^\circ \subseteq A$ and $\text{tr}_{EU} \rho^\circ = \rho$.

Recall that we use different letters for different kinds of variables (cf. page 4), so the above definition implicitly assumes that $X$ are program variables, $E$ are entangled ghost variables, and $U$ are unentangled ghost variables. In the remainder of this work, we assume that these conventions are understood. Note that if $E = U = \emptyset$, then **Definition 1** specializes to the definition given in the recap above, namely $\rho \models A \iff \text{supp} \rho \subseteq A$.

Given the definition of satisfying a predicate, it is straightforward to define our Hoare logic:
Definition 2 (Hoare logic with ghosts) Let \( A \) be a predicate over \( X^{\text{all}}EU \), and \( B \) a predicate over \( X^{\text{all}}E'U' \), and \( \epsilon \) a program.

Then \( \{ A \} \epsilon \{ B \} \) iff for all mixed memories \( \rho \) over \( X^{\text{all}} \) with \( \rho \models A \), we have that \( [\epsilon](\rho) \models B \).

Note that \( A \) and \( B \) do not need to use the same ghosts. Ghosts are local to the interpretation of a given predicate. In particular, if ghost variables are chosen in a particular way when showing \( \rho \models A \), this does not mean that they have to be chosen in a related way in \( \rho \models B \).

Example. Consider the following situation. We have two variables \( x, y \) of type \( \{0, 1\} \). Initially, they are entangled in the state \( \psi := \frac{1}{\sqrt{2}} |00\rangle + \frac{1}{\sqrt{2}} |11\rangle \). Now we initialize \( y \) with \( |0\rangle \). What do we know about \( x \)? The initial state of \( x, y \) is represented by the predicate \( xy = q \psi \) in our notation (see page 6). So, we are asking for a predicate \( B \) involving \( x \) such that \( \{ xy = q \psi \} \text{init} y \{ B \} \).

Lemma 1 (Irrelevance of sets of ghosts) Let \( \rho \) be a mixed memory over \( X \). Let \( \rho \models EU A \) denote \( \rho \models A \) (as in Definition 1) where \( A \) is interpreted as a predicate over \( X^{\text{all}}EU \).

Assume that \( E_1U_1, E_2U_2 \supseteq \text{fv}(A) \setminus X \). Then \( \rho \models E_1U_1 A \) iff \( \rho \models E_2U_2 A \).

Proof. For clarity, we write \( A_V \) when we interpret \( A \) as a predicate over \( V \).

Due to symmetry, we only need to prove \( \rho \models E_1U_1 A \implies \rho \models E_2U_2 A \). Assume \( \rho \models E_1U_1 A \). Then there exists a \( (XE_1, U_1) \)-separable mixed memory \( \rho^o \) over \( XE_1U_1 \) with \( \text{supp} \rho^o \subseteq \text{AXE}_1U_1 \) and \( \text{tr}_{E_1U_1} \rho^o = \rho \).

Let \( \rho^o := \text{tr}_{E_1U_1} \rho \). Then \( \rho^o \) is a mixed memory over \( X(E_1 \cap E_2)(U_1 \cap U_2) \). And since \( \rho^o \) was \( (XE_1, U_1) \)-separable, \( \rho^o \) is \( (X(E_1 \cap E_2), U_1 \cap U_2) \)-separable. And since \( \text{supp} \rho^o \subseteq \text{AXE}_1U_1 \), we have \( \text{supp} \rho^o \subseteq \text{AX}(X(E_1 \cap E_2)(U_1 \cap U_2)) \). (The last step uses that \( X(E_1 \cap E_2)(U_1 \cap U_2) \supseteq \text{fv}(A) \).

Let \( \rho^o := \rho^o \otimes \sigma_{E_2 \setminus E_1} \otimes \sigma_{U_2 \setminus U_1} \), where \( \sigma_{E_2 \setminus E_1} \) and \( \sigma_{U_2 \setminus U_1} \) are arbitrary mixed memories of trace 1 over \( E_2 \setminus E_1 \) and \( U_2 \setminus U_1 \), respectively. Then \( \rho^o \) is is \( (XE_2U_2) = (X(E_1 \cap E_2)(E_2 \setminus E_1), (U_1 \cap U_2)(U_2 \setminus U_1)) \)-separable since \( \rho^o \) is \( (X(E_1 \cap E_2), U_1 \cap U_2) \)-separable. And \( \text{supp} \rho^o \subseteq \text{supp} \rho^o \otimes \ell^2[E_2U_2 \setminus E_1U_1] \subseteq \text{AX}(X(E_1 \cap E_2)(U_1 \cap U_2)) \otimes \ell^2[E_2U_2 \setminus E_1U_1] = \text{AXE}_2U_2 \). Furthermore:

\[
\text{tr}_{E_2U_2} \rho^o = \text{tr}_{(E_1 \cap E_2)(U_1 \cap U_2)} \rho^o = \text{tr}_{X(E_1 \cap E_2)(U_1 \cap U_2)} \text{tr}_{E_1U_1 \setminus E_2U_2} \rho^o = \text{tr}_{E_1U_1} \rho^o = \rho.
\]

Thus \( \rho \models E_2U_2 A \).

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5 Predicates with Ghosts

In this section, we describe three important kinds of predicates that can be expressed using ghosts.

5.1 Variables with a certain distribution

First, we show that entangled ghosts can be used to express that a variable has a certain distribution. Given a distribution $D$ on $T$, we define $\psi_{DD} := \sum_i \sqrt{D(i)} |i\rangle \otimes |i\rangle$, a state on two variables of type $T$. This state has the property that, if we erase (or measure) the second part, we get a $D$-distributed classical value $|i\rangle$ in the first part. So, if $xe$ is in state $\psi_{DD}$, then, since $e$ is a ghost, $e$ is, in effect, erased. Thus the predicate $xe = \psi_{DD}$ effectively means that $x$ is $D$-distributed. Thus we introduce syntactic sugar for predicates:

- $\mathsf{distrib}(X, D)$ ($X$ is $D$-distributed). $\mathsf{distrib}(X, D)$ is short for $xe =_q \psi_{DD}$ where $e$ is a fresh entangled ghost (i.e., one that does not occur elsewhere in the predicate we are formulating) of the same type as $X$.

- $\mathsf{uniform}(X)$ ($X$ is uniformly distributed). This is short for $\mathsf{distrib}(X, D)$ where $D$ is the uniform distribution on the type of $X$.

(As a special case, if $D$ is the uniform distribution on a single bit, then $\psi_{DD}$ is the state $\psi$ from the example in the previous section. So the postcondition $B$ in that example can indeed be written as $\mathsf{uniform}(x)$ as was already hinted there.)

So far, we gave only a relatively hand-waving explanation why $\mathsf{distrib}(X, D)$ means that $X$ is $D$-distributed. But the following lemma makes this formal:

Lemma 2 (Distribution predicates) Let $D$ be a distribution over $T$. Let $\rho$ be a mixed memory over $Y$. Let $X \subseteq Y$ have type $T$. Let $\rho_D := \sum_i D(i)\mathsf{proj}(|i\rangle)$ be a mixed memory over $X$. (I.e., $\rho_D$ contains a $D$-distributed classical value $i$.) Then the following are equivalent:

- $\rho \models \mathsf{distrib}(X, D)$.
- There exists a mixed memory $\rho'$ over $Y \setminus X$ such that $\rho = \rho' \otimes \rho_D$.

In other words, $\mathsf{distrib}(X, D)$ means that $X$ is $D$-distributed and independent of other variables.

Proof. First, we check that $\rho_D$ is the result of removing variable $e$ from the quantum memory $\psi_{DD}$ (we interpret $\psi_{DD}$ as a quantum memory over $xe$):

$$\mathsf{tr}_e \mathsf{proj}(\psi_{DD}) = \mathsf{tr}_e \mathsf{proj}\left(\sum_i \sqrt{D(i)} |i\rangle_X \otimes |i\rangle_e\right) = \sum_i D(i)\mathsf{proj}(|i\rangle_X) = \rho_D. \tag{1}$$

$\mathsf{distrib}(X, D)$ is syntactic sugar for $xe =_q \psi_{DD}$ and thus is a predicate over some variables $\mathsf{YEU}$ with $X \subseteq Y$ and $e \in E$.

"

First we show that if $\rho \models \mathsf{distrib}(X, D)$, then $\rho = \rho' \otimes \rho_D$ for some $\rho'$. Since $\rho \models \mathsf{distrib}(X, D)$, there exists a $\rho'$ over $\mathsf{YEU}$ with $\mathsf{supp}\rho' \subseteq \mathsf{distrib}(X, D)$ and $\mathsf{tr}_{\mathsf{EU}} \rho' = \rho$. Thus $\rho' = \sum_i \mathsf{proj}(\psi_i)$ for some $\psi_i$ with

$$\psi_i \in \mathsf{distrib}(X, D) = (xe =_q \psi_{DD}) = \mathsf{span}\{\psi_{DD}\} \otimes \mathbb{C}^2[\mathsf{Xe}^6].$$
Hence ψi = ψDD ⊗ ψ′i for some ψ′i over YEU \ Xe. Thus
\[ ρ = \text{tr}_{EU} \rho^o = \text{tr}_{EU} \sum_i \text{proj}(ψDD) ⊗ \text{proj}(ψ′i) = \text{tr}_{EU} \text{proj}(ψDD) ⊗ \text{tr}_{EU \setminus e} \sum_i \text{proj}(ψ′i) \uplus ρD ⊗ ρ′. \]

This shows the \( \Rightarrow \)-direction.

\( \Leftarrow \): We next show that if \( ρ = ρ' ⊗ ρ_D \), then \( ρ ⇐\text{distrib}(X, D) \). Let \( ρ^o := ρ' ⊗ \text{proj}(ψDD) ⊗ σ_{E \setminus e} ⊗ σ_U \) for some arbitrary mixed memories \( σ_{E \setminus e}, σ_U \) of trace 1 on \( E \setminus e \) and \( U \), respectively. The \( ρ^o \) is (YE, U)-separable and \( \text{supp} ρ^o ⊆ \text{span}{ψDD} ⊗ ℓ^2[|Xe|^2] = \text{distrib}(X, D) \).

Furthermore, \( \text{tr}_{EU} ρ^o = ρ' ⊗ \text{tr}_{proj}(ψDD) \uplus ρ' ⊗ ρ_D \). This shows the \( \Leftarrow \)-direction. \( \square \)

We will see examples of this predicate in the rule \text{SAMPLE} for sampling statements (\( y \leftarrow D \)), and in our analysis of the quantum one-time-pad in Section 8.3.

### 5.2 Separable variables

A concept specific to the quantum setting is for a variable to be separable, i.e., not entangled with any other variables. (But a separable variable may be probabilistically correlated!)

Expressing that a variable \( x \) is separable seems, at the first glance, impossible to do using predicates (that are modeled as subspaces): Such a predicate would have to contain, e.g., the states \( |00\rangle_{xy} \) and \( |11\rangle_{xy} \) (since in both cases, \( x \) and \( y \) are equal but not entangled) but not the state \( \frac{1}{\sqrt{2}}|00\rangle_{xy} + \frac{1}{\sqrt{2}}|11\rangle_{xy} \). But that would mean that the predicate is not closed under linear combinations, hence not a subspace.

Yet, by introducing ghosts, we can model separable variables. To understand how, we first need to recall a concept from [19], namely the quantum equality (between two variables):

**Definition 3 (Quantum equality [19, Defs. 22, 23])** Let \( W, W' \subseteq V \) be disjoint lists of quantum variables. (\( W \) and \( W' \) have the same type.) Let \text{SWAP} be the unitary that swaps the content of \( W \) and \( W' \). That is, \( \text{SWAP}(|i⟩_W ⊗ |j⟩_W ⊗ ψ'') := |j⟩_W ⊗ |i⟩_W' ⊗ ψ'' \) for all \( i, j \in T \) and all quantum memories \( ψ'' \) over \( V \setminus WW' \).

Then \( W ≡_q W' \) is the set of all quantum memories \( ψ \) on \( V \) such that \( \text{SWAP}ψ = ψ \).

([19] also presents a number of useful lemmas for rewriting and simplifying predicates involving \( ≡_q \)).

In other words, we consider \( W \) and \( W' \) to have equal content (\( W ≡_q W' \)) iff a state is invariant under swapping \( W \) and \( W' \). Now, it turns out that if \( W ≡_q W' \), but \( W \) and \( W' \) are not entangled with each other, then \( W \) and \( W' \) also cannot be entangled with any other variables:

**Lemma 3 (Quantum equality & separable states [19, Coro. 25])** Fix quantum memories \( ψ \) over \( V \supseteq W \) and \( ψ' \) over \( V' \supseteq W' \). Then \( ψ ⊗ ψ' \in (W ≡_q W') \) iff \( ψ \) and \( ψ' \) are of the form \( ψ = ψ_W ⊗ ψ_{V \setminus W} \) and \( ψ' = ψ'_W ⊗ ψ'_{V' \setminus W'} \) and \( ψ_W = ψ'_{W', W} \uplus ψ'_{W', W} \) for some quantum memories \( ψ_W, ψ_{V \setminus W}, ψ'_{V \setminus W}, ψ'_{V' \setminus W'}, ψ_{W'} \uplus ψ'_{W' \setminus W'} \) over \( W, V \setminus W, W', V' \setminus W' \), respectively.

\(^{14}\)The original definition of \( ≡_q \) is more general because we can write something like \( Ux ≡_q U'y \) meaning that \( x \) and \( y \) are equal up to operations \( U, V \). Since we will no explicitly make use of this in this paper, we only gave the definition of the special case here. But the more general definition is, of course, also admissible in predicates as defined here.

\(^{15}\)Up to renaming of variables, formally \( ψ_W = U_{W' \setminus W} ψ'_{W'} \).
But this means that a program variable \( x \) is separable iff \( x \equiv_q u \) for some unentangled ghost! (Remember from Definition 1 that an unentangled ghost \( u \) will, by definition, not be entangled with \( x \)) Thus we can introduce the following syntactic sugar for predicates:

- \( \text{separable}(X) \) (\( X \) is separable). \( \text{separable}(X) \) is short for \( X \equiv_q u \) where \( u \) is a fresh unentangled ghost (i.e., one that does not occur elsewhere in the predicate we are formulating) of the same type as \( X \).

The following lemma formalizes our informal reasoning above, \( \text{separable}(X) \) indeed characterizes separability:

**Lemma 4 (Separability predicates)** Let \( \rho \) be a mixed memory on \( Y \). Let \( X \subseteq Y \). Then the following are equivalent:

- \( \rho \models \text{separable}(X) \).
- \( \rho \) is \((X, Y \setminus X)\)-separable.

**Proof.** \( \text{separable}(X) \) is syntactic sugar for \( X \equiv_q u \) and thus is a predicate over some variables \( \text{YE} \) with \( X \subseteq Y \) and \( u \in U \). And \( X \) and \( u \) have the same type.

\( \implies \): First we show that if \( \rho \models \text{separable}(X) \), then \( \rho \models (X, Y \setminus X)\)-separable. Since \( \rho \models \text{separable}(X) \), there exists a \((\text{YE}, U)\)-separable \( \rho^2 \) with \( \text{supp} \rho^2 \subseteq \text{separable}(X) \) and \( \text{tr}_{\text{EU}} \rho^2 = \rho \). Thus \( \rho^2 = \sum_i \text{proj}((\psi_{\text{YE}, i} \otimes \psi_{1, i})) \) for some \( \psi_{\text{YE}, i}, \psi_{1, i} \) over \( \text{YE} \) and \( U \), respectively. Then

\[
\psi_{\text{YE}, i} \otimes \psi_{1, i} \in \text{supp} \rho^2 \subseteq \text{separable}(X) = (X \equiv_q u).
\]

By Lemma 3, this implies that \( \psi_{\text{YE}, i} = \psi_{X, i} \otimes \psi_{\text{YE} \setminus X, i} \) for some \( \psi_{X, i}, \psi_{\text{YE} \setminus X, i} \) over \( X \) and \( \text{YE} \setminus X \), respectively. Thus \( \text{proj}((\psi_{\text{YE}, i})) \) is \((X, \text{YE} \setminus X)\)-separable. Thus \( \text{tr}_{\text{E}} \text{proj}((\psi_{\text{YE}, i})) \) is \((X, Y \setminus X)\)-separable. Hence

\[
\rho = \text{tr}_{\text{EU}} \rho^2 = \sum_i \text{tr}_{\text{E}} \text{proj}((\psi_{\text{YE}, i}))
\]

is \((X, Y \setminus X)\)-separable as well. This shows the \( \implies \)-direction.

\( \impliedby \): We next show that if \( \rho \models (X, Y \setminus X)\)-separable, then \( \rho \models \text{separable}(X) \). Since \( \rho \models (X, Y \setminus X)\)-separable, \( \rho = \sum_i \text{proj}(\psi_{X, i} \otimes \psi_{Y \setminus X, i}) \) for some quantum memories \( \psi_{X, i}, \psi_{Y \setminus X, i} \) over \( X \) and \( Y \setminus X \), respectively. Without loss of generality, \( \|\psi_{X, i}\| = 1 \). Let

\[
\psi_i^0 := \psi_{X, i} \otimes \psi_{Y \setminus X, i} \otimes \psi_{E, i} \otimes \psi_{1, i} \otimes \psi_{U \setminus 1, i}
\]

where \( \psi_{E, i}, \psi_{U \setminus 1, i} \) are arbitrary quantum memories of norm 1 on \( E \) and \( U \setminus u \), respectively, and \( \psi_{1, i} := \psi_{X, i} \) except that \( \psi_{1, i} \) is a quantum memory over \( u \) and not over \( X \). By Lemma 3, \( \psi_i^0 \in (X \equiv_q u) \). Let \( \rho^2 := \sum_i \text{proj}(\psi_i^0) \). Then \( \rho^2 \) is \((\text{YE}, U)\)-separable and \( \text{supp} \rho^2 = \text{span} \{\psi_i^0\} \subseteq (X \equiv_q u) = \text{separable}(X) \). And

\[
\text{tr}_{\text{EU}} \rho^2 = \sum_i \text{proj}(\psi_{X, i} \otimes \psi_{Y \setminus X, i}) = \rho.
\]

(Using that \( \psi_{E, i}, \psi_{1, i}, \psi_{U \setminus 1, i} \) all have norm 1.) Hence \( \rho \models \text{separable}(X) \). This shows the \( \impliedby \)-direction. \( \square \)

As an example for the relationship between different predicates, notice that \( \text{distrib}(x, D) \) implies \( \text{separable}(x) \) since \( \text{distrib}(x, D) \) implies that \( x \) is distributed independently from all other
variables (Lemma 2). This also follows within our logic by an application of the rule Transmute below, see the example after rule Transmute.

