Local Variables and Quantum Relational Hoare Logic

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Abstract
We add local variables to quantum relational Hoare logic (Unruh, POPL 2019). We derive reasoning rules for supporting local variables (including an improved “adversary rule”). We extended the qrhl-tool for computer-aided verification of qRHL to support local variables and our new reasoning rules.

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1 Introduction

In this work, we add local variables to the programming language underlying the quantum relational Hoare logic (qRHL) from [28], develop some reasoning rules related to this change, and added support for our extensions to the qrhl-tool [23] that enables computer-verified reasoning in qRHL.
qRHL is a logic that allows us to establish pre- and postconditions of pairs of quantum programs, thereby reasoning about the relationship between those two programs. (E.g., in the simplest case, establish that they do the same thing.) qRHL was designed with security proofs for quantum cryptography in mind, following the example of probabilistic relational Hoare logic (pRHL) \[4\] using in the EasyCrypt tool for classical security proofs.

To understand the motivation for and challenges in adding local variables, we first explain a bit of the background and motivation behind qRHL:

**Post-quantum security.** Quantum computers have long been known to be a potential threat to cryptographic protocols, in particular public key encryption. Shor’s algorithm \[20\] allows us to efficiently solve the integer factorization and discrete logarithm problems, thus breaking RSA and ElGamal and variants thereof. This breaks all commonly used public key encryption and signature schemes. Of course, as of today, there are no quantum computers that even come close to being able to execute Shor’s algorithm on reasonable problem sizes. Yet, there is constant progress towards larger and more powerful quantum computers (see, e.g., the recent breakthrough by Google \[1\]). In light of this, it is likely that quantum computers will be able to break today’s public key encryption and signature schemes (and possibly other kinds of cryptosystems) in the foreseeable future. Since the development, standardization, and industrial deployment of a cryptosystem can take many years, we need to develop and analyze future post-quantum secure protocols already today. One important step in this direction is the NIST post-quantum competition \[17\] that will select a few post-quantum public-key encryption and signature schemes for industrial standardization.

**Verifying classical cryptography using pRHL.** Cryptographic security proofs tend to be complex, and, due to their complexity, error prone. Small mistakes in a proof can be difficult to notice and may invalidate the whole proof. For example, the proof of the OAEP construction \[6\] went through a number of fixes \[21, 11, 12\] until it was finally formally proven in \[3\] after years of industrial use. The PRF/PRP switching lemma was a standard textbook example for many years before it was shown that the standard proof is flawed \[7\]. And more recently, an attack on the ISO standardized blockcipher mode OCB2 \[15\] was found \[14\], even though OCB2 was believed to be proven secure by \[19\].

While a rigorous and well-structured proof style (e.g., using sequences of games as advocated in \[7, 22\]) can reduce the potential for hidden errors and imprecisions, it is still very hard to write a proof that is 100% correct. And especially if a mistake in a proof happens in a step that seems very intuitive, it is quite likely that the mistake will also not be spotted by a reader.

To avoid this, formal (computer-aided) verification can be employed. Typically, a formal version of the sequences-of-games approach is used. In this approach, roughly speaking, the security of a cryptographic scheme is represented by the probability that a certain event happens in a certain program (encoding both the adversary and the scheme), and then this game is rewritten step-by-step, and on each step, it is shown that the old and new game stand in some relationship, until a final game is reached for which determining the probability of the event of interest is trivial to bound.

A number of frameworks/tools use this approach for verifying classical cryptography: CryptoVerif \[9\], CertiCrypt \[4\], EasyCrypt \[2\], FCF \[18\], CryptHOL \[5\], and Verypto \[8\]. CryptoVerif tries to automatically determine a sequence of games by using a set of fixed rewriting rules for games. This has the advantage of reducing user effort, but it also means that the framework is more limited in terms of what game transformations are possible. In contrast, the other frameworks require the user to explicitly specify the games that constitute the security proof (as is done in a pen-and-paper proof), and to additionally provide justification for the fact that two
consecutive games are indeed related as claimed. This justification will often be considerably
more detailed than in a pen-and-paper proof where the fact that two slightly different games are
equivalent will often be declared to be obvious.

One approach for proving the relationship of consecutive games is to give a proof in rela-
tional Hoare logic. Relational Hoare logic is a logic that allows us to express the relationship
between two programs by specifying a relational precondition and a relational postcondition.

A relational Hoare judgment of the form \( \{ A \} \texttt{c} \leadsto \texttt{d} \{ B \} \) intuitively means that if the variables
of the programs \( \texttt{c} \) and \( \texttt{d} \) are related as described by the precondition \( A \) before execution, and
we execute \( \texttt{c} \) and \( \texttt{d} \), then afterwards their variables will be related as described by \( B \).