5.3 Classical variables

A third application of ghost variables is to formulate predicates that imply that a variable has a classical state. We say a mixed memory $\rho$ over $Y$ is classical in $X \subseteq Y$ iff it is of the form $\rho = \sum_i \text{proj}(\ket{i}_X) \otimes \rho_i$ for some mixed memories $\rho_i$ over $Y \setminus X$. (This is often called a \textit{cq-state}.)

Expressing that a variable $x$ is classical seems, at the first glance, impossible to do using predicates (that are modeled as subspaces): Such a predicate would have to contain, e.g., the states $\ket{0}_x$ and $\ket{1}_x$ (since those are classical) but not the state $\frac{1}{\sqrt{2}} \ket{0}_x + \frac{1}{\sqrt{2}} \ket{1}_x$. But that would mean that the predicate is not closed under linear combinations, hence not a subspace.

Yet, by introducing ghosts, we can model classicality. In order to see how, we introduce a different equality notion between quantum variables, $\equiv_d$. Intuitively, two variables are classically equal iff measuring both in the computational basis will always give the same outcome. (So, $\ket{0}_x$ and $\ket{0}_y$ would be classically equal, but $\frac{1}{\sqrt{2}} \ket{0}_x + \frac{1}{\sqrt{2}} \ket{1}_x$ and $\frac{1}{\sqrt{2}} \ket{0}_y + \frac{1}{\sqrt{2}} \ket{1}_y$ would not be.)

Formally:

\textbf{Definition 4 (Classical equality)} Let $W, W' \subseteq V$ be disjoint lists of quantum variables, ($W$ and $W'$ have the same type $T$.)

Then $W \equiv_d W'$ is the span of all quantum memories of the form $\ket{i}_W \otimes \ket{i}_W' \otimes \psi$ with $i \in T$ and $\psi$ a quantum memory on $V \setminus WW'$.

If we think of two variables $x, u$ both having the same state $\psi$, then $x \equiv_d u$ holds if $\psi = \ket{i}$ for some $i$ (i.e., if $\psi$ is a classical state). But if $\psi$ is a superposition of different $\ket{i}$, then measuring both $x$ and $u$ in the computational basis gives different results with non-zero probability. Hence $x \not\equiv_d u$ in that case. This suggests that $x$ is classical iff it is classically equal to some unentangled ghost variable $u$. That is, we introduce the following syntactic sugar for predicates:

- $\text{class}(X)$ ($X$ is classical). $\text{class}(X)$ is short for $X \equiv_d u$ where $u$ is a fresh unentangled ghost (i.e., one that does not occur elsewhere in the predicate we are formulating) of the same type as $X$.

The following lemma formalizes our informal reasoning above, $\text{class}(X)$ indeed characterizes classicality:

\textbf{Lemma 5 (Classicality predicates)} Let $\rho$ be a mixed memory over $Y$. Let $X \subseteq Y$. Then the following are equivalent:

- $\rho \models \text{class}(X)$
- $\rho$ is classical in $X$. (As defined at the beginning of this section.)

\textit{Proof.} $\text{class}(X)$ is syntactic sugar for $X \equiv_d u$ and thus is a predicate over some variables $YEU$ with $X \subseteq Y$ and $u \in U$.

$\Rightarrow$": First we show that if $\rho \models \text{class}(X)$, then $\rho$ is classical in $X$. Since $\rho \models \text{class}(X)$, there exists a $(YE, U)$-separable $\rho^0$ with $\text{supp} \rho^0 \subseteq \text{class}(X)$ and $\text{tr}_U \rho^0 = \rho$. Thus $\rho^0 = \sum_i \text{proj}(\psi_{YE,i} \otimes \psi_{U,i})$ for some $\psi_{YE,i}, \psi_{U,i}$ over $YE$ and $U$, respectively. Without loss of generality, $\|\psi_{U,i}\| \neq 0$ for all $i$. And $\psi_{YE,i} \oplus \psi_{U,i} \in \text{supp} \rho^0 \subseteq \text{class}(X)$. Fix some $i$. (We will

16Somewhat counterintuitively, $x$ and $y$ are also classically equal if they are in the entangled state $\frac{1}{\sqrt{2}} \ket{00}_{xy} + \frac{1}{\sqrt{2}} \ket{11}_{xy}$. But this will not matter in our setting since we will apply $\equiv_d$ only to unentangled variables.

17Classical equality to some entangled ghost would not be sufficient due to the situation described in footnote 16.
More interesting are the rules for operations on quantum states (isometries, initialization): 

Sample* for measurements and random sampling. We discuss the predicate this section. We can "forget" Definition 2 and build only on the rules from this section. (Convenient particular, all "derived rules" in Section 7 are a consequence of these core rules. That is, after primitive, plus some useful structural rules) that form the basis of the rest of this paper. In logic semantically (Definition 2), the set of rules is not fixed a priori (since we can always prove in this section, we present the core reasoning rules for our logic. Since we have defined the 

6 Core Rules

In this section, we present the core reasoning rules for our logic. Since we have defined the logic semantically (Definition 2), the set of rules is not fixed a priori (since we can always prove additional rules sound). Nevertheless, we identify a set of important rules (one per language primitive, plus some useful structural rules) that form the basis of the rest of this paper. In particular, all “derived rules” in Section 7 are a consequence of these core rules. That is, after this section we can “forget” Definition 2 and build only on the rules from this section. (Convenient additional rules will be derived in later sections as corollaries.)

6.1 Rules for individual statements

For each command of our language (sequence, skip, initialization, application, if, while), we introduce one rule that derives a Hoare judgment for that command from judgments about its subterms. The rules for sequence and skip are quite obvious and follow directly from the definition:

\[
\begin{align*}
\text{SEQ} & : \{A\} e \{B\} \quad \{B\} \delta \{C\} \\
\text{SKIP} & : A \subseteq B
\end{align*}
\]

More interesting are the rules for operations on quantum states (isometries, initialization):

\[
\begin{align*}
\text{APPLY} & : \{A\} \text{apply } U \text{ to } X \{(U \text{ on } X) \cdot A\} \\
\text{INIT} & : \{A\} \text{init } x \{A\{e/x\}, x =_q |0\}
\end{align*}
\]
**Apply** says that applying an isometry $U$ to variables $X$ has the effect of multiplying the predicate $A$ with $U$ (after suitably lifting $U$ to operate on quantum memories, see page 5 for the definition of $U$ on $X$). **Init** is more interesting because it is the first rule that introduces ghosts. Since initialization “overwrites” the original value of $x$, $x$ becomes an engangeded ghost, thus the precondition $A$ is replaced by $A\{e/x\}$, i.e., $x$ is replaced by a fresh ghost $e$. ($e$ is fresh, i.e., $\notin fv(A)$, because otherwise $\{e/x\}$ would not be welltipped.) Additionally, $x$ will afterwards be in the state $\ket{0}$, so the postcondition additionally contains $x =_{q} \ket{0}$. The rules **Apply** and **Init** are shown in Lemmas 10 and 11 in Section 6.3.

The rules for if and while do not introduce ghosts and are the same as in “regular” quantum Hoare logic:

\[
\begin{align*}
\textbf{If} & \quad \{ (\text{proj}(\ket{1}) \text{ on } x) \cdot A \} \epsilon \{ B \} \quad & \textbf{While} & \quad \{ (\text{proj}(\ket{1}) \text{ on } x) \cdot A \} \epsilon \{ A \}
\end{align*}
\]

Since the if-statement measures $x$ before executing $\epsilon$ or $\delta$ (see Section 3), the precondition $A$ becomes $(\text{proj}(\ket{1}) \text{ on } x) \cdot A$ when that measurement returns $1$ and $\epsilon$ is executed (as $\text{proj}(\ket{1})$ is the projector corresponding to measurement outcome $1$), and it becomes $(\text{proj}(\ket{0}) \text{ on } x) \cdot A$ if the measurement returns $0$ and $\delta$ is executed. Thus analyzing **if** then $A$ else $B$ reduces to analyzing $\epsilon$ and $\delta$ with those two respective preconditions.

Similarly, **while** $x \text{ do } \epsilon$ executes $\epsilon$ after measuring $x$ and getting $1$. Thus, if we use $A$ as the loop invariant, the postcondition for the loop body becomes $(\text{proj}(\ket{1}) \text{ on } x) \cdot A$. And to end the loop, the measurement of $x$ must return $0$, hence we get the postcondition $(\text{proj}(\ket{0}) \text{ on } x) \cdot A$ for the overall loop. The rules **If** and **While** are proven in Lemmas 12 and 13 in Section 6.3.

### 6.2 Further core rules

Besides the per-statement rules from the previous section, we will use five more rules, related to case-distinctions and to the modification of ghosts. First, we consider case-distinctions. In classical Hoare logic, we can easily show the following rule: $\forall z. \{ x = z, A \} \epsilon \{ B \} \Rightarrow \{ A \} \epsilon \{ B \}$. That is, to show $\{ A \} \epsilon \{ B \}$, it is sufficient to consider each possible value $z$ of $x$ separately and prove $\{ A \} \epsilon \{ B \}$ under the additional assumption that $x = z$ holds in the precondition. An immediate quantum analogue would be: $\forall \psi. \{ x =_{q} \psi, A \} \epsilon \{ B \} \Rightarrow \{ A \} \epsilon \{ B \}$. There are two problems with such this rule. First, it does not hold in this generality: $x =_{q} \psi$ implies that $x$ is not entangled with any other variables (because it is in the specific pure state $\psi$), so proving $\{ x =_{q} \psi, A \} \epsilon \{ B \}$ for all $\psi$ does not guarantee anything about the behavior of $\epsilon$ in the presence of entanglement. And even if we fix this by adding suitable extra conditions, the rule will force us to always quantify over all possible $\psi$. But if, for example, $x$ is guaranteed to be classical (e.g., $A = \text{class}(x)$) then we would like to only consider the cases $x = \ket{z}$. To formulate a rule that solves both problems, we introduce an additional concept:

**Definition 5 (Disentangling)** A predicate $A$ on $XU$ is $M$-disentangling (for a set $M \subseteq \ell^{2}[X]$) iff: For all sets of variables $VX$ (disjoint from $XU$), all quantum memories $\psi_{VX} \neq 0$ over $VX$, and all quantum memories $\psi_{U} \neq 0$ over $U$ with $\psi_{VX} \otimes \psi_{U} \in A$, we have that $\psi_{VX} = \psi_{V} \otimes \psi_{X}$ for some $\psi_{V} \in \ell^{2}[V]$ and some $\psi_{X} \in M$.

What does this definition mean? Roughly speaking, it means that if variables $X$ and $U$, jointly, satisfy $A$, and variables $U$ are not entangled with variables $X$ or $V$, then we know that variables

\[\text{Formally, a counterexample would be: } A := (\text{xy} =_{q} \ket{00} + \ket{11}), B := \bot, \text{ and } \epsilon := \text{skip}. \text{ Then for all } \psi, (x =_{q} \psi, A) = \bot, \text{ hence } \{ x =_{q} \psi, A \} \text{skip } \{ B \}. \text{ But } \{ A \} \epsilon \{ B \} \text{ does not hold.}\]
are also not entangled with variables \( V \), and additionally that variables \( X \) will be in one of the states in \( M \).

A trivial example would be \( A := (xu = \phi_1 \otimes \phi_2) \) which is \( \{ \phi_1 \} \)-disentangling. That is, if \( xu \) are in state \( \phi_1 \otimes \phi_2 \), then \( x \) is in state \( \phi_1 \) (unsurprisingly). Similarly, for any non-separable \( \phi \), \( S = \text{span}\{\phi\} \) is \( \sigma \)-disentangling (as the variables \( xu \) cannot at the same time be non-entangled and in state \( \phi \)). The following lemma gives two more interesting examples of disentangling predicates:

**Lemma 6** Let \( T \) be the type of \( X \). Then \( X \equiv_d U \) and separable\((X)\) are \( \ell^2[X] \)-disentangling. And \( X \equiv_d U \) and class\((X)\) are \( \{ i \} \}_{i \in T} \)-disentangling.

**Proof.** We first show that \( X \equiv_d U \) is \( \ell^2[X] \)-disentangling. (This also implies that separable\((X)\) is \( \ell^2[X] \)-disentangling since separable\((X)\) is simply syntactic sugar for \( X \equiv_d u \).) Fix some variables \( V \), and quantum memories \( \psi_{VX} \) and \( \psi_U \) over \( VX \) and \( U \), respectively, with \( \psi_{VX} \otimes \psi_U \in (X \equiv_d U) \). By Lemma 3 (with \( \psi = VX \), \( W = X \), \( V' = W' = U \)), this implies that \( \psi_{VX} \) can be written as \( \psi_{VX} = \psi_V \otimes \psi_X \) for some quantum memories \( \psi_V, \psi_X \) over \( V, X \), respectively. And trivially, \( \psi_X \in \ell^2[X] \). Thus \( X \equiv_d U \) is \( \ell^2[X] \)-disentangling by Definition 5.

Now we show that \( X \equiv_d U \) is \( \{ i \} \)\(_{i \in T}\)-disentangling. (This also implies that class\((X)\) is \( \{ i \} \)\(_{i \in T}\)-disentangling since class\((X)\) is simply syntactic sugar for \( X \equiv_d u \).) Fix some variables \( V \), and quantum memories \( \psi_{VX} \) and \( \psi_U \) over \( VX \) and \( U \), respectively, with \( \psi_{VX} \otimes \psi_U \in (X \equiv_d U) \) and \( \psi_U \neq 0 \). By Definition 5, we need to show that \( \psi_{VX} = \psi_V \otimes |i\rangle_X \) for some \( i \in T \) and \( \psi_V \) over \( V \). We decompose \( \psi_{VX} = \sum \lambda_i \psi_{V,i} \otimes |i\rangle_X \) and \( \psi_U = \sum \lambda'_j |j\rangle_U \) for some \( \psi_{V,i} \neq 0 \) over \( V \). Since \( \psi_U \neq 0 \), there exists a \( j \) such that \( \lambda'_j \neq 0 \). If \( \lambda_i \neq 0 \) for some \( i \neq j \), then \( \psi_{VX} \otimes \psi_U \) is not in the span of states of the form \( \nu_X \otimes \nu_U \otimes \ldots \), in contradiction to \( \psi_{VX} \otimes \psi_U \in (X \equiv_d U) \). Thus \( \lambda_i = 0 \) for all \( i \neq j \), hence \( \psi_{VX} = \lambda_j \psi_{V,j} \otimes |j\rangle_X \) as desired. Thus \( X \equiv_d U \) is \( \{ i \} \)\(_{i \in T}\)-disentangling. \( \square \)

Armed with the definition of disentangling predicates, we can formulate the rule for case distinctions:

**Case**

\[
\begin{align*}
\text{C is M-disentangling predicate on } XU & \quad A \subseteq C \quad \forall \psi \in M, \{ X =_q \psi, A \} \in \{ B \} \\
\{ A \} & \in \{ B \}
\end{align*}
\]

As a special case (with \( C := \text{class}(x) \) and using Lemma 6), we can recover a rule for case distinction over classical variables: \( \forall z. \{ X =_q |z\rangle, \text{class}(X), A \} \in \{ B \} \Rightarrow \{ \text{class}(X), A \} \in \{ B \} \). See the derived rule CASECLASSICAL on page 34 for details. Notice that we would not have been able to even state such a case rule without using ghosts! The Case rule is proven in Lemma 14 in Section 6.3.

The Case rule has the disadvantage that we need to have a disentangling predicate in the precondition. As described above, this is necessary because the variable under consideration might be entangled with other variables. However, if we make a case distinction over the state of all variables, then this requirement disappears. In fact, it turns out that it is enough to make a case distinction over the state of the free variables in program and pre-/postconditions plus one extra variable \( x \) (this is not obvious because those variables might still be entangled with other variables that are not used but nevertheless present, even variables with uncountable type):

**Case**

\[
\begin{align*}
\text{Universe} & \quad XEU \supseteq \text{fv}(A,c) \quad X \supseteq \text{progvars}(\text{fv}(B)) \quad x \notin X \quad \text{type of } x \text{ is infinite} \\
\forall \psi \in \ell^2[XxE], \psi' \in \ell^2[U], \psi, \psi' \neq 0. \{ XxE =_q \psi, U =_q \psi', A \} \in \{ B \} \\
\{ A \} & \in \{ B \}
\end{align*}
\]

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(We call this rule **Universe** since we do a case distinction over the state of all variables, i.e., of the whole universe.) We will see an example where the **Universe** rule is useful in the analysis of the quantum one-time pad (Section 8.3, general case). Note that it is important in this rule that we can fix one concrete set $\mathbf{XXEU}$ of variables to quantify over. Otherwise, we would have to quantify over all states *over all possible sets of variables*; depending on the precise formalization the “set” of all possible sets of variables might not even be a set, and a rigorous formalization of the rule may not be possible in logical foundations that do not allow us to quantify over large classes (e.g., higher-order logic as formalized in Isabelle/HOL [17]). The rule is proven in Lemma 16 in Section 6.3.

For stating the next rules more readable, we introduce another notation: We write $A \Rightarrow B$ for $\{A\} \text{skip \{B\}}$ (which in turn is equivalent to $\forall \rho. \rho \models A \implies \rho \models B$). By rules **Seq** and **Skip** (and the fact that **skip** is the neutral element of $\Rightarrow$) we immediately have that $\Rightarrow$ is a preorder that refines $\subseteq$. Also note that rule **Seq** implies that $A \Rightarrow A', \{A'\} \in \{B\} \land B \Rightarrow \{A\} \in \{B\}$, so $\Rightarrow$ can be used for rewriting Hoare judgments.

The next three rules are specific to ghost variables and allow us to rewrite predicates.

\[
\text{**Rename**} \\
\forall i. \text{rank } M_i \leq 1 \quad \sum_i M_i \cdot M_i = \text{id} \\
A \Rightarrow A\{E'/E, U'/U\}
\]

\[
\text{**Transmute**} \\
G \text{ either all entangled or all unentangled ghosts} \\
G' \text{ either all entangled or all unentangled ghosts} \\
A \Rightarrow \bigvee_i \left( (M_i \text{ on } G') \cdot A\{G'/G\} \right)
\]

\[
\text{**Shift**} \\
\text{tr} \text{ proj}(\psi) = \text{tr} \text{ proj}(\psi') \land (E' \cup E') \cap \text{fv}(A) = \emptyset \\
(X \in_q \psi, A) \Rightarrow (X \in_q \psi', A)
\]

Rule **Rename** simply allows us to rename ghosts, this mainly allows us to tidy up judgments. Rule **Rename** follows directly from Definitions 1 and 2. When reading **Transmute**, recall that $G, G'$ may refer to both entangled and unentangled ghosts. The purpose of the **Transmute** rule is to change an entangled ghost into an unentangled ghost or vice versa. (That is, we will usually have $G = e$ and $G' = u$ or vice versa.) Ideally, we would like to have something like $A \Rightarrow A\{u/e\} =: A'$ and vice versa, i.e., being able to change the kinds of ghost variables freely. But of course, that would mean that entangled and unentangled ghosts are equivalent, and we would not have to had to distinguish between those different kinds of variables in the first place. Instead, we get a somewhat more complicate rule where, after replacing $u$ by $e$ or vice versa, we also need to replace $A'$ by $\bigvee_i ((M_i \text{ on } G') \cdot A')$. (Recall that $\bigvee$ is the disjunction of predicates, i.e., the sum of subspaces, see page 5. Hence $\bigvee_i$ is a disjunction of a family of predicates $(M_i \text{ on } G') \cdot A'$.) The rule will be most useful if we can chose the $M_i$ in such a way that $\bigvee_i ((M_i \text{ on } G') \cdot A') = A'$. We will see later that this is often possible when classical variables are involved (i.e., when the precondition contains **class(X)**).

An example of using rule **Transmute** analyzes the predicate $\text{distrib}(X, D)$:

\[
\text{distrib}(X, D) = (Xe =_q \psi_{DD}) \Rightarrow \bigvee_i (\text{proj}(i)) \text{ on } u \cdot (Xu =_q \psi_{DD}) \\
= \bigvee_i (Xu =_q \sqrt{D(i)} \otimes |i\rangle) \subseteq \begin{cases} (X =_q u) = \text{separable}(X) \\ (X =_q u) = \text{class}(X). \end{cases}
\]

Here rule **Transmute** is applied with $M_i := \text{proj}(i)$, $G := e$, $G' := u$. Thus $\text{distrib}(X, D)$ implies that $X$ is separable and classical.
The main purpose of ShapeShift, in contrast, is to rewrite the state $\psi$ in predicates of the form $XE = q \psi$. The ShapeShift rule has the precondition $tr_E \proj(\psi) = tr_E \proj(\psi')$. That is, after tracing out (erasing) $E, E'$, the two states $\psi, \psi'$ (interpreted as density operators by applying $\proj(\cdot)$) should be identical. Or, stated differently, looking only at $X$, $\psi$ and $\psi'$ have to look identical. Thus the rule says, roughly, that in a predicate $XE = q \psi$, we can replace $\psi$ by any state that looks identical from the point of view of $X$. For example, $xe = q |00\rangle + |11\rangle \Rightarrow xe = q |01\rangle + |10\rangle$.

Both Transmute and ShapeShift are be extensively used in the derivations of derived rules in Section 7.1. We refer to those derivations for examples as to how and where Transmute and ShapeShift can be used. ShapeShift is also used as the core step in the security proof of the quantum one-time pad (Section 8.3). The rules are proven in Lemmas 17 and 18, respectively.

6.3 Proofs of core rules
We begin with some auxiliary lemmas:

**Lemma 7** Let $\rho$ be a mixed memory over $VW$ and $A$ a predicate over $V$. Then $\supp \rho \subseteq A \otimes \ell^2(W)$ iff $\supp trW \rho \subseteq A$.

**Proof.** For a predicate $B$, let $P_B$ denote the projector onto $B$. Then for a mixed memory $\sigma = \sum_i \proj(\psi_i)$, $\supp \sigma \subseteq B$ iff $\forall i. \psi_i \in B$ iff $\forall i. \|P_B \psi_i\| = \|\psi_i\|$ iff $\forall i. tr_{P_B} \proj(\psi_i) = tr \proj(\psi_i)$ iff $tr_{P_B} \sigma = tr \sigma$. (The last step uses that $tr_{P_B} \proj(\psi_i) P_B^* = tr \proj(\psi_i)$ for all $i$.)

We have

$$tr_{P_B \otimes \ell^2(W)} \rho P_A \otimes \ell^2(W) = tr(\rho \otimes id_W) \rho(\rho \otimes id_W)^* = tr tr_W(\rho \otimes id_W) \rho(\rho \otimes id_W)^* = tr \rho \rho^*$$

Thus $\supp \rho \subseteq A \otimes \ell^2(W)$ iff $\supp trW \rho \subseteq A$. □

**Lemma 8** If $A$ is a predicate, and $\rho_i$ are a family of mixed memories with $\rho_i \models A$ for all $i$, and $\sum_i \rho_i$ exists, then $\sum_i \rho_i \models A$.

**Proof.** A is a predicate over $XEU$, and $\rho_i$ are mixed memories over $X$ for some $XEU$. Since $\rho_i \models A$, there are $(XEU, U)$-separable $\rho_i^U$ with $\supp \rho_i^U \subseteq A$ and $tr_{EUX} \rho_i^U = \rho_i$. We have $\sum tr \rho_i^U = \sum \rho_i < \infty$, since $\sum \rho_i$ exists. Thus $\rho^U := \sum \rho_i^U$ exists.

Then $tr EUX \rho^U = \sum tr_{EUX} \rho_i^U = \sum \rho_i$. And since all $\rho_i^U$ are $(XEU, U)$-separable, so is $\rho^U$. Finally, $\supp \rho^U = \supp \rho_i^U = \sum \rho_i \subseteq A$. Thus $\sum \rho_i \models A$, as desired. □

**Lemma 9** Let $\rho$ be a mixed memory over $X$, let $A$ be a predicate, and assume $\rho \models A$.

(i) Let $M$ be an operator from $\ell^2[X]$ to $\ell^2[X]$. Then $M \rho M^* \models (M \otimes I)[A]$.

(ii) Let $Y \subseteq X$ and $fv(A) \cap Y = \emptyset$ and $N$ be an operator from from $\ell^2[Y]$ to $\ell^2[Y]$. Then $(N \otimes I)[A] \models N \rho N^*$. □

**Proof.** We first prove (i). Let $E(\sigma) := M \sigma M^*$ for all $\sigma$. Then $\rho := E(\rho)$ is a mixed memory over $X'$, and we need to show $\rho \models (M \otimes I)[A]$. And in the judgment $\rho \models A$, $A$ is a predicate over some variables $XEU$ for some variables $EU$, and in the judgment $\rho' \models M \cdot A$, it is interpreted as a predicate over variables $X'EU$ (see page 7).

Since $\rho \models A$, there exists a $(XE, U)$-separable $\rho^U$ with $\supp \rho^U \subseteq A$ and $tr_{EUX} \rho^U = \rho$. Let
\( \tilde{\rho} := (\mathcal{E} \otimes \text{id}_{\mathcal{EU}})(\rho^o) \). Then \( \tilde{\rho}^o \) is \((\mathcal{X}^E, \mathcal{U})\)-separable. Furthermore,

\[
\text{tr}_{\mathcal{EU}} \tilde{\rho}^o = (\text{id}_{\mathcal{X}} \otimes \text{tr}) \circ (\mathcal{E} \otimes \text{id}_{\mathcal{EU}})(\rho^o) = (\mathcal{E} \otimes \text{tr})(\rho^o) = \mathcal{E}(\text{tr}_{\mathcal{EU}} \rho^o) = \mathcal{E}(\rho) = \rho'.
\]

(Here \( \text{tr} \) is seen as a superoperator from the trace-class operators over \( \mathcal{EU} \) to the trace-class operators on the 1-dimensional space \( \mathbb{C} \).)

And finally, we can write \( \rho^o = \sum_i \text{proj}(\psi_i) \) for some \( \psi_i \in \ell^2[\mathcal{X}] \) and thus

\[
\text{supp } \rho^o = \text{supp } (\mathcal{E} \otimes \text{id}_{\mathcal{EU}})(\rho^o) = \text{supp } (\mathcal{M} \otimes \text{id}_{\mathcal{X}})(\rho^o)^* = \text{supp } \sum_i \text{proj}(\mathcal{M} \otimes \text{id}_{\mathcal{X}})(\psi_i) = \mathcal{M} \otimes \text{id}_{\mathcal{X}} \cdot \text{span}\{\psi_i\} = \mathcal{M} \otimes \text{id}_{\mathcal{X}} \cdot \mathcal{A}.
\]

Thus \( \rho' \models (\mathcal{M} \otimes \text{id}_{\mathcal{X}}) \cdot \mathcal{A} \). This shows (i).

We now show (ii) by reduction to (i). Let \( \mathcal{M} := (\mathcal{N} \otimes \mathcal{Y}) \). Then by (i), \( \mathcal{M} \models (\mathcal{N} \otimes \mathcal{Y})^\dagger \models (\mathcal{M} \otimes \mathcal{Y}) \cdot \mathcal{A} \). Thus we need to show that \( (\mathcal{M} \otimes \mathcal{Y}) \cdot \mathcal{A} \). Fix \( \psi \in (\mathcal{M} \otimes \mathcal{Y}) \cdot \mathcal{A} \). Then there exists \( \psi' \in \mathcal{A} \) with \( \psi = (\mathcal{M} \otimes \mathcal{Y}) \cdot \psi' \). \( \mathcal{A} \) is a predicate on \( \mathcal{X} \) for some \( \mathcal{EU} \). Let \( \mathcal{P} \) be the projector onto \( \mathcal{A} \). Since \( \text{tr} = 0 \), we can write \( \mathcal{P} = \text{id}_{\mathcal{Y}} \otimes \mathcal{P} \) for some projector \( \mathcal{P} \) on \( \mathcal{X} \). And when \( \mathcal{A} \) is interpreted as a predicate on \( \mathcal{X} \), we can write \( \mathcal{P} = \text{id}_{\mathcal{Y}} \otimes \mathcal{P} \). We have

\[
(\text{id}_{\mathcal{Y}} \otimes \mathcal{P}) = (\mathcal{M} \otimes \text{id}_{\mathcal{X}})(\psi) = (\mathcal{M} \otimes \text{id}_{\mathcal{X}})(\psi') = (\mathcal{M} \otimes \text{id}_{\mathcal{X}})(\psi) = (\mathcal{M} \otimes \text{id}_{\mathcal{X}})(\psi) = \psi.
\]

This shows (ii).

**Lemma 10** Rule APPLY is sound.

**Proof.** The predicate \( \mathcal{A} \) is a space of quantum memories over some variables \( \mathcal{X} \subseteq \mathcal{X} \). In this proof, we will encounter both the term \( \text{U on } \mathcal{X} \) interpreted as an operator on quantum memories over \( \mathcal{X} \), and over \( \mathcal{X} \). Since the syntax \( \text{U on } \mathcal{X} \) does not disambiguate between the two (the space we are operating on is left implicit), we write \( (\text{U on } \mathcal{X})_{\mathcal{X}} \) and \( (\text{U on } \mathcal{X})_{\mathcal{X}} \), respectively. Note that \( (\text{U on } \mathcal{X})_{\mathcal{X}} = (\text{U on } \mathcal{X})_{\mathcal{X}} \otimes \text{id}_{\mathcal{EU}} \).

We need to show that for any mixed memory \( \rho \) over \( \mathcal{X} \), \( \rho \models \mathcal{A} \) implies \( \mathcal{A} \models (\text{U on } \mathcal{X})_{\mathcal{X}} \). Since \( \rho \models \mathcal{A} \), there exists an \( (\mathcal{X}, \mathcal{U}) \)-separable \( \rho^o \) with \( \text{supp } \rho^o \subseteq \mathcal{A} \) and \( \text{tr}_{\mathcal{EU}} \rho^o = \rho \). Since \( \rho^o \) is \((\mathcal{X}, \mathcal{U}) \)-separable, we can write it as \( \rho^o = \sum_i \text{proj}(\psi_{\mathcal{X}, \mathcal{U}, i} \otimes \psi_{\mathcal{U}, i}) \). Since \( \text{supp } \rho^o \subseteq \mathcal{A} \), this implies that \( \psi_{\mathcal{X}, \mathcal{U}, i} \otimes \psi_{\mathcal{U}, i} \in \mathcal{A} \) for all \( i \).

Let

\[
\rho^o := \sum_i \text{proj}(\psi_{\mathcal{X}, \mathcal{U}, i} \otimes \psi_{\mathcal{U}, i}).
\]

Then \( \rho^o \) is \((\mathcal{X}, \mathcal{U}) \)-separable. And

\[
(\text{U on } \mathcal{X})_{\mathcal{X}} \otimes \psi_{\mathcal{U}, i} = (\text{U on } \mathcal{X})_{\mathcal{X}} (\psi_{\mathcal{X}, \mathcal{U}, i} \otimes \psi_{\mathcal{U}, i}) \in (\text{U on } \mathcal{X})_{\mathcal{X}} \cdot \mathcal{A}.
\]
So \( \text{supp} \hat{\rho}^\circ \in (U \downarrow X)_{X^{\text{all}}EU} \cdot A \). Finally,

\[
\text{tr}_{EU} \hat{\rho}^\circ = (U \downarrow X)_{X^{\text{all}}} \left( \text{tr}_{EU} \sum_i \text{proj}(\psi_{X^{\text{all}}I_i} \otimes \psi_{U,I_i}) \right) (U \downarrow X)_{X^{\text{all}}}
= (U \downarrow X)_{X^{\text{all}}} (\text{tr}_{EU} \rho^\circ)(U \downarrow X)_{X^{\text{all}}} = (U \downarrow X)_{X^{\text{all}}} \rho(U \downarrow X)_{X^{\text{all}}} = [\text{apply } U \downarrow X](\rho).
\]

Hence \([\text{apply } U \downarrow X](\rho) \models (U \downarrow X)_{X^{\text{all}}EU} \cdot A\). \(\square\)

**Lemma 11** **Rule INIT** is sound.

**Proof.** \(A\) is a predicate on some variables \(X^{\text{all}}EU\). We also have that \(e \notin E\) and that \(e\) and \(x\) have the same type because otherwise \(A[e/x]\) would not be well-typed. Let \(B := (A[e/x], x =_{\ell_0} 0)\) (the postcondition). Note that there is an implicit conversion happening: By definition, \(A[e/x]\) is a predicate on \(X^{\text{all}}EeU \setminus x\), so it does not make sense to intersect it \((\land)\) with \(x =_{\ell_0} 0\). But, as discussed at the end of Section 2 (page 7), we identify any predicate \(A\)' with \(A\otimes \ell^2[x]\). In particular, \(A[e/x]\) is identified with \(A[e/x] \otimes \ell^2[x] := A[e/x]_{X^{\text{all}}EU}\) on \(X^{\text{all}}EeU\). In that notation, \(B\) is actually \(B := (A[e/x]_{X^{\text{all}}EU}, x =_{\ell_0} 0)\), a predicate over \(X^{\text{all}}EeU\).

To show the rule, we need to show that for any mixed memory \(\rho\) on \(X^{\text{all}}\), \(\rho \models A\) implies \(\rho \models B\). \(\rho \models A\) implies that there is a \((X^{\text{all}}E, U)\)-separable \(\rho^\circ\) such that \(\text{supp} \rho^\circ \subseteq A\) and \(\text{tr}_{EU} \rho^\circ = \rho\).

Let \(E\) be the canonical mapping from mixed memories over \(x\) to mixed memories over \(e\). (Formally, \(E(\sigma) = U_{x \to e} \sigma U_{x \to e}^\ast\) where \(U_{x \to e}\) was defined on page 6.) Then \(E \otimes \text{id}_{X^{\text{all}}EU \setminus x}\) maps mixed memories over \(X^{\text{all}}EU\) to mixed memories over \(X^{\text{all}}EeU \setminus x\) by renaming \(x\) to \(e\). We define:

\[
\hat{\rho}^\circ := (E \otimes \text{id}_{X^{\text{all}}EU \setminus x})(\rho^\circ) \quad \text{and} \quad \hat{\rho}^\circ := \hat{\rho}^\circ \otimes \text{proj}(0)_{x}.
\]

Since \(\hat{\rho}^\circ\) is \((X^{\text{all}}E, U)\)-separable, and \(E \otimes \text{id}_{X^{\text{all}}EU \setminus x}\) is the identity on \(U\), we have that \(\hat{\rho}^\circ\) is \((X^{\text{all}}Ee \setminus x, U)\)-separable, and thus \(\hat{\rho}^\circ\) is \((X^{\text{all}}E, U)\)-separable.

We have

\[
\text{supp} \hat{\rho}^\circ = \text{supp}(U_{x \to e} \otimes \text{id}_{X^{\text{all}}EU \setminus x}) \rho^\circ (U_{x \to e} \otimes \text{id}_{X^{\text{all}}EU \setminus x})^\ast
= (U_{x \to e} \otimes \text{id}_{X^{\text{all}}EU \setminus x}) \cdot \text{supp} \rho^\circ \subseteq (U_{x \to e} \otimes \text{id}_{X^{\text{all}}EU \setminus x}) \cdot A \subseteq A[e/x].
\]

Here \((\ast)\) is the definition of \(A[e/x]\) (page 6). Thus

\[
\text{supp} \hat{\rho}^\circ \subseteq \text{supp} \rho^\circ \otimes \ell^2[x] \subseteq A[e/x] \otimes \ell^2[x] = A[e/x]_{X^{\text{all}}EU}.
\]

And \(\text{supp} \hat{\rho}^\circ \subseteq (x =_{\ell_0} 0)\) by definition of \(\hat{\rho}^\circ\). Thus \(\text{supp} \hat{\rho}^\circ \subseteq B\). Finally,

\[
\text{tr}_{EU} \hat{\rho}^\circ = (\text{tr}_{EU} \hat{\rho}^\circ) \otimes \text{proj}(0)_{x} \subseteq \text{tr}_{EU} \rho^\circ \otimes \text{proj}(0)_{x}
= \text{tr}_{EU} \rho^\circ \otimes \text{proj}(0)_{x} = \text{tr}_{x} \rho \otimes \text{proj}(0)_{x} = [\text{init } x]_{x}(\rho).
\]

Here \((\ast)\) uses that \(\hat{\rho}^\circ\) is the result of renaming \(x\) to \(e\) in \(\rho^\circ\), so tracing out \(e\) in \(\hat{\rho}^\circ\) is the same as tracing out \(x\) in \(\rho^\circ\).