A very simple example would be \( \{ x_1 \leq x_2 \} x \leftarrow x + 1 \leadsto x \leftarrow x + 1 \{ x_1 \leq x_2 \} \). This means that the variable \( x \) in the left program is smaller-equal than in right one, and both programs increase
\( x \), then \( x \) in the left program will still be smaller-equal than in the right one. As this example
shows, relational Hoare logic can express more complex relationships than simple equivalence
of two games. This makes the approach very powerful. To reason about cryptography, one needs
a variant of relational Hoare logic that supports probabilistic programs. Such a probabilistic
relational Hoare logic (pRHL) was developed for this purpose by Barthe, Grégoire, and Zanella
Béguelin [4]. Both CertiCrypt \([4]\) and its popular successor EasyCrypt use pRHL for proving
the relationship between cryptographic games.

### Verifying quantum cryptography using qRHL.

If we wish to follow the EasyCrypt approach to verify security proofs of quantum cryptographic schemes (be it actual quantum protocols, or merely post-quantum secure schemes that withstand quantum attacks), we cannot use pRHL but need a logic that allows us to reason about quantum programs, i.e., programs that can operate on quantum data. Such a logic was proposed in [28], namely quantum relational Hoare logic (qRHL). Inspired by qPRHL, this logic allows us to write judgments of the form \( \{ A \} \texttt{c} \leadsto \texttt{d} \{ B \} \) which mean, informally, that if the predicate \( A \) is satisfied by a pair of quantum memories \( M_1, M_2 \), and we execute the quantum programs \( \texttt{c}, \texttt{d} \) on those memories, then \( M_1, M_2 \)
satisfy \( B \) afterwards. Since the quantum memories do not contain classical values, the predicates
\( A, B \) are not predicates in the classical sense. We will make this more formal later, for now it is
sufficient to understand that those predicate can express conditions both about the classical and
quantum variables in the memories \( M_1, M_2 \), analogously to what is done in qRHL. (E.g., state
that they are equal.)

It was argued in [28] that qRHL is suitable for reasoning about cryptography in the quantum
setting. To demonstrate this, they developed a tool for computer-aided verification of proofs in
qRHL (called the qrhl-tool henceforth), and did several example verifications, such as a
verification of quantum teleportation and one of the post-quantum security of a very simple en-
cryption scheme. However, those were toy examples only, and did not shed light on the scalability
of the approach. To resolve this issue, [25] attempted formal computer-aided verification of a
non-trivial post-quantum cryptographic proof of a state-of-the-art construction of an encryption
scheme (a variant of the Fujisaki-Okamoto transform [10] analyzed in [13]). This verification was
performed using the qrhl-tool. The upshot of that case study was that, in principle, qRHL is
suitable for analyzing more complex cryptographic schemes, but several limitations were identi-
fied. One of them concerned the absence of support for local variables in qRHL. It turned out
that without support for local variables, formalizing the whole proof was at least very difficult.  

\(^1\)

\(^1\)Changes in one subproof tended to need a refactoring of most other subproofs (affecting the variables the other subproofs talked about). And this refactoring then required new changes in other subproofs. It was not clear whether this process would end eventually (without the additions to the logic introduced in the present work). On the other hand, seen separately, each subproof seemed easy to finish. (Which is why the toy examples from [28] did not uncover this difficulty.)
Unfortunately, the quantum equality is more peculiar than the classical one. It is not the same as \( q_r \) to \( q \) for quantum predicates) and does not imply \( q_l \) holds. Then, if \( x \) is not entangled with anything else but that is not implied by \( \{ \} \). Using the reasoning rules from [28], it is easy to show that \( \{ x_1 = x_2 \} c_1 \sim d_1 \{ x_1 = x_2 \} \) holds (we do not need to include \( y_1, y_2 \) in the precondition since \( y \) is overwritten in both programs), and then use the fact that \( (x_1, y_1) = (x_2, y_2) \implies x_1 = x_2 \) to conclude \( \{ x_1 = x_2 \} c_1 \sim d_1 \{ x_1 = x_2 \} \).

Now consider an analogous example involving quantum variables. Say \( q \) is a global quantum variable and \( r \) is pseudo-local. Let \( c_2 := d_2 := (r \# \{ 0 \}; \text{apply } U \text{ to } q_r) \). That is, \( r \) is initialized with a fixed state \( 0 \), and then the unitary \( U \) is jointly applied to \( q_r \). E.g., \( U \) could be a CNOT. Again, we want to show that \( c \) and \( d \) have the same observable behavior (given access only to \( q \)). This can be expressed in qRHL \( \{ q_1 \equiv_{\text{quant}} q_2 \} c_2 \sim d_2 \{ q_1 \equiv_{\text{quant}} q_2 \} \). Here \( \equiv_{\text{quant}} \) is the quantum equality introduced in [28], intuitively it expresses that two variables (or two tuples of variables) have the same value. We try to follow the same approach as in the classical case. Using the reasoning rules from [28], it is easy to show that \( \{ q_1 \equiv_{\text{quant}} q_2 \} c_2 \sim d_2 \{ q_1 \equiv_{\text{quant}} q_2 \} \) holds. Then, if \( q_1 r_1 \equiv_{\text{quant}} q_2 r_2 \) (meaning that \( q_r \) in memory \( M_1 \) jointly are equal in content to \( q_r \) in \( M_2 \)) we could conclude \( \{ q_1 \equiv_{\text{quant}} q_2 \} c_2 \sim d_2 \{ q_1 \equiv_{\text{quant}} q_2 \} \).