Altogether, we have \([\text{init } x]_{x}(\rho) \models B\). \(\square\)

**Lemma 12** **Rule IF** is sound.
Lemma 13 \textbf{Rule While is sound.}

Proof. The predicate $A$ is a subspace of quantum memories over some variables $X^{\text{all}}E'U$. We need to show that for any mixed memory $\rho$ on $X^{\text{all}}$, if $\rho \equiv A$, then $[\text{while } x \text{ do } c ](\rho) \equiv B$. Recall that $[\text{if } x \text{ then } c \text{ else } d ](\rho) = [c](\rho) + [d](\rho)$ where $\rho_i := \downarrow_i(\rho) = (\text{proj}(i) \circ \text{proj}([i]) \circ \text{proj}(i)) \circ \rho$.

By Lemma 9, we have $\rho_i = (\text{proj}(i))\rho(\text{proj}(i)) \equiv (\text{proj}([i]) \circ \rho(\text{proj}([i])) \circ \text{proj}(i)) \circ \rho$. Since $\{ (\text{proj}([i]) \circ \text{proj}(i)) \circ \rho(\text{proj}(i)) \circ \text{proj}(i) \circ \rho \}$, by assumption of the induction step, it follows that $[c](\rho) \equiv B$ and $[d](\rho) \equiv B$. Thus with Lemma 8, $[\text{if } x \text{ then } c \text{ else } d ](\rho) = [c](\rho) + [d](\rho) \equiv B$. \hfill \qed

Lemma 14 \textbf{Rule Case is sound.}

Proof. The predicate $A$ is a subspace of quantum memories over $X^{\text{all}}E'U$ for some variables $E'U$ with $U \subseteq U$. And $B$ is a subspace of quantum memories over $X^{\text{all}}E'U'$ for some variables $E'U'$. We need to show that if $\rho \equiv A$ then $[c](\rho) \equiv B$. Since $\rho \equiv A$, there is a $(X^{\text{all}}E, \hat{U})$-separable $\rho^\circ$ with $\text{supp } \rho^\circ \subseteq A$ and $\text{supp } \rho^\circ = \rho$. For making the notation more compact in the remainder of the proof, let $V := X^{\text{all}}E \times X$ and $W := \hat{U} \setminus U$. In that notation, $\rho^\circ$ is $(X^V, UV)$-separable. Thus $\rho^\circ$ can be written as $\rho^\circ = \sum_{i=1}^n \text{proj}(\psi_{i,1,i})$ where $\psi_{i,1,i} = \psi_{X^V,i} \otimes \psi_{UV,i}$ for some quantum memories $\psi_{X^V,i} \neq 0$ over $X^V$ and $\psi_{UV,i} \neq 0$ over $UW$.

Fix some $i$. (We will omit $i$ from the subscripts for now.) We can write $\psi_{UV} \neq 0$ as a nonempty sum $\psi_{UV} = \sum_j \phi_{U,j} \otimes \phi_{W,j}$ with quantum memories $\phi_{U,j} \otimes \phi_{W,j} \neq 0$ over $U$ and $W$ respectively where the $\phi_{W,j}$ are orthogonal. We have $\psi_{i,1,i} \in \text{supp } \rho \subseteq A \subseteq C$. Thus

$$\psi_{X^V} \otimes \phi_{U,j} \otimes \phi_{W,j} = (\text{proj}(\phi_{W,j}) \circ \text{proj}(\phi_{W,j})) \circ \psi_{i,1,i} \neq 0 \text{ over } X^V \text{ and } UV.$$
(X^{allE, U})-separable. Hence \( \rho_{all} := \text{tr}_{EU} \text{proj}(\psi_{all}) \supseteq (X =q \psi_X) \land A \). By assumption of the rule CASE, \( X = q \psi_X \), \( A \vdash B \). Thus \([\mathbf{e}]((\rho_{all})') \vdash B \).

We now “unfix” \( i \). We thus have \([\mathbf{e}]((\rho_{all,i})') \vdash B \) for \( \rho_{all,i} := \text{tr}_{EU} \text{proj}(\psi_{all,i}) \). Furthermore,

\[
[\mathbf{e}]'(\rho) = [\mathbf{e}](\text{tr}_{EU} \rho) = [\mathbf{e}]
\left(\text{tr}_{EU} \left(\sum_{i \in I} \text{proj}(\psi_{all,i})\right)\right)
= [\mathbf{e}]
\left(\sum_{i \in I} \rho_{all,i}\right)
= [\mathbf{e}](\rho_{all}).
\]

By Lemma 8, \( \forall i. [\mathbf{e}]((\rho_{all,i})') \vdash B \) implies \( [\mathbf{e}](\rho) = \sum_i [\mathbf{e}](\rho_{all,i})' ) \vdash B \). □

The following is an auxiliary lemma needed for the proof of rule UNIVERSE. But it is also of independent interest because it says that the choice of the set of program variables with respect to which we evaluate a program (denoted \( X^{all} \) on page 7) does not matter as long as it is large enough.

**Lemma 15 (Changing the set of program variables)** Let \( \{A \} \mathbf{e} \{B\}^{X} \) denote Hoare judgments \( \{A \} \mathbf{e} \{B\} \) as in Definition 2, except that the set \( X \) is used instead of \( X^{all} \). (I.e., the semantics of the program \( \mathbf{e} \) are defined with respect to memories containing variables \( X \), not \( X^{all} \).

Assume that \( \text{fv}(\mathbf{e}), \text{progvars}(\text{fv}(A)), \text{progvars}(\text{fv}(B)) \subseteq X_1, X_2 \). Let \( Y_i := X_i \setminus \text{fv}(\mathbf{e}) \setminus \text{fv}(A) \setminus \text{fv}(B) \).

Let \( T_i \) be the type of \( Y_i \). Assume that \( |T_1| \geq |T_2| \) or \( |T_1| = \infty \). Then \( \{A \} \mathbf{e} \{B\}^{X_1} \implies \{A \} \mathbf{e} \{B\}^{X_2} \).

**Proof.** We fix some \( E, U \) such that \( EU \) contains all ghosts from \( \text{fv}(A), \text{fv}(B) \). By Lemma 1, we can interpret \( A, B \) in judgments \( \rho \vdash A, \rho \vdash B \) as predicates over \( X EU \) (where \( \rho \) is over \( X \)), i.e., we can without loss of generality use the same \( EU \) everywhere. Note that \( X_1 \setminus Y_1 = X_2 \setminus Y_2 \) since both are equal to \( \text{fv}(\mathbf{e}) \cup \text{progvars}(\text{fv}(A)) \cup \text{progvars}(\text{fv}(B)) \).

Assume \( \{A \} \mathbf{e} \{B\}^{X_1} \). To show \( \{A \} \mathbf{e} \{B\}^{X_2} \), we fix a mixed memory \( \rho \) over \( X_2 \) with \( \rho \vdash A \), and we need to show \( [\mathbf{e}](\rho) \vdash B \).

Let \( S := \text{supp} \text{tr}_{X_1 \setminus Y_2} \rho \subseteq \ell^2(Y_2) \). The operator \( \text{tr}_{X_1 \setminus Y_2} \rho \) can be written as \( \sum_{i \in I} p_i \text{proj}(\psi_i) \) with some orthonormal \( \psi_i \in \ell^2(Y_2) \) and some \( p_i > 0 \) with \( \sum_{i \in I} p_i = \text{tr}(\text{tr}_{X_1 \setminus Y_2} \rho) < \infty \). Thus \( I \) is countable (otherwise \( \sum_{i \in I} p_i \) cannot converge). Hence \( \dim S = \text{dim} \text{span}(\psi_i)_{i \in I} = |I| \) is countable. Furthermore \( \dim S \leq \text{dim} \ell^2(Y_2) = |T_2| \). Since \( |T_1| \geq |T_2| \) or \( |T_1| = \infty \), it follows that \( \dim S \leq |T_1| = \text{dim} \ell^2(Y_1) \). Thus there exists an isometry \( U \) from \( S \) to \( \ell^2(Y_1) \) by setting \( U = 0 \) on the orthogonal complement of \( S \). Then \( U^*U \) is the projector \( P_S \) onto \( S \). Since \( S = \text{supp} \text{tr}_{X_1 \setminus Y_2} \rho \), \( S \subseteq \ell^2(X_2 \setminus Y_2) \supseteq \text{supp} \rho \).

And \((P_S \text{on} Y_2) \) is the projector onto \( S \otimes \ell^2(X_2 \setminus Y_2) \). Hence \( \text{supp} \rho \) is fixed by \((P_S \text{on} Y_2) \).

Let \( \mathcal{E}(\sigma) := U\sigma U^* \) for all \( \sigma \) over \( Y_2 \). And let \( \mathcal{E}(\sigma) := (U \text{on} Y_2)\sigma(U \text{on} Y_2)^* \) for all \( \sigma \) over \( X_2 \), i.e., \( \mathcal{E} = \text{id}_{X_2 \setminus Y_2} \otimes \mathcal{E} \).

Let \( \mathcal{E}^*(\sigma) := U^*\sigma U \) for all \( \sigma \) over \( Y_1 \). And let \( \mathcal{E}^*(\sigma) := (U^* \text{on} Y_1)\sigma(U^* \text{on} Y_1)^* \) for all \( \sigma \) over \( X_1 \), i.e., \( \mathcal{E}^* = \text{id}_{X_1 \setminus Y_1} \otimes \mathcal{E}^* \).

We have \( \mathcal{E}^* \circ \mathcal{E}(\rho) = (P_S \text{on} Y_2)\rho(P_S \text{on} Y_2)^* = \rho \). Here the last equality is because \( \text{supp} \rho \) is fixed by \((P_S \text{on} Y_2) \).

Since \( \text{fv}(A) \cap Y_2 = \emptyset \) and \( \rho \vdash A \), by Lemma 9 (ii), \( \mathcal{E}(\rho) \vdash A \). Note that \( \mathcal{E}(\rho) \) is a mixed memory over \( X_2 \setminus Y_2 \cup Y_1 = X_1 \). Since \( \{A \} \mathbf{e} \{B\}^{X_1} \), we have \([\mathbf{e}][X_1](\mathcal{E}(\rho)) \vdash B \). Here \([\mathbf{e}][X_1] \) denotes the semantics \([\mathbf{e}] \) of \( \mathbf{e} \) defined with respect to the set of variables \( X_1 \) instead of \( X^{all} \).

Note that \([\mathbf{e}][X_1] = [\mathbf{e}][X_1 \cap Y_1] \otimes \text{id}_{Y_1} \) and \([\mathbf{e}][X_2] = [\mathbf{e}][X_2 \cap Y_2] \otimes \text{id}_{Y_2} \) (since \( \text{fv}(\mathbf{e}) \cap Y_1 = \text{fv}(\mathbf{e}) \cap Y_2 = \emptyset \).
Lemma 17

\[ \mathcal{E}^* \left( [\mathbf{c}]^{X_1} (\mathcal{E}(\rho)) \right) = (id_{X_1 \x Y_1} \otimes \mathcal{E}^*) \circ ([\mathbf{c}]^{X_1} \otimes id_{Y_1}) \circ (id_{X_2 \x Y_2} \otimes \mathcal{E})(\rho) \]

Hence, the rule \( \mathcal{E}^* \) is sound.

Lemma 16 Rule Universe is sound.

Most of the work for the proof has already been done in Lemma 15.

Proof. By Lemma 15 (with \( X_1 := \mathbf{Xx} \) and \( X_2 := \mathbf{Xall} \)), we have that \( \{A\} \mathbf{c} \{B\}^{XX} \) (in the notation of Lemma 15) implies \( \{A\} \mathbf{c} \{B\} \). (For this, note that \( \mathbf{Xx} \) contains \( \mathbf{x} \) and thus has infinite type.) Thus to prove the soundness of Universe, it is sufficient to prove \( \{A\} \mathbf{c} \{B\}^{XX} \).

To show \( \{A\} \mathbf{c} \{B\}^{XX} \), fix some \( \rho \) over \( \mathbf{Xx} \) with \( \rho \models A \). Then there is a \( \{\mathbf{Xx}, \mathbf{U}\} \)-separable \( \rho^\perp \) over \( \mathbf{XxU} \) with \( \text{tr}_{\mathbf{U}} \rho^\perp = \rho \) and \( \text{supp} \rho^\perp \subseteq A \).

Since \( \rho^\perp \) is \( \{\mathbf{Xx}, \mathbf{U}\} \)-separable, we can write \( \rho^\perp = \sum_i \text{proj}(\psi_i \otimes \psi'_i) \) with \( \psi_i \in \mathcal{E}^2[\mathbf{Xx}] \) and \( \psi'_i \in \mathcal{E}^2[\mathbf{U}] \) and \( \psi_i, \psi'_i \neq 0 \). Since \( \text{supp} \rho^\perp \subseteq A \), we have \( \psi_i \otimes \psi'_i \in A \) for all \( i \). Furthermore, we have \( \psi_i, \psi'_i \in \{\mathbf{Xx} = \psi, \mathbf{U} = \psi'\} \). Thus \( \psi_i, \psi'_i \in A_i := \{\mathbf{Xx} = \psi, \mathbf{U} = \psi\} \). We then have that \( \text{tr}_{\mathbf{U}} \rho^\perp = \mathcal{E}^2[\mathbf{Xx}] \)-separable and \( \text{supp} \rho^\perp \subseteq A \). Thus \( \rho_i := \text{tr}_{\mathbf{U}} \rho^\perp \models A_i \). By assumption of the rule Universe we have \( \{A_i\} \mathbf{c} \{B\} \).

The cardinality of the type of \( \mathbf{Xall} \) at least as big as that of \( \mathbf{Xx} \). Since \( \rho_i \models A_i \), we have \( [\mathbf{c}](\rho_i) \models B \).

This holds for all \( i \).

We have \( \rho = \text{tr}_{\mathbf{U}} \rho^\perp = \sum_i \text{tr}_{\mathbf{U}} \rho^\perp \models \psi_i \otimes \psi'_i \) \( \models \psi_i \otimes \psi'_i \) \( \models \sum_i \rho_i \). Thus \( [\mathbf{c}](\rho) = \sum_i [\mathbf{c}](\rho_i) \). Since for all \( i \), \( [\mathbf{c}](\rho_i) \models B \), by Lemma 8 we have \( [\mathbf{c}](\rho) = \sum_i [\mathbf{c}](\rho_i) \models B \). Since this holds for all \( \rho \) over \( \mathbf{Xx} \) with \( \rho \models A \), we have shown \( \{A\} \mathbf{c} \{B\}^{XX} \).

As mentioned in the beginning of the proof, by Lemma 15 this implies \( \{A\} \mathbf{c} \{B\} \).

Lemma 17 Rule Transmute is sound.

Proof. We distinguish four cases: \( \mathbf{G}, \mathbf{G}' \) are entangled ghosts (EE-case), \( \mathbf{G}, \mathbf{G}' \) are unentangled ghosts (UU-case), \( \mathbf{G} \) is entangled and \( \mathbf{G}' \) is unentangled ghosts (EU-case), and \( \mathbf{G} \) are unentangled and \( \mathbf{G}' \) are entangled ghosts (UE-case). Most of the proof is the same in all four cases, we make case distinctions in individual proof steps as necessary.

\( \mathbf{A} \) is a predicate over \( \mathbf{XallEU} \) for some \( \mathbf{E, U} \). And \( \mathbf{A}' := \mathbf{A} \{\mathbf{G}/\mathbf{G}'\} \) is a predicate over \( \mathbf{XallEU}' \) for some \( \mathbf{E}', \mathbf{U}' \). (What variables are in \( \mathbf{E}', \mathbf{U}' \), respectively, depends on the case, e.g., in the EU-case, \( \mathbf{E}' = \mathbf{E} \setminus \mathbf{G} \) and \( \mathbf{U}' = \mathbf{U} \cup \mathbf{G} \).)

To show \( \mathbf{A} \models \bigvee_i ((M_i \text{ on } \mathbf{G}') \cdot \mathbf{A} \{\mathbf{G}/\mathbf{G}'\}) \) \( \models B \), we fix some mixed memory \( \rho \) over \( \mathbf{Xall} \) with \( \rho \models A \). We have to show that \( \rho \models B \).

Since \( \rho \models A \), there exists a \( \{\mathbf{Xall}, \mathbf{U}\} \)-separable \( \rho^\perp \) over \( \mathbf{XallEU} \) with \( \text{supp} \rho^\perp \subseteq A \) and
Lemma 18 \textbf{Rule \textsc{ShapeShift} is sound.}

\begin{proof}
Since $\langle \mathbf{E} \cup \mathbf{E}' \rangle \cap \text{fv}(\mathbf{A}) = \emptyset$, we can interpret $\mathbf{A}$ as a predicate over $\text{Xall} \mathbf{E} \mathbf{U}$ for some $\mathbf{E} \mathbf{U}$ with $\mathbf{E} \cap (\mathbf{E} \cup \mathbf{E}') = \emptyset$. (See the discussion on page 7 about identifying predicates over different sets.) Then the pre- and postconditions $(\mathbf{X} \mathbf{E} = q \psi, \mathbf{A})$ and $(\mathbf{X} \mathbf{E}' = q \psi', \mathbf{A})$ can be written more explicitly as predicates $(\mathbf{X} \mathbf{E} = q \psi, \mathbf{A} \otimes \ell^2[\mathbf{E}])$ and $(\mathbf{X} \mathbf{E}' = q \psi', \mathbf{A} \otimes \ell^2[\mathbf{E}'])$ over $\text{Xall} \mathbf{E} \mathbf{U}$ and $\text{Xall} \mathbf{E} \mathbf{U}'$, respectively. (Justified by Lemma 1.) And $\psi, \psi'$ are quantum memories over $\mathbf{X} \mathbf{E}$ and $\mathbf{X} \mathbf{E}'$, respectively.

Fix a mixed memory $\rho$ over $\text{Xall}$ with $\rho \vdash (\mathbf{X} \mathbf{E} = q \psi, \mathbf{A} \otimes \ell^2[\mathbf{E}])$. To show rule \textsc{ShapeShift}, we need to show that $\rho \vdash (\mathbf{X} \mathbf{E}' = q \psi', \mathbf{A} \otimes \ell^2[\mathbf{E}'])$.

Since $\rho \vdash (\mathbf{X} \mathbf{E} = q \psi, \mathbf{A} \otimes \ell^2[\mathbf{E}])$, there is an $(\text{Xall} \mathbf{E} \mathbf{U}, \mathbf{U})$-separable $\rho^0$ with $\text{supp} \rho^0 \subseteq \mathbf{U}$.
(XE_\rho = \psi, A \otimes \ell^2[E]) \text{ and } \text{tr}_{\text{EEU}} \rho^o = \rho.

Thus \text{supp} \rho^o \subseteq (XE_\rho = \psi). Hence \rho^o = (\text{tr}_{XE} \rho^o) \otimes \text{proj}(\psi). Let \bar{\rho}^o := (\text{tr}_{XE} \rho^o) \otimes \text{proj}(\psi'). Then

\[ \text{tr}_E \rho^o = \text{tr}_E ( (\text{tr}_{XE} \rho^o) \otimes \text{proj}(\psi) ) = (\text{tr}_{XE} \rho^o) \otimes \text{tr}_E \text{proj}(\psi) \]

\[ \supseteq (\text{tr}_{XE} \rho^o) \otimes \text{tr}_E \text{proj}(\psi') = \text{tr}_E ( (\text{tr}_{XE} \rho^o) \otimes \text{proj}(\psi) ) = \text{tr}_E \bar{\rho}^o. \] (3)

Here (*) is by assumption from rule \text{ShapeShift}. Then

\[ \text{tr}_{\text{EEU}} \bar{\rho}^o = \text{tr}_{\text{EEU}} \text{tr}_E \bar{\rho}^o \supseteq \text{tr}_{\text{EEU}} \text{tr}_E \rho^o = \text{tr}_{\text{EEU}} \rho^o = \rho. \]

Since \rho^o is (X_{\text{all}} \text{EE}, \bar{U})-separable, tr_{XE} \rho^o is (X_{\text{all}} \text{EE} \setminus X, \bar{U})-separable, and hence \bar{\rho}^o = (\text{tr}_{XE} \rho^o) \otimes \text{proj}(\psi') is (X_{\text{all}} \text{EE} \setminus X \cup X_{\text{E}'}, \bar{U}) = (X_{\text{all}} \text{EE'}, \bar{U})-separable.

Since \text{supp} \rho^o \subseteq (XE_q = \psi, A \otimes \ell^2[E]), we have \text{supp} \rho^o \subseteq A \otimes \ell^2[E']. By Lemma 7, this implies \text{supp} \text{tr}_E \rho^o \subseteq A. Then by (3), \text{supp} \text{tr}_E \rho^o \subseteq A. And by Lemma 7, \text{supp} \rho^o \subseteq A \otimes \ell^2[E']. And since \bar{\rho}^o = (\text{tr}_{XE} \rho^o) \otimes \text{proj}(\psi'), we also have \text{supp} \bar{\rho}^o \subseteq (XE' = \psi'). Thus \text{supp} \bar{\rho}^o \subseteq (XE' = \psi, A \otimes \ell^2[E']).

Since \rho^o is (X_{\text{all}} \text{EE'}, \bar{U})-separable and satisfies \text{supp} \bar{\rho}^o \subseteq (XE' = \psi', A \otimes \ell^2[E']) and tr_{EEU} \rho^o = \rho, it follows that \rho \models (XE' = \psi, A \otimes \ell^2[E']). Since \rho was arbitrary with \rho \models (XE = \psi, A \otimes \ell^2[E]), we have shown (XE = \psi, A \otimes \ell^2[E]) \Rightarrow (XE' = \psi', A \otimes \ell^2[E']), the conclusion of the rule. \qed

7 Derived rules

In this section, we show that our eleven core rules are powerful enough to derive a number of new rules without having to refer to the semantics of Hoare judgments with ghosts from Definition 2 (That is, the rules in this section would hold for any definition of Hoare judgments satisfying the eleven core rules.)

This first derived rule is relatively trivial but of high importance:

\[ \text{CONSEQ} \quad A \subseteq A' \quad \{A' \} \epsilon \{B'\} B' \subseteq B \]

\[ \{A\} \epsilon \{B\} \]

\textbf{Proof.} From \textit{Skip} and \textit{Seq}, we get \{A\} \textit{skip}; c; \textit{skip} \{B\}. Since \textit{skip} is the neutral element for \epsilon (page 7), this implies \{A\} \epsilon \{B\}. \qed

7.1 Derived rules for derived language elements

\textbf{Initialization.} The next rules deal with the initialization of variables. They are generalizations of rule \textit{Init}, dealing with the syntactic sugar \ X \leftarrow \psi \ (\text{initialization}) \text{ and } X \leftarrow z \ (\text{classical initialization}).

\text{InitQ} \quad \{A\} X \leftarrow \psi \ A[e/X], X = \psi \}

\text{InitC} \quad \{A\} X \leftarrow z \ A[e/X], X = z \ \text{class}(X) \}

The derivation of rule \textit{InitQ} is not difficult, but the proof of rule \textit{InitQ} provides a nice first example of reasoning with sequences of Hoare judgments. The derivation of rule \textit{InitC} is a little more involved, and it gives an example how to use rules \text{ShapeShift} and \text{Transmute} to show that the content of a variable is classical.

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Proof of \texttt{InitQ}. \( X \triangleq \psi \) is syntactic sugar for \texttt{init} \( x_1; \ldots; \texttt{init} \ x_n; \texttt{apply} \ U_\psi \texttt{to} \ X \) where \( U_\psi(0, \ldots, 0) = \psi \) and \( x_1 \ldots x_n := X \). For variables \( E := e_1 \ldots e_n \) and \( e \) of the same type as \( X \), we have:

\[
\{ A \} \ \texttt{init} \ x_1 \ \{ A[e_1/x_1], \ x_1 =_q |0 \} \\
\texttt{init} \ x_2 \ \{ A[e_1 e_2/x_1 x_2], \ x_1 =_q |0, \ x_2 =_q |0 \} \\
\ldots \ \{ A[e_1 \ldots e_{n-1}/x_1 \ldots x_{n-1}], \ x_1 =_q |0, \ldots, x_{n-1} =_q |0 \} \\
\texttt{init} \ x_n \ \{ A[E/X], \ X =_q |0 \} \\
\texttt{apply} \ U_\psi \texttt{to} \ X \ \{(U_\psi \texttt{on} \ X) \cdot (A[E/X], \ X =_q |0)\} \\
= \{ A[E/X], \ X =_q \psi \} \\
\Rightarrow \{ A[e/E], \ X =_q \psi \}. \\
\]

Then by rule \texttt{Seq}, we get \( \{ A \} \ X \triangleq \psi \{ A[e/E], \ X =_q \psi \}. \quad \square \)

Proof of \texttt{rule InitC}. Recall that \( X \leftarrow z \) is syntactic sugar for \( X \triangleq |z\). Thus we have

\[
\{ A \} \ X \leftarrow z \ \{ A[e/E], \ X =_q |z\} \quad \text{(rule InitQ)} \\
\Rightarrow \{ A[e/E], \ X =_q |z\} \quad \text{(rule Shapeshift with} \ E := \emptyset, \ E' := e') \\
\Rightarrow \{ \bigvee_i \{ (\texttt{proj}(i) \texttt{on} \ u) \cdot (A[X/E], \ X =_q |z\otimes |z\} \} \}
\]

\[
\quad \text{(rule Transmute with} \ M_i := \texttt{proj}(i), \ G := e', \ G' := u) \\
\downarrow \quad \{ A[e/E], \ X =_q |z\} \quad \subseteq \quad \{ A[e/E], \ X =_q |z\} \quad \text{(class}(X)\} \\
\subseteq \quad \{ A[e/E], \ X =_q |z\} \Rightarrow \{ A[e/E], \ X =_q |z\} \quad \text{(class}(X)\}. \\
\]

Measurements. More interesting is the rule for measurements because it actively makes use of ghosts to record the distribution of outcomes. We first look at the rule for measurements that forget the outcome (\texttt{measure} \( X \) instead of \( Y \leftarrow \texttt{measure} \ X \)) because it is a bit simpler, and the underlying ideas are the same:

\[
\texttt{MeasureForget} \\
\{ A \} \ \texttt{measure} \ X \ \{ U_{\text{copy},X \rightarrow e} \cdot A \} \\
\]

Here \( U_{\text{copy},V \rightarrow W} \) is the isometry from \( V \) to \( VW \) defined by \( U_{\text{copy},V \rightarrow W} \cdot i \cdot v = |i\rangle v \otimes |i\rangle w \). Thus \( U_{\text{copy},X \rightarrow e} \) is the operation that “classically copies” (in the computational basis) the content of \( X \) to the fresh entangled ghost \( e \). (We have \( e \notin \text{fv}(A) \) is fresh because otherwise \( U_{\text{copy},X \rightarrow e} \cdot A \) would not be well-defined since it would contain two \( e \)’s.)

In other words, \texttt{rule MeasureForget} says that after measuring \( X \), the result is simply to get \( X \) entangled with a fresh entangled ghost \( e \). Since \( e \) is a ghost, being entangled with it effectively means that \( X \) has been measured. (It is a well-known fact in quantum information that entangling with a subsystem that is not observed any more effectively measures a state.) Thus, the predicate \( U_{\text{copy},X \rightarrow e} \cdot A \) encodes the fact that \( X \) has been measured. At the same time, this predicate does not forget about the probabilities of the different measurement outcomes.
This is best illustrated by an example: Let $x$ be of type integer and $\psi := \sqrt{2/3|1\rangle + \sqrt{1/3}|2\rangle}$. We have $\{ x =_q \psi \} \\text{measure} \ x \{ U_{\text{copy}, x \rightarrow e} \cdot (x =_q \psi) \} = \{ xe =_q U_{\text{copy}, x \rightarrow e}\psi \} = \{ xe =_q \psi' \}$ with $\psi' := \sqrt{2/3|1\rangle + \sqrt{1/3}|2\rangle}$. As we see, the postcondition encodes the probabilities of measuring 1 and 2 (namely, 2/3 and 1/3). Note that the postcondition $xe =_q \psi'$ does not mean that $x$ is actually entangled with something. Since $e$ is a ghost, it only means that $x$ is in a state that can be seen as a hypothetical entanglement with some $e$. In fact, it is easy to see (Lemma 2) that the only mixed memory on $x$ satisfying $xe =_q \psi'$ is $\rho = \frac{1}{2} \text{proj}(|1\rangle) + \frac{1}{2} \text{proj}(|2\rangle)$, as expected. Thus the postcondition faithfully encodes the probabilities of the measurement outcome, something that would not have been possible without using ghosts.

Since measurements are merely syntactic sugar in our language, it turns out that rule MeasureForget can be easily derived from the more basic rules we saw so far:

**Proof of MeasureForget.** Recall from page 8 that measure $X$ is syntactic sugar for “$z \in\Downarrow |0\rangle$; apply CNOT to $Xz$; $z \in\Downarrow |0\rangle$” for some fresh $z$ (in particular, $z \not\in \text{fv}(A), X$). We then have for some fresh $e$:

\[
\begin{align*}
\{ A \} & \ z \in\Downarrow |0\rangle \ \{ A|e/z\}, \ z =_q |0\rangle \} = \{ A, z =_q |0\rangle \} \quad \text{(rule INITQ)} \\
& \subseteq \{ U_{\text{copy}, x \rightarrow e} \cdot A \} \\
\text{apply CNOT to } Xz & \ \{ (\text{CNOT on } Xz) \cdot (A, \ z =_q |0\rangle) \} \quad \text{(rule APPLY)} \\
& \subseteq \{ U_{\text{copy}, x \rightarrow e} \cdot A \}. \\
\end{align*}
\]

Here ($\ast$) follows since $(\text{CNOT on } Xz)(\psi \otimes |0\rangle) = U_{\text{copy}, x \rightarrow e}\psi$.

Then by rules Seq and Conseq, we get $\{ A \} \text{ measure } X \{ U_{\text{copy}, x \rightarrow e} \cdot A \}$. ⊳

The postcondition of rule MeasureForget encodes both the distribution of outcomes, as well as the state after the measurement. Sometimes, it may not be necessary to remember the distribution (only which outcomes are possible). In this case we can use the following weaker rule:

\[
\begin{align*}
\{ A \} & \ \text{measure } X \ \{ \text{class}(X), \ \bigvee_i (\text{proj}(i) \ on \ X) \cdot A \} \\
\end{align*}
\]

To understand the rule, it is easiest to look at the same example as above. Recall that $\psi = \sqrt{2/3|1\rangle + \sqrt{1/3}|2\rangle}$ and $x$ is of type integer. Then MeasureForget* implies

\[
\{ x =_q \psi \} \ \text{measure } x \ \{ \text{class}(x), \ \bigvee_i (\text{proj}(i) \ on \ x) \cdot (x =_q \psi) \} = \{ \text{class}(x), \ \bigvee_i x =_q \text{proj}(i)\psi \}.
\]

Since $\text{proj}(i)\psi = 0$ for $i \not\in \{ 1, 2 \}$ and $\text{proj}(i)\psi = |i\rangle$ up to scalar factor for $i = 1, 2$, we have that $\bigvee_i x =_q \text{proj}(i)\psi$ equals $x =_q |1\rangle \lor x =_q |2\rangle$. Thus

\[
\{ x =_q \psi \} \ \text{measure } x \ \{ \text{class}(x), \ x =_q |1\rangle \lor x =_q |2\rangle \}.
\]

In other words, after measuring $x$, $x$ will be classical and have a state $|1\rangle$ or $|2\rangle$. Rule MeasureForget* is derived from MeasureForget by rule Transmute:
Proof of MeasureForget*.  

\[ \{ A \} \; \text{measure} \; X \; \{ U_{\text{copy}, X \rightarrow e} \cdot A \} \]  
\[ \Rightarrow \{ \bigvee_i ((\text{proj}(|i\rangle) \; \text{on} \; u) \cdot (U_{\text{copy}, X \rightarrow u} \cdot A)) \} \]  
\[ \text{(rule MeasureForget)} \]  
\[ \subseteq \{ \bigvee_i ((\text{proj}(|i\rangle) \; \text{on} \; X) \cdot A, \; u \equiv_q |i\rangle) \} \]  
\[ \subseteq \{ \bigvee_i ((\text{proj}(|i\rangle) \; \text{on} \; X) \cdot A, \; X \equiv_q |i\rangle, \; u \equiv_q |i\rangle) \} \]  
\[ \subseteq \{ \bigvee_i ((\text{proj}(|i\rangle) \; \text{on} \; X) \cdot A, \; X \equiv_d u) \} \]  
\[ \subseteq \{ \bigvee_i ((\text{proj}(|i\rangle) \; \text{on} \; X) \cdot A, \; X \equiv_d u) \} \]  
\[ \subseteq \{ \text{class}(X), \; \bigvee_i ((\text{proj}(|i\rangle) \; \text{on} \; X) \cdot A \} \]  
\[ \text{=} \{ \text{class}(X), \; \bigvee_i ((\text{proj}(|i\rangle) \; \text{on} \; X) \cdot A \} \]. \]

Here \((*)\) follows since \((\text{proj}(|i\rangle) \; \text{on} \; u) U_{\text{copy}, X \rightarrow u} \phi = (\text{proj}(|i\rangle) \; \text{on} \; X) \phi \otimes |i\rangle_u \) for all \(\phi\). And \((***)\) follows since \((\text{proj}(|i\rangle) \; \text{on} \; X) \cdot A \subseteq (X = q |i\rangle) \). \(\Box\)

Above, we studied measurements that forget their outcome (measure \(X\)). When we consider measurement that remember their outcome \((Y \leftarrow \text{measure} \; X)\), we get the following analogues to MeasureForget and MeasureForget*:

**Measure**  
\[ \{ A \} \; Y \leftarrow \text{measure} \; X \; \{ U_{\text{copy}, X \rightarrow e'} \cdot U_{\text{copy}, X \rightarrow Y} \cdot A \{ e / Y \} \} \]

**Measure**  
\[ \{ A \} \; Y \leftarrow \text{measure} \; X \; \{ \text{class}(X), \; \text{class}(Y), \; \bigvee_i ((\text{proj}(|i\rangle) \; \text{on} \; X) \cdot A \{ e / Y \}, \; Y = q |i\rangle) \} \]

As one can see, the only differences to MeasureForget and MeasureForget* is that the measurement is additionally written to \(Y\) (either via \(U_{\text{copy}, X \rightarrow Y}\) or via \(Y = q |i\rangle\)). And additionally, \(Y\) is replaced by \(e\) in \(A\) if it occurs there because it is overwritten (analogous to rule INIT, rule INITQ, rule INITC). For example, with \(\psi\) and \(X\) as above, we get \(\{ X = q \psi \} Y \leftarrow \text{measure} \; X \; \{ \text{class}(X), \; \text{class}(Y), \; X \equiv_q |i\rangle \} \) with \(\psi'' := \sqrt{2/3} |11\rangle + \sqrt{1/3} |22\rangle\) and \(\{ X = q \psi \} Y \leftarrow \text{measure} \; X \; \{ \text{class}(X), \; \text{class}(Y), \; X \equiv_q |11\rangle \lor X \equiv_q |22\rangle \} \). The proofs of these rules are very similar to those of MeasureForget and MeasureForget*:

Proof of Measure. Recall from page 8 that \(Y \leftarrow \text{measure} \; X\) is syntactic sugar for \("Y \leftarrow \text{init} \; z = q |0\rangle; \text{apply CNOT to XY}; \text{apply CNOT to Xz}; \text{z = q |0\rangle}"\) for some fresh \(z\) (in particular, \(z \not\equiv f(A), X, Y\)). Then we have for some fresh \(e, e'\):

\[ \{ A \} \; Y \equiv_{cl} |0\rangle \; \{ A \{ e / Y \}, \; Y = q |0\rangle \} \]  
\[ \text{z = q} \; |0\rangle \; \{ (A \{ e / Y \}, \; Y = q |0\rangle) \cdot (e'/z), \; z = q |0\rangle \} \]  
\[ = \{ A \{ e / Y \}, \; Y = q |0\rangle, \; z = q |0\rangle \} \]  
\[ \text{(rule INITQ)} \]  
\[ \text{(rule INITQ)} \]  
\[ \text{(z \not\equiv f(A), Y, e)} \]  
\[ \text{apply CNOT to XY} \; \{ (\text{CNOT on XY}) \cdot (A \{ e / Y \}, \; Y = q |0\rangle), \; z = q |0\rangle \} \]  
\[ \text{(rule APPLY, z \not\equiv XY)} \]  
\[ \text{apply CNOT to Xz} \; \{ (\text{CNOT on Xz}) \cdot (U_{\text{copy}, X \rightarrow Y} \cdot A \{ e / Y \}, \; z = q |0\rangle) \} \]  
\[ \text{(rule APPLY)} \]  
\[ \text{apply CNOT to Xz} \; \{ (\text{CNOT on Xz}) \cdot (U_{\text{copy}, X \rightarrow Y} \cdot A \{ e / Y \}, \; z = q |0\rangle) \} \]  
\[ \text{(rule APPLY)} \]  
\[ \text{z = q} \; |0\rangle \; \{ U_{\text{copy}, X \rightarrow e'} \cdot U_{\text{copy}, X \rightarrow Y} \cdot A \{ e / Y \}, \; z = q |0\rangle \} \]  
\[ \text{z = q} \; |0\rangle \; \{ U_{\text{copy}, X \rightarrow e'} \cdot U_{\text{copy}, X \rightarrow Y} \cdot A \{ e / Y \}, \; z = q |0\rangle \} \]  
\[ \subseteq \{ U_{\text{copy}, X \rightarrow e'} \cdot U_{\text{copy}, X \rightarrow Y} \cdot A \{ e / Y \} \}. \]
Finally, we consider sampling for some $\text{Sample}^*$. Here is the support of the distribution $D$, i.e., $\text{supp} D = \{ i : D(i) \neq 0 \}$. That is, the postcondition from $\text{Sample}^*$ says that $X$ is distributed according to $D$ ($\text{distrib}(X, D)$), while the postcondition from rule $\text{Sample}^*$ merely says that $X$ is classical and has value $i (X = q_i)$ for some $i \in \text{supp} D$. Both rules can be derived easily using the definition of $\text{distrib}(X, D)$ as syntactic sugar and the rules we have derived above.
Proof of Sample. Recall that $X \stackrel{\Psi}{\rightarrow} D$ is syntactic sugar for \texttt{“X \{\Psi\}$measure X”} where $\Psi = \sum_{i \in T} \sqrt{D(i)}|i\rangle$. And \texttt{distrib(X, D)} is syntactic sugar for $X e =_q \Psi_{DD}$ where $\Psi_{DD} = \sum_i \sqrt{D(i)}|i\rangle$ and $e$ is fresh. We have (with fresh $e, e'$):

\[
\{A|X \stackrel{\Psi}{\rightarrow} D\} \{A(e/X), X =_q \Psi_D\} \quad (\text{rule INITQ})
\]

\[
\text{measure X } \{U_{copy, X \rightarrow e'} \cdot (A(e/X), X =_q \Psi_D)\} \quad (\text{rule MeasureForget})
\]

\[
= \{A(e/X), U_{copy, X \rightarrow e'} \cdot (X =_q \Psi_D)\}
\]

\[
= \{A(e/X), Xe =_q \Psi_{DD}\} = \{A(e/X), \text{distrib}(X, D)\}.
\]

Rule \texttt{Sample} then follows by rule \texttt{Seq}.

Proof of Sample*. Recall that $X \stackrel{\Psi}{\rightarrow} D$ is syntactic sugar for \texttt{“X \{\Psi\}$measure X”} where $\Psi = \sum_{i \in T} \sqrt{D(i)}|i\rangle$. We have (with fresh $e$):

\[
\{A|X \stackrel{\Psi}{\rightarrow} D\} \{A(e/X), X =_q \Psi_D\} \quad (\text{rule INITQ})
\]

\[
\text{measure X } \{\text{class}(X), \bigvee_i (\text{proj}(|i\rangle) \text{on } X) \cdot (A(e/X), X =_q \Psi_D)\} \quad (\text{rule MeasureForget*})
\]

\[
= \{\text{class}(X), \bigvee_i (A(e/X), X =_q \text{proj}(|i\rangle) \Psi_D)\}
\]

\[
\subseteq \{A(e/X), \text{class}(X), \bigvee_i X =_q \text{proj}(|i\rangle) \Psi_D\}
\]

\[
\overset{(\ast)}{=} \{A(e/X), \text{class}(X), \bigvee_{i \in \text{supp } D} X =_q |i\rangle\}.
\]

Here (\ast) follows since $\text{proj}(|i\rangle) \Psi_D = 0$ for $i \notin \text{supp } D$, and $0 \neq \text{proj}(|i\rangle) \Psi_D \propto |i\rangle$ for $i \in \text{supp } D$. Rule \texttt{Sample*} then follows by rules \texttt{Seq} and \texttt{Conseq}.

Final note. Without the concept of ghosts, we would not have been able to express rule \texttt{Init} and thus not have been able to derive the above rules. Instead, we would have had to directly prove rules for measurements and sampling directly from the semantics. And without ghosts, those rules would not have been as expressive, for example, \texttt{Sample} would not have been expressible (i.e., we cannot express what distribution $X$ has after sampling), and rule \texttt{Sample*} would lack the predicate $\text{class}(X)$, i.e., we cannot express that $X$ is not a superposition between different $|i\rangle$ with $i \in \text{supp } D$.

7.2 Programs with classical variables

In this section, we show how programs using classical variables can be conveniently treated in our logic, even though the definition of our programming language does not contain classical variables. The lack of classical variables in language and logic has, at the first glance, a number of negative consequences:

(i) Any classical values in a program need to be encoded as quantum states. In particular, reasoning steps that hold only for classical variables cannot be applied. (E.g., a case distinction over the value of the classical variable.)

(ii) Quantum operations cannot be parametrized by classical values. For example, we might wish to model a program step such as $\texttt{apply } U_y \texttt{ to } x$, i.e., $U_i$ is a family of isometries, and the classical variable $y$ selects which of them is applied to $x$. For example, in [19], every program step can be parametrized by all classical variables, and this possibility is essential for expressing more complicated programs (e.g., the cryptographic schemes analyzed there).
(iii) Predicates cannot depend on classical values. For example, we might wish to say something like $x \in_\psi S_y$, i.e., $S_y$ is a family of subspaces, and $x$ lies in the subspaces $S_y$ selected by the classical variable $y$. For example, \cite{19} handles this by defining predicates to be families of subspaces indexed by the values of the classical variables (and not simply subspaces as is the case here). Such predicates are necessary for more complex analyses, e.g., think of Grover’s algorithm \cite{10} where the loop invariant would have to state that the quantum register is in a state that depends on how many iterations have been performed so far (the iteration counter being a classical variable).

As we see, a special treatment of classical variables is almost essential for convenient reasoning about hybrid programs (i.e., programs that contain both classical and quantum values), yet such a special treatment comes with a large formal overhead (the semantics are more complex, all proofs need to distinguish between classical and quantum variables). In this section, we will see how ghost variables allow us to recover the benefits of classical variables without the formal overhead, simply by introducing additional syntactic sugar and some derived rules.

**Syntactic sugar for programs.** In our language, apply $U$ to $X$ requires $U$ to be a constant. Since $X \triangleleft \psi$, $X \leftarrow z$, and $X \triangleleft D$ are all syntactic sugar based on apply, they inherit this restriction, i.e., $\psi, z, D$ are constants as well. Thus we cannot even write something as simple as $x \leftarrow y$, meaning we assign the content of the classical variable $y$ to $x$. We introduce some syntactic sugar for apply that solves this problem:

Consider the term apply $U$ to $X$ where $U$ is an expression containing program variables $Y$ of type $T$ (disjoint from $X$). For any assignment $z$ to the variables $Y$, $U\{z/Y\}$ defines an isometry $U[z]$ ($U$ evaluated for $Y := z$). Let $U[Y]$ be the isometry on $Y\times$ defined by $U[Y](|i\rangle\otimes\psi) := |i\rangle\otimes U[i]\psi$. (That is $U[Y]$ is a controlled operation, like CNOT.) Finally, apply $U$ to $X$ is syntactic sugar for apply $U[Y]$ to $Y\times$.

This notation is best understood by looking at a typical example. Consider apply $e^{-2i\pi yH}$ to $x$ where $H$ is some fixed Hermitian operator, and $y$ has type $\mathbb{R}$. Since $U := e^{-2i\pi yH}$ contains the variable $y$, it defines the family $U[z] := e^{-2i\pi zH}$ of unitaries. Then $U[y](|z\rangle\otimes\psi) = |z\rangle\otimes e^{-2i\pi zH}\psi$. Then apply $e^{-2i\pi yH}$ to $x = \text{apply } U[y] \text{ to } y\times$ applies $U[z] := e^{-2i\pi zH}$ to $x$ if $y$ is in state $|z\rangle$, as expected.

Note that this notation does not require that $Y$ refers to classical variables. It is meaningful to use this notation when $Y$ does not contain classical data. However, in the remainder of this paper, we will only use this notation when we think of $Y$ as classical variables.

Since $X \triangleleft \psi$, $X \leftarrow z$, and $X \triangleleft D$ are all syntactic sugar based on apply, this notation automatically carries over to those constructs, too. For example, $x \leftarrow y$ is syntactic sugar for init $x$; apply $U[y]$ to $x$ with $U[z]|0\rangle := |z\rangle$ which is syntactic sugar for init $x$; apply $(U[y])[y]$ to $y\times$ where $(U[y])[y]|z\rangle|0\rangle = |z\rangle|z\rangle$. Hence $x \triangleleft y$ will initialize $y$ with $|z\rangle$ when $x$ contains $|z\rangle$, as expected. Similarly, had we chosen to define a more complicated measurement command in Section 3 (instead of $Y \leftarrow \text{measure } X$) that takes the measurement basis as an additional argument, then that measurement command would generalize analogously and allow us specify a basis that depends on classical variables.

**Syntactic sugar for predicates.** We use similar syntactic sugar for writing predicates that depend on classical variables. Without such syntactic sugar, predicates such as $x \equiv_\psi \psi$ can only contain a constant $\psi$, i.e., $\psi$ cannot depend on classical variables. An expression $A$ containing some (supposedly classical) variables $Y$ of type $T$ defines a family $A[z]$ ($z \in T$) of predicates with $\forall (A[z]) \cap Y = \emptyset$, resulting from substituting $Y$ by $z$ in the expression $A$. We then define the predicate $A[Y] := \bigvee_z (Y =_\psi |z\rangle, A[z])$. (That is, $|z\rangle\otimes\psi \in A[Y]$ iff $\psi \in A[z]$.) We can now
use the notation $A^{[Y]}$ in pre-/postconditions to parametrize predicates by the values of classical variables. In most cases, we omit the $[Y]$, writing simply the predicate $A$. While this notation is potentially ambiguous, in most cases it will be clear where the $[Y]$ has to be added since otherwise the pre-/postconditions will not be welltyped.

We illustrate this by example: Consider the judgment $\{\text{class}(y), x =_q [0]\} \text{apply}\ e^{-2i\pi y H} \to x\ \{\text{class}(y), x =_q e^{-2i\pi y H}[0]\}$. We have seen in the previous paragraph how to read $\text{apply}\ e^{-2i\pi y H} \to x$. The precondition does not contain any syntactic sugar related to classical variables. We now translate the postcondition. Without omission of the implicitly understood $[Y]$, it reads $\text{class}(y), (x =_q e^{-2i\pi y H}[0])^{[Y]}$. (The $[Y]$ cannot be placed elsewhere since including the $\text{class}(y)$ in it would be mean that our postcondition contain non-welltyped subterms $\text{class}(z)$ for real $z$. And we cannot have $[xy]$ instead of $[y]$ since that would lead to non-welltyped subterms $z_1 = q \ldots$ where $z_1$ is not a variable.) Then $x =_q e^{-2i\pi y H}[0]$ defines a family of predicates $x =_q e^{-2i\pi y H}[0]$ for real $z$, and $(x =_q e^{-2i\pi y H}[0])^{[Y]}$ means $\bigvee_z (y =_q |z|, x =_q e^{-2i\pi z H}[0])$. Thus the postcondition would, without the syntactic sugar, read $\text{class}(y), \bigvee_z (y =_q |z|, x =_q e^{-2i\pi z H}[0])$. Of course, given appropriate rules such as $\text{ApplyParam}$ below, one rarely needs to actually explicitly unfold the syntactic sugar.

**Derived rules.** Since the syntactic sugar introduced in this section expands to language constructs for which we already have introduced rules, we could, in principle, reason about programs involving classical variables with only the rules above. However, in practice this may be cumbersome. Therefore we will now introduce a few derived rules specifically for the dealing with such programs. The first is a simple consequence of rule $\text{CaseClassical}$:

$$\forall z. \{Y =_q |z|, \text{class}(Y), A^{[z]} \} \varepsilon \{B\} \\Rightarrow \{\text{class}(Y), A^{[Y]} \} \varepsilon \{B\}$$

**Proof.** Let $T$ be the type of $Y$. For any $z \in T$, we have $(Y =_q |z|, A^{[z]}) = (Y =_q |z|, \bigvee_z (Y =_q |z'|, A^{[z']})) = (Y =_q |z|, A^{[Y]})$. (The first equality follows since $(Y =_q |z|, Y =_q |z'|, A^{[z']}) = 0$ for $z \neq z'$.) Thus the premise of $\text{CaseClassical}$ becomes $\forall z. \{Y =_q |z|, \text{class}(Y), A^{[Y]} \} \varepsilon \{B\}$. By $\text{Case}$ (with $A := (\text{class}(Y), A^{[Y]}), C := \text{class}(X), M := \{|z|\}_{z \in T}$, we get $\{\text{class}(Y), A^{[Y]} \} \varepsilon \{B\}$. (Using Lemma 6 to show $\text{class}(X)$ is $\{|z|\}_{z \in T}$-disentangling.)

From this rule, we can derive a rule for our classically parametrized $\text{apply}$-command:

$$\text{ApplyParam} \quad \text{fv}(e) \subseteq Y \quad Y \cap X = \emptyset \quad \frac{}{\{\text{class}(Y), A^{[Y]} \} \text{apply} e \to X \{\text{class}(Y), \{((e \text{ on } X) \cdot A)^{[Y]}\}\}}$$

Note that his rule is basically the same as rule $\text{Apply}$ (especially if we write it with omitted $[Y]$), except that we allow expression $e$ that specifies the operation to apply to contain variables $Y$ that must be guaranteed to be classical in the preconditional $\{\text{class}(Y)\})$.

**Proof.** Let $Y' := \text{fv}(e)$. Let $Y'' := Y \setminus Y'$. Let $T, T', T''$ be the types of $Y, Y', Y''$, respectively. Then $T = T' \times T''$ (up to a canonical bijection). Then $\text{apply} e \to X$ is syntactic sugar for
apply $e^{[Y']} \text{ to } Y'X$ where $e[z'] := e\{z'/Y'\}$ for $z' \in T'$. For any $z = (z', z'') \in T$, we have:

\[
\{ Y = \_ \, | \, z \}, \text{ class}(Y), \, A^{[z]} \}
\]
\[
\text{apply } e^{[Y']} \text{ to } Y'X \{ (e^{[Y']} \text{ on } Y'X) \cdot (Y = \_ \, | \, z), \, \text{ class}(Y), \, A^{[z]} \} \]
\[
\overset{\text{def}}{=} \{ (e[z'] \text{ on } X) \cdot (Y = \_ \, | \, z), \, \text{ class}(Y), \, A^{[z]} \} \]
\[
= \{ Y = \_ \, | \, z \}, \, \text{ class}(Y), \, (e[z'] \text{ on } X) \cdot A^{[z]} \}
\]
\[
= \{ Y = \_ \, | \, z \}, \, \text{ class}(Y), \, ((e \text{ on } X) \cdot A)^{[z]} \}
\]
\[
\overset{\text{def}}{=} \{ Y = \_ \, | \, z \}, \, \text{ class}(Y), \, \bigvee_{\tilde{z}} (Y = \_ \, | \tilde{z}), \, ((e \text{ on } X) \cdot A)^{[z]} \}
\]
\[
= \{ Y = \_ \, | \, z \}, \, \text{ class}(Y), \, ((e \text{ on } X) \cdot A)^{[Y]} \}
\]
\[
\subseteq \{ \text{ class}(Y), \, ((e \text{ on } X) \cdot A)^{[Y]} \}.
\]

Here (\*) follows from the fact that by definition, $U^{[Y']}$ operates as $U^{[z]}$ on quantum memories in $Y = \_ \, | \, z$. And (\**) follows since $(Y = \_ \, | \tilde{z}), \, Y = \_ \, | \tilde{z}, \, A^{[\tilde{z}]} \) = 0$ for $z \neq \tilde{z}$.

Thus (using rule CONSEQ and the syntactic sugar for apply):

\[
\{ Y = \_ \, | \, z \}, \, \text{ class}(Y), \, A^{[z]} \} \text{ apply } e \text{ to } X \{ \text{ class}(Y), \, ((e \text{ on } X) \cdot A)^{[Y]} \}
\]

By rule CASECLASSICAL (with $B := (\text{ class}(Y), \, ((e \text{ on } X) \cdot A)^{[Y]}))$, we get the conclusion of rule APPLYPARAM.  

For a simple example of using this rule see the correctness of the quantum one-time pad (Section 8.1).

8 Case Study: Quantum One-time Pad

In this section, we give a more advanced example of using Hoare logic with ghosts. We analyze the quantum one-time pad (QOTP, [3, 16]), a simple encryption scheme for quantum data. First, we analyze its correctness (i.e., the fact that decryption correctly yields the original plaintext). This is entirely unproblematic and can be done in most variants of quantum Hoare logic. We include this case as a warm-up example for reasoning with mixed quantum and classical data. Then we turn to the security of the QOTP, i.e., the fact that an encrypted qubit looks like random data if the key is not known. For reasons described below (Section 8.2), this is hard or impossible with prior variants of quantum Hoare logic. It thus shows nicely the power of ghosts.

The QOTP, presented here in its version for single qubits, is very simple: The key $x = (x_1, x_2)$ are two uniformly random classical bits. The plaintext $y$ is a qubit. To encrypt, we apply the Pauli-Z operator $Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ iff $x_1 = 1$. Then we apply the Pauli-X operator $X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ iff $x_2 = 1$. Or, written more compactly, to encrypt $y$, we apply $X^{x_2}Z^{x_1}$ to it.

Decryption works by inverting the sequence of operations, i.e., by applying $Z^{x_1}X^{x_2}$ to $y$.

In our language, the QOTP, consisting of key generation, encryption, and decryption, is expressed as follows:

\[
\begin{align*}
\text{Keygen} & := x \overset{\$}{\leftarrow} K, \quad \text{Enc} := \text{apply } X^{x_2}Z^{x_1} \text{ to } y \\
\text{Dec} & := \text{apply } Z^{x_1}X^{x_2} \text{ to } y
\end{align*}
\]

Here $x$ has type $K := \{0, 1\}^2$ (the key space), $y$ has type $M := \{0, 1\}$ (the message space). In slight abuse of notation, we also use $K$ and $M$ for the uniform distributions over $K$ and
8.1 Correctness of the QOTP

The correctness of the QOTP can be expressed by the following Hoare judgment:

\[ \forall z, \psi. \quad \text{\{\(yz =_q \psi\}\} \text{Keygen; Enc; Dec \{\(yz =_q \psi\}\}} \]  

(5)

We introduced an extra variable \(z\) here to model that even if \(y\) is entangled with some other system \(z\), decryption correct restores the state of \(y\) and its entanglement with \(z\). Using the rules from this paper, the derivation of (5) is elementary:

\[
\{y =_q \psi\} \xleftarrow{S} K \{y =_q \psi, \text{class}(x), \bigvee_y x =_q \psi\} \]  

(rule \text{SAMPLE*})

\[
\subseteq \{\text{class}(x), yz =_q \psi\} \]

\[
\text{apply } X^{x_2}Z^{x_1} \text{ to } y \{\text{class}(x), (X^{x_2}Z^{x_1} \text{ on } y) \cdot (yz =_q \psi)\} \]  

(rule \text{APPLYPARAM})

\[
\text{apply } Z^{x_1}X^{x_2} \text{ to } y \{\text{class}(x), (Z^{x_1}X^{x_2} \text{ on } y) \cdot (X^{x_2}Z^{x_1} \text{ on } y) \cdot (yz =_q \psi)\} \]  

(rule \text{APPLYPARAM})

\[
= \{\text{class}(x), (Z^{x_1}X^{x_2}X^{x_2}Z^{x_1} \text{ on } y) \cdot (yz =_q \psi)\} \]

\[
\subseteq \{\text{class}(x), (id \text{ on } y) \cdot (yz =_q \psi)\} = \{\text{class}(x), yz =_q \psi\} \]

Here (+) uses that \(ZZ = XX = \text{id}\). By rules \text{SEQ} and \text{CONSEQ}, and the definitions of \text{Keygen, Enc, Dec, we then get} (5).

8.2 The Quantum One-time Pad and Other Logics

In this section, we explain why it is hard or even impossible to analyze the security of the QOTP in existing quantum Hoare logics (without ghosts). This section is not required for understanding the security proof and can be skipped. However, it illustrates why we need ghosts. Since this section is about logics from prior work, and it would be beyond the scope of this section to introduce those logics in more detail, in this section we assume some familiarity with the logics referenced here.

Security of the QOTP means that, after encrypting, the variable \(y\) is indistinguishable from a uniformly random bit. (More precisely, after running \text{Keygen; Enc.}) How can we model/prove this in different Hoare logics?

Quantum Hoare logic with subspace predicates. Probably the simplest and most obvious variant of quantum Hoare logic is quantum Hoare logic with subspaces. Here pre-/postconditions are modeled as subspaces (a.k.a. sharp predicates, Birkhoff-von Neumann quantum logic). See the “Recap Hoare logic” paragraph on page 9 for additional details. In this logic, we cannot express that \(y\) is uniformly distributed. Specifically, any predicate \(A\) on \(y\) that holds when \(y\) is a uniformly distributed bit has to also hold for any other distribution! Namely, since \(y\) can be \([0]\) or \([1]\) (or anything else), \(A\) needs to contain \([0]\) and \([1]\). But the only subspace containing both \([0]\) and \([1]\) is the full space \(\ell^2[y] = \mathbb{T}\). Thus, the only postcondition on \(y\) that would be satisfied by the QOTP encryption is \(\mathbb{T}\) which would also be satisfied by any insecure encryption scheme. So we cannot formulate (let alone prove) any judgment in this variant of quantum Hoare logic that would express the security of the QOTP.

\footnote{A more elementary statement would be \(y \psi, \{y =_q \psi\} \text{Keygen; Enc; Dec \{y =_q \psi\}.}\) Alternatively, we could also state a stronger statement \(\{A\} \text{Keygen; Enc; Dec \{A\} for all } A \text{ with } x \notin \text{fv}(A).\) Both can be proven with essentially the same derivation as (5).}
Quantum Hoare logic with expectations. A more expressive variant of quantum Hoare logic is Hoare logic with expectations. Here, predicates are quantitatively "expectations";20 that is, for a given state $\rho$, satisfaction of a predicate $A$ is not binary (true/false), but a predicate $\rho$ is satisfied to a certain degree. (Formally, $A$ is a Hermitian operator and the degree of satisfaction is defined as $\text{tr} A \rho$. And a Hoare judgment $\{A\} \cdot c \{B\}$ means that $[c] (\rho)$ satisfies $B$ at least as much as $\rho$ satisfies $A$. Such a logic can be expressed in two ways, either via Hoare triples (e.g., (20)) or equivalently in terms of weakest preconditions [7].

We know that the weakest preconditions of a quantum program determines the denotational semantics of said program [7], that is, if $c$ and $d$ have the same weakest preconditions, then $\llbracket c \rrbracket = \llbracket d \rrbracket$. (Where $\llbracket \cdot \rrbracket$ is defined as in Section 3.) Or equivalently: $\llbracket c \rrbracket = \llbracket d \rrbracket$ iff for all predicates $A, B$, $\{A\} \cdot c \{B\} \iff \{A\} \cdot d \{B\}$. (This holds only if the predicates $A, B$ are expectations!) Thus we could define security of the QOTP by requiring that $\text{Keygen}; \text{Enc}$ has the same weakest preconditions as the program $y \leftarrow M$. (Where we do not allow predicates to refer to $x$ since security only holds when the key is secret. For simplicity, we will assume that $y$ is the only variable left after execution.) The weakest precondition for $y \leftarrow M$ and postcondition $B$ is $\frac{1}{2} \text{tr} B \cdot \text{id}$. Thus we can define security of the QOTP as follows: The QOTP is secure iff for all $B$, the weakest precondition of $\text{Keygen}; \text{Enc}$ for postcondition $B$ is $\frac{1}{2} \text{tr} B \cdot \text{id}$. Or in terms of Hoare judgments: The QOTP is secure iff for all $A, B$ with $A \leq \frac{1}{2} \text{tr} B \cdot \text{id}$, we have $\{A\} \cdot \text{Keygen}; \text{Enc} \{B\}$ and for all $A, B$ with $A \leq \frac{1}{2} \text{tr} B \cdot \text{id}$, we do not have $\{A\} \cdot \text{Keygen}; \text{Enc} \{B\}$.

This is formally correct (except for the fact that we glossed over the fact that there are variables beyond $y$), and security of the one-time pad can be derived due to the completeness of the calculus from [7]. However, the definition is very awkward. In order to prove the security of the one-time pad, not only do we need to prove that $\{A\} \cdot \text{Keygen}; \text{Enc} \{B\}$ holds for certain $A, B$ but also that is does not hold for certain others. This is problematic since usually we reason only in terms of judgments that hold, and not in terms of judgments that do not hold. (Or, in terms of weakest precondition, we reason about inequalities, not equalities.) Especially in the presence of partial specifications, proving that certain judgments do not hold might be very difficult.

What happens if we simply omit the requirement that some judgments do not hold? I.e., we use the following definition: The QOTP is secure iff for all $A, B$ with $A \leq \frac{1}{2} \text{tr} B \cdot \text{id}$, we have $\{A\} \cdot \text{Keygen}; \text{Enc} \{B\}$. As it turns out, this works for the QOTP (we can show that this condition is equivalent to the original one). However, this is accidental, and for slight variations of the QOTP, this might not work any more.

To illustrate this, consider the following slightly artificial variant $\frac{1}{2} \text{QOTP}$ of the QOTP: This variant has an encryption algorithm $\text{Enc}_{1/2}$ that terminates only with probability $\frac{1}{4}$, but that works correctly when it terminates. That is $\text{Enc}_{1/2} := T; \text{Enc}$ where $T$ is a program that does not touch any variables and terminates with probability $\frac{1}{2}$ (i.e., $[T](\rho) = \frac{1}{2} \rho$, e.g., implemented as a loop). Analogous to the above, we can say that the $\frac{1}{2} \text{QOTP}$ is secure iff for all $A, B$ with $A \leq \frac{1}{2} \text{tr} B \cdot \text{id}$, we have $\{A\} \cdot \text{Keygen}; \text{Enc}_{1/2} \{B\}$. (Note that $\frac{1}{2}$ was replaced by $\frac{1}{4}$, since we now compare with the program $T; y \leftarrow M$ which only satisfies these judgments.) But now consider a program $c$ that with probability $\frac{1}{4}$ runs $\text{skip}$, and with probability $\frac{1}{2}$ runs the original QOTP.21 This is clearly not a secure encryption scheme (with probability $\frac{1}{4}$ the plaintext is leaked by the program $\text{skip}$). Yet, we can check that when $A \leq \frac{1}{2} \text{tr} B \cdot \text{id}$, we have $\{A\} \cdot c \{B\}$. Hence the insecure $c$ also satisfies our definition of security! Thus, our security definition of the $\frac{1}{2} \text{QOTP}$ does not guarantee any reasonable security.

Summarizing, if we want to analyze the security of the QOTP or variants in quantum Hoare logic with expectations, it can be done in principle, but we need complicated definitions (we

20 Analogous to the classical expectations by Kozen [14].
21 Formally, $c := x \leftarrow M; \text{if } x \text{ then } \text{Keygen}; \text{Enc} \text{ else } \text{skip}$. }
cannot express the security as a single judgment but through an infinite family). And we need to not only prove that judgments hold but also that some judgments do not hold. (Except in some cases like the QOTP proper where positive judgments are sufficient. But seeing this needs additional extra-logical reasoning and does not generalize, e.g., to the 1/2-QOTP.) And even if we surmount these difficulties, it is not clear how we can reason with such families of judgments in a larger context (e.g., if the security of the QOTP is needed to derive some property of a larger program).

Quantum relational Hoare logic. Another variant of Hoare logic that seems particularly suitable for the analysis of the QOTP is quantum relational Hoare logic (qRHL [19]). This logic was specifically designed with cryptographic proofs in mind, inspired by the success of probabilistic relational Hoare logic [2]. In qRHL, Hoare judgments apply to pairs of programs. Very roughly speaking, a judgment such as \( \{ A \} e \sim d \{ B \} \) means that, if the memories of \( e \) and \( d \) jointly satisfy the predicate \( A \) before the execution of \( e \) and \( d \), they will jointly satisfy \( A \) afterwards. For example, if \( X_1, X_2 \) are the variables of \( e, d \), respectively, then \( \{ X_1 \equiv X_2 \} e \sim d \{ X_1 \equiv X_2 \} \) means that for identical initial states, \( e, d \) have identical final states. In other words, \( [e] = [d] \).

And \( \{ \top \} e \sim d \{ X_1 \equiv X_2 \} \) would mean that the final states are identical, no matter what the initial states are, i.e., \( \forall \rho, \rho'. [e](\rho) = [d](\rho') \).

Thus, at the first glance, it seems very easy to model the security of the one-time pad. To specify that \( y \) is uniformly random after execution of the QOTP (no matter what its initial state was), we simply require that \( y \) after the QOTP is the same as \( y \) after \( y \stackrel{\$}{\leftarrow} M \). That is, we say the QOTP is secure iff \( \{ \top \} \text{Keygen}: Enc \sim y \stackrel{\$}{\leftarrow} M \{ y_1 \equiv y_2 \} \). (Here \( y_1, y_2 \) refer to the \( y \) from the left/right program, respectively.) Unfortunately, this does not work. We can show that \( \{ \top \} \text{Keygen}: Enc \sim y \stackrel{\$}{\leftarrow} M \{ y_1 \equiv y_2 \} \) does not hold in qRHL. Intuitively, the reason is that after encrypting, \( y_1 \) is still correlated with the key \( x_1 \). This means that it could still be decrypted to the original plaintext, and therefore qRHL does not consider it equivalent to a uniformly random \( y_2 \) (that is independent of any other variables).

To resolve this, we need to erase the key after encrypting. So the definition becomes: The QOTP is secure iff

\[
\{ \top \} \text{Keygen}: Enc; x \leftarrow 00 \sim y \stackrel{\$}{\leftarrow} M \{ y_1 \equiv y_2 \}.
\] (6)

This judgment is indeed a good definition for the security of the QOTP. It is not hard to prove that it holds by explicitly computing the superoperators \([\text{Keygen}: Enc; x \leftarrow 00]\) and \([y \stackrel{\$}{\leftarrow} M]\), and then showing (6) directly from the semantic definition of qRHL. In that sense, qRHL is superior to the two Hoare logic variants above: at least we can state the security of the QOTP concisely. (And for variants of it such as 1/2-QOTP, similar definitions work.)

Unfortunately, it seems hard (or impossible) to derive (6) within the logic. (That is, by an application of a sequence of reasoning rules.) While we do not have a proof that (6) cannot be derived from the rules from [19], a natural proof would seem to go along the following lines: First, we show \( \{ \top \} \text{Keygen}: Enc \sim y \stackrel{\$}{\leftarrow} M \{ B \} \) for some \( B \), then we show \( \{ B \} x \leftarrow 00 \sim \text{skip} \{ y_1 \equiv y_2 \} \), and then we use the qRHL-analogue to rule \text{Seq} to conclude (6). Unfortunately, we can show that there exists no predicate \( B \) such that both \( \{ \top \} \text{Keygen}: Enc \sim y \stackrel{\$}{\leftarrow} M \{ B \} \) and \( \{ B \} x \leftarrow 00 \sim \text{skip} \{ y_1 \equiv y_2 \} \) are true. Hence this proof approach is doomed.

To summarize, in qRHL, while it is easy to formulate the security of the QOTP, there are reasons to believe that the security proof is difficult or even impossible.

\footnote{Or alternatively, we could define security as \( \{ \top \} \text{Keygen}: Enc \sim \text{Keygen}: Enc \{ y_1 \equiv y_2 \} \) which means that the ciphertexts \( y_1, y_2 \) have the same distribution, no matter what the plaintexts (initial values of \( y_1, y_2 \)) are. The difficulties described here apply in the same way to that definition.}
8.3 Security of the Quantum One-time Pad

We will now demonstrate how to prove the security of the QOTP using quantum Hoare logic with ghosts. Security of the QOTP means that, after encrypting, the variable \( y \) is indistinguishable from a uniformly random bit, as long as the key is not known. We formalize this by requiring that after key generation, encryption, and subsequent deletion of the key, \( y \) is uniformly random. As a Hoare judgment, we write this as:

\[
\{ \top \} \text{Keygen; Enc} \colon x \leftarrow 00 \{ \text{uniform}(y) \}. 
\]  

(7)

The \( x \leftarrow 00 \) overwrites the key \( x \) and is added to model the fact that we do not know the key.\(^{23}\) The precondition is \( \top \) since we do not want to make any assumption about the initial state of \( y \), i.e., about the plaintext. (In particular, the plaintext can be entangled with other variables.)

**Warm up.** Before we show (7), we prove a weaker claim as a warm up:

\[
\forall \psi \neq 0. \ \{ y =_q \psi \} \text{Keygen; Enc} \colon x \leftarrow 00 \{ \text{uniform}(y) \}. 
\]  

(8)

This equation say that the QOTP is secure as long as the plaintext \( y \) is some (arbitrary) state \( \psi \). That is, it only guarantees security for unentangled plaintexts. We will do the general case (7) below, but the simplified case is simpler and contains already many of the needed ideas.

Recall that \( \text{Keygen} = x \xleftarrow{\$} K \) and \( \text{Enc} = \text{apply } X^{x_2}Z^{x_1} \text{ to } y \). We first derive a postcondition for \( \text{Keygen; Enc; } x \leftarrow 00 \) by simply applying the reasoning rules step by step:

\[
\{ y =_q \psi \} \ x \xleftarrow{\$} K \ \{ y =_q \psi, \ \text{uniform}(x) \} \tag{rule SAMPLE}
\]

\[
\text{apply } X^{x_2}Z^{x_1} \text{ to } y \ \{ (X^{x_2}Z^{x_1})^{[x]} \text{ on } xy \} \cdot \{ y =_q \psi, \ \text{uniform}(x) \} \tag{rule APPLY}
\]

\[
x \leftarrow 00 \ \{ (X^{e_2}Z^{e_1})^{[e]} \text{ on } ey \} \cdot \{ y =_q \psi, \ \text{uniform}(e) \}, \ x =_q 00, \ \text{class}(x) \} \tag{rule InitC}
\]

\[
\subseteq \ \{ (X^{e_2}Z^{e_1})^{[e]} \text{ on } ey \} \cdot \{ y =_q \psi, \ \text{uniform}(e) \} \}
\]

For the application of rule SAMPLE, recall that \( \text{uniform}(x) \) is syntactic sugar for \( \text{distrib}(x, K) \) where \( K \) is the uniform distribution on the type of \( x \). For the application of rule APPLY, recall that \( \text{apply } X^{x_2}Z^{x_1} \text{ to } y \) is syntactic sugar for \( \text{apply } (X^{x_2}Z^{x_1})^{[x]} \text{ to } xy \) (page 33). By rules \( \text{Seq} \) and \( \text{Conseq} \), we immediately get

\[
\{ y =_q \psi \} \text{Keygen; Enc; } x \leftarrow 00 \ \{ (X^{e_2}Z^{e_1})^{[e]} \text{ on } ey \} \cdot \{ y =_q \psi, \ \text{uniform}(e) \} \} =: \{ B \} \tag{9}
\]

While this is not yet the final result (8) we wanted, we see that the application of the \( \text{InitC} \) rule already achieved one important thing: Since \( x \) was turned into a ghost, the postcondition \( B \) refers only to the ciphertext \( y \) and not other variables, i.e., we got rid of the dependence between \( y \) and \( x \). What is left to do is to prove that the postcondition \( B \) implies \( \text{uniform}(y) \).

Analyzing \( B \) involves some calculations. (This is to be expected because the QOTP relies on the properties of the involved matrices, so we have to calculate somewhere.) We first unfold the syntactic sugar. \( \text{uniform}(e) \) means \( ee'^{e} =_q \psi_{KK} \) for some fresh \( e' \). Thus

---

\(^{23}\) One might think that it should be sufficient to simply not mention the key in the postcondition. I.e., to define security as \( \{ \top \} \text{Keygen; Enc } \{ \text{uniform}(y) \} \). However, from Lemma 2 we know that in a state satisfying \( \text{uniform}(y) \), \( y \) is uniform and independent of all other variables. This is clearly not the case after encryption (\( y \) is not independent of the key \( x \)). Thus \( \{ \top \} \text{Keygen; Enc } \{ \text{uniform}(y) \} \) does not hold.
\[ (y = q, \text{uniform}(e)) = (yee' = q \psi \otimes \psi_{KK}). \] Furthermore \((X^{e_2}Z^{e_1})^{[e]} = \sum_{k \in K} \text{proj}(k) \otimes X^{k_2}Z^{k_1}\) (see page 33). Thus

\[
B = \left( \left( \sum_{k \in K} \text{proj}(k) \otimes X^{k_2}Z^{k_1} \right) \text{on } ey \right) \cdot (yee' = q \psi \otimes \psi_{KK})
\]

\[
= \sum_{\phi} \left( yee' = q \left( \sum_{k \in K} X^{k_2}Z^{k_1} \otimes \text{proj}(k) \otimes \text{id} \right) (\psi \otimes \psi_{KK}) \right).
\]

(Note that in (*), the tensor product factors in the sum are written in a different order because the \((\ldots \text{on } ey)\)-term and the \((yee' = q \ldots)\)-term list the variables in a different order.) Since \(B\) is now of the form \(yee' = \phi\), it is amenable to rewriting using rule \text{SHAPESHIFT}. Furthermore, our intended postcondition \text{uniform}(y) is syntactic sugar for \(yee' = q \psi_{MM}\), which is also compatible with \text{SHAPESHIFT}. Specifically, if we can show \(\text{tr}_{ee'} \text{proj}(\phi) = \text{tr}_{ee'} \text{proj}(\psi_{MM})\), then \text{rule SHAPESHIFT} implies

\[
B = (yee' = q \phi) \Rightarrow (y =_{q} \psi_{MM}) = \text{uniform}(y). \tag{10}
\]

(Recall that \(M\) is the uniform distribution on the type of \(y\), i.e., on \(\{0,1\}\).) We now show \(\text{tr}_{ee'} \text{proj}(\phi) = \text{tr}_{ee'} \text{proj}(\psi_{MM})\) by computation. Since \(\psi_{KK} = \sum_{l \in K} \frac{1}{2} |l\rangle \otimes |l\rangle\) by definition, we have:

\[
\phi = \sum_{kl} \frac{1}{2} X^{k_2}Z^{k_1} \psi \otimes \text{proj}(k) \otimes |l\rangle \otimes |l\rangle_{w'}. \quad \sum_{k} \frac{1}{2} X^{k_2}Z^{k_1} \psi \otimes |k\rangle_{a} \otimes |k\rangle_{a'}. \]

Thus

\[
\text{tr}_{ee'} \text{proj}(\phi) = \text{tr}_{ee'} \sum_{k} \frac{1}{2} X^{k_2}Z^{k_1} \text{proj}(\psi)(X^{k_2}Z^{k_1})^{*} \otimes |k\rangle_{a} \otimes |k\rangle_{a'}. \]

\[
= \sum_{k} \frac{1}{2} X^{k_2}Z^{k_1} \text{proj}(\psi)(X^{k_2}Z^{k_1})^{*} = \sum_{k} \frac{1}{4} \text{proj}(X^{k_2}Z^{k_1} \psi). \]

Here (*) follows from the facts that \(\text{tr}_{ee'} \sigma \otimes \tau = \sigma \text{tr} \tau\) and that \(\text{tr}|k\rangle \langle k'| = 1\) if \(k = k'\) and \(= 0\) otherwise. Without loss of generality, we can assume that \(\|\psi\| = 1\) (because the predicate \(y = q\) does not change if we multiply \(\psi\) with a nonzero scalar.) Thus \(\psi = (\gamma)\) for some \(\alpha, \beta \in \mathbb{C}\) with \(\alpha^{*} + \beta \beta^{*} = 1\). Then \(\sum_{k} \frac{1}{4} \text{proj}(X^{k_2}Z^{k_1} \psi)\) can be explicitly computed (a sum of four \(2 \times 2\)-matrices), and simplifies to \(\frac{1}{2} \text{id}\). Furthermore, we easily compute that \(\text{tr}_{ee'} \psi_{MM} = \frac{1}{2} \text{id}\). Thus \(\text{tr}_{ee'} \text{proj}(\phi) = \text{tr}_{ee'} \text{proj}(\psi_{MM})\). Hence (10) follows by rule \text{SHAPESHIFT}. From (9), (10), with rule \text{SEQ}, we get (8). This shows the security of the QOTP in the special case that the plaintext is unentangled.

**General case.** We have shown the security of the QOTP in the special case (8) that the plaintext is not entangled with anything else but is in a fixed but arbitrary state \(\psi\). We now show the general case (7). To do so, we first show something similar to the special case (8), namely that the QOTP is secure when the plaintext \(y\) and one further variable \(z\) are in a fixed state \(\psi\). (And, for technical reasons we also include the variable \(x\), but that variable is less interesting since it is overwritten by Keygen.) Formally,

\[
\forall \psi \neq 0. \quad \{yzx = q \psi\} \text{Keygen} := x \leftarrow 00 \{\text{uniform}(y)\}. \tag{11}
\]

Here \(z\) is a program variable of infinite cardinality (e.g., of type integer). Intuitively, this already means that the QOTP is secure when the plaintext \(y\) is entangled. And indeed, the general
case (7) then is an immediate consequence of (11) and rule Universe (with X := xy, x := z, E := U := ∅, A := T, B := uniform(y)).

We are left to show (11). This is done similarly to (8), except that the computations are a bit more complex. First, we have

\[
\{yzx =_q \psi \} \times \overset{\times}{K} \{yze'' =_q \psi, \text{uniform}(x)\} \quad \text{(rule Sample)}
\]

apply \(X^{x_2}Z^{x_1}\) to y \(\{(X^{x_2}Z^{x_1})[x] \mid \text{on } xy\} \cdot (yze'' =_q \psi, \text{uniform}(x))\) \(\text{(rule Apply)}\)

\[
x \leftarrow \{00\} \{(X^{e_2}Z^{e_1})[e] \mid \text{on } ey\} \cdot (yze'' =_q \psi, \text{uniform}(e), x =_q [00], \text{class}(x)) \quad \text{(rule Initial)}
\]

\[
\subseteq \{(X^{e_2}Z^{e_1})[e] \mid \text{on } ey\} \cdot (yze'' =_q \psi, \text{uniform}(e))\}.
\]

Thus with rule Seq and rule Conseq:

\[
\{yzx =_q \psi\} \text{ Keygen; Enc; } x \leftarrow \{00\} \{(X^{e_2}Z^{e_1})[e] \mid \text{on } ey\} \cdot (yze'' =_q \psi, \text{uniform}(e))\} =: \{B'\}. \quad (12)
\]

As in the special case, we unfold syntactic sugar and we get:

\[
B' = (yze''e' =_q \left(\sum_{k \in K} X^{k_2}Z^{k_1} \otimes \text{id}_{ze''} \otimes \text{proj}([k]_e) \otimes \text{id}_{e''}) (\psi \otimes \psi_{Kk})\).
\]

Quite analogous to the special case, we compute

\[
\phi' = \sum_k \frac{1}{2} (X^{k_2}Z^{k_1} \otimes \text{id}_{ze''}) \psi \otimes [k]_e \otimes [k]_{e'} \quad \text{ and } \quad \text{tr}_{ee'} \text{proj}(\phi') = \sum_k \frac{1}{2} \text{proj}((X^{k_2}Z^{k_1} \otimes \text{id}_{ze''}) \psi).
\]

\(\text{(We will additionally need to trace out } e'', \text{ but the computation is easier if we do not do that yet.) We can write } \psi \text{ as } [0]_y \otimes \psi_0 + [1]_y \otimes \psi_1 \text{ for some } \psi_0, \psi_1 \text{ over } ze'. \) By substituting this in the rhs of the second equation in (13), and multiplying out and canceling terms, we get

\[
\text{tr}_{ee'} \text{proj}(\phi') = \frac{1}{2} (\text{proj}([0])_y + \text{proj}([1])_y) \otimes (\text{proj}(\psi_0) + \text{proj}(\psi_1)) = \frac{1}{2} \text{id}_y \otimes \rho_{ze''}.
\]

Let \(e_y, e_z\) be additional entangled ghosts. Then \(\text{tr}_{ee'} \text{proj}(\psi_{MM}) = \frac{1}{2} \text{id}_y\) (if we interpret \(\psi_{MM}\) as a quantum memory over \(ye_y\)). And there exists a \(\gamma\) over \(ze' e_z\) such that \(\text{tr}_{ee'} \text{proj}(\gamma) = \rho_{ze''}\). Thus \(\text{tr}_{ee'} \text{proj}(\phi') = \text{tr}_{ee'} e_y e_z \text{proj}(\psi_{MM} \otimes \gamma)\). Hence \(\text{tr}_{ee'} \text{proj}(\phi') = \text{tr}_{ee'} e_y e_z \text{proj}(\psi_{MM} \otimes \gamma)\). Using rule ShapeShift for \((*)\), we thus have

\[
B' = (yze''e' =_q \phi') \Rightarrow (ye_y z e'' e_z =_q \psi_{MM} \otimes \gamma)
\]

\[
= (ye_y =_q \psi_{MM}, ze' e_z =_q \gamma) \subseteq (ye_y =_q \psi_{MM}) = \text{uniform}(y).
\]

Then (11) follows with (12), rule Seq and rule Conseq. And, as mentioned above, the general case (7) is an immediate consequence of (11) and rule Universe. This shows the security of the QOTP.
### Symbol index

| Symbol | Description                                                                 | Page |
|--------|----------------------------------------------------------------------------|------|
| supp M | Support of an operator $M$                                                  | 9    |
| $Z$    | Pauli-Z operator                                                          | 35   |
| CNOT   | (Generalized) CNOT                                                         | 5    |
| skip   | Program: does nothing                                                     | 7    |
| $\downarrow_i(\rho)$ | Mixed state restricted to measurement outcome $i$               | 8    |
| $[\mathfrak{c}]$ | Denotation of a program $\mathfrak{c}$                           | 7    |
| tr$_V\rho$ | Partial trace (removing variables $V$)                        | 5    |
| $\psi_D$ | State encoding the distribution $D$                              | 8    |
| $\psi_{DD}$ | State encoding the distribution $D$ (on two variables)                | 12   |
| distrib(X, $D$) | Predicate: $X$ has distribution $D$                           | 12   |
| uniform(X) | Predicate: $X$ has uniform distribution                  | 12   |
| $X \leftarrow \psi$ | Program: Initialize $X$ with quantum state $\psi$       | 8    |
| separable(X) | Predicate: $X$ is separable from all other variables         | 13   |
| $A\{v/w\}$ | Predicate $A$ with $w$ substituted by $v$        | 6    |
| $A \Rightarrow B$ | “Implication” of predicates            | 19   |
| $M \cdot A$ | Operator $M$ applied to subspace $A$ | 5    |
| Enc | Encryption algorithm of the QOTP                                                                 | 35   |
| measure X | Program: Measure $X$ in computational basis, forget outcome | 8    |
| $X \leftarrow D$ | Program: Sample $X$ according to distribution $D$ | 8    |
| progsavars(V) | Set of program variables in $V$                           | 4    |
| $V \in S$ | Predicate: $V$ has a value in $S$                           | 6    |
| $\text{span } A$ | Span, smallest subspace containing $A$ | 6    |
| $V \equiv_q \psi$ | Predicate: $V$ is in state $\psi$ | 6    |
| $W \equiv_q W'$ | Predicate: $W$ and $W'$ are in the same state | 13   |
| $U \text{ on } V$ | Operator $U$ applied to variables $V$ | 5    |
| $A, B, C$ | (Quantum) predicates                                                           | 5    |
| $\|\psi\|$ | Norm of vector $\psi$                                                     | 4    |
| $|x|$ | Absolute value/cardinality                                                  |      |
| tr$M$ | Trace of matrix/operator $M$                                               |      |
| id | Identity                                                                 |      |
| proj($\psi$) | Projector onto $\psi$, i.e., $\psi\psi^*$               | 4    |
| $a^*$ | Adjoint of operator/vector $a$                                             | 4    |
| $V \equiv_d V'$ | Predicate: $V$ and $V'$ are classically in the same state | 15   |
| SWAP | Unitary that swaps $W$ and $W'$                                           | 13   |
| while $x$ do $\mathfrak{c}$ | Program: While (loop)                                           | 7    |
| $\mathfrak{c}, \mathfrak{d}$ | Program: execute $\mathfrak{c}$ then $\mathfrak{d}$ | 7    |
| $\mathbb{N}$ | Natural numbers $1, 2, 3, \ldots$                                       |      |
| Dec | Decryption algorithm of the QOTP                                                                 | 35   |
| $\mathbb{C}$ | Complex numbers                                                            |      |
\(\mathbb{R}\)  \(\text{Real numbers}\)

\(v, w\)  \(\text{Variable}\)

\(x, y, z\)  \(\text{Program variable}\)

\(u\)  \(\text{Unentangled ghost variable}\)

\(e\)  \(\text{Entangled ghost variable}\)

\(X, Y, Z\)  \(\text{List/set of program variables}\)

\(g\)  \(\text{Ghost variable}\)

\(X\)  \(\text{Pauli-X operator}\)

\(y \leftarrow \text{measure X}\)  \(\text{Program: Measure X in computational basis, assign outcome to y}\)

\(\{A\} c \sim d \{B\}\)  \(\text{Relational Hoare judgment}\)

\(\text{if } x \text{ then } c \text{ else } d\)  \(\text{Program: If (conditional)}\)

\(\text{class}(X)\)  \(\text{Predicate: X is classical}\)

\(A^X\)  \(\text{Predicate } A_i \text{ depending on } X\)

\(U^X\)  \(\text{Unitary } U_i \text{ controlled by } X\)

\(0\)  \(\text{Default value (in every variable type)}\)

\(\text{rank } M\)  \(\text{Rank of operator } M\)

\(U_{\text{cop}}, V \rightarrow W\)  \(\text{Copies classically from } V \text{ into } W\)

\(U_{V \rightarrow W}\)  \(\text{Rename variables } V \text{ into } W\)

\(\cup\)  \(\text{Disjoint union}\)

\(\text{im } M\)  \(\text{Image of operator } M\)

\(\text{Keygen}\)  \(\text{Key generation algorithm of the QOTP}\)

\(\rho \models A\)  \(\text{Mixed quantum memory } \rho \text{ satisfies predicate } A\)

\(E\)  \(\text{List/set of entangled ghost variables}\)

\(U\)  \(\text{List/set of unentangled ghost variables}\)

\(V, W\)  \(\text{List/set of variables}\)

\(G\)  \(\text{List/set of ghost variables}\)

\(\langle x \mid \rangle\)  \(\text{Adjoint of } |x\rangle, \text{i.e., } |x\rangle^*\)

\(|x\rangle\)  \(\text{Basis state } x\)

\(\ell^2[V]\)  \(\text{Pure quantum assignments on } V\)

\(\ell^2(X)\)  \(\text{Hilbert space with basis indexed by } X\)

\(A \otimes B\)  \(\text{Tensor product of vectors/operators/spaces } A \text{ and } B\)

\(m\)  \(\text{An assignment}\)

\(\perp\)  \(\text{Predicate: never satisfied}\)

\(\top\)  \(\text{Predicate: always satisfied}\)

\(\text{init } x\)  \(\text{Program: Initialize x with } |0\rangle\)

\(\text{apply } U \text{ to } V\)  \(\text{Program: Apply } U \text{ to variables } V\)

\(c, d\)  \(\text{A program}\)

\(f v(a)\)  \(\text{Free variables of predicate/program } a\)

\(A \lor B\)  \(\text{Sum of predicates (disjunction)}\)

\(\{A\} \epsilon \{B\}\)  \(\text{Hoare judgment}\)

\(X^{\text{all}}\)  \(\text{Set of program variables that can be used in the execution of a program}\)
| Symbol | Definition |
|--------|------------|
| $A \land B$, $A, B$ | Intersection of predicates (conjunction) |
| $\text{Enc}_{1/2}$ | Encryption algorithm of QOTP |
| $\text{supp } D$ | Support of a distribution $D$ |
| $X \leftarrow z$ | Program: Initialize $X$ with classical value $z$ |
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