Unfortunately, the quantum equality is more peculiar than the classical one. \( q_1 r_1 \equiv_{\text{quant}} q_2 r_2 \) is not the same as \( q_1 \equiv_{\text{quant}} q_2 \cap r_1 \equiv_{\text{quant}} r_2 \) (intersection \( \cap \) is the analogue of conjunction \( \land \) for quantum predicates) and does not imply \( q_1 \equiv_{\text{quant}} q_2 \); this is because a quantum equality \( Q_1 \equiv_{\text{quant}} Q_2 \) not only implies that \( Q_1 \) and \( Q_2 \) have the same content but that also that \( Q_1 \) and \( Q_2 \) are not entangled with any other variables. Thus \( q_1 \equiv_{\text{quant}} q_2 \) would imply that \( q_1, q_2 \) are not entangled with anything else but that is not implied by \( q_1 r_1 \equiv_{\text{quant}} q_2 r_2 \) (and in fact does not even hold after running \( c, d \)).

For example, we could adopt a disciplined naming strategy that prefixes local variables with the names of the procedures they are used in, and to initialize all local variables before use. This would make sure that local variables are never accessed outside their intended scopes. (In the presence of recursion this would not work because recursive invocations would access the same variables at the same time. But the language of qRHL does not support recursion anyway.)

The converse holds: \( q_1 \equiv_{\text{quant}} q_2 \cap r_1 \equiv_{\text{quant}} r_2 \) implies \( q_1 r_1 \equiv_{\text{quant}} q_2 r_2 \).
This issue means that even though \( r \) has no relevance outside of \( c, d \), we have to carry information about \( r \) in our postconditions. The effect of this is that local variables “spread” through the invariants used in other parts of the proof as described previously, making it very hard to find consistent invariants and breaking the modularity of proofs.

Can this problem be resolved? Instead of \( c, d \) as defined above, we could define them as:

\[
\begin{align*}
    c_3 & := d_3 := (r \cdot |0\rangle; \text{apply $U$ to $qr$}; r \cdot |0\rangle) \\
\end{align*}
\]

(Or stated more generally, initialize any pseudo-local variable initialized before use, overwrite it at the end of its scope.) We have that

\[
\begin{align*}
    \{ q_1 \equiv \text{quant} q_2 \} r \cdot |0\rangle & \approx r \cdot \emptyset \cdot |0\rangle \{ q_1 \equiv \text{quant} q_2 \},
\end{align*}
\]

in other words, if we overwrite a quantum variables occurring in a quantum equality, that variable can be removed from the quantum equality. Then \( \{ q_1 \equiv \text{quant} q_2 \} c_3 \approx d_3 \{ r_1 \equiv \text{quant} r_2 \} \) follows immediate from \( \{ q_1 \equiv \text{quant} q_2 \} c_2 \approx d_2 \{ q_1 \equiv \text{quant} q_2 \} \) (from the previous paragraph) and \( (1) \) by the \text{Seq} rule from [28]. Judgment \( (1) \) cannot be proven using the rules from [28]. One of the results of the present work is a reasoning rule \text{JointQInitEq} from which \( (1) \) is an immediate consequence.

Proving rule \text{JointQInitEq} would probably be enough to have rudimentary support for pseudo-local variables (when following all the guidelines mentioned above about keeping names separate, and initializing and overwriting). However, it seems quite inconvenient to do so in a larger project. Furthermore, if local variables are not explicitly declared as such, they will show up in, e.g., the set of free variables of a program. For example, the \text{Adversary} rule from [28] allows us to reason about program fragments as a black box (i.e., without needing to look at their concrete implementation, more about that later) but it depends on the set of free variables of a program. Since the rule would not recognize that some of the free variables are pseudo-local, the pseudo-local variables would creep back into the pre-/post conditions produced by the adversary rule.

In light of those challenges, it seems that for making qRHL and \text{qrhl-tool} usable for larger projects, built-in support for local variables is a high priority. This is what we set out to do in the present work.

1.1 Our contribution

We add local variables to the programming language underlying qRHL and prove sound reasoning rules to work with local variables. Furthermore, we extend the \text{qrhl-tool} to support reasoning with local variables. In more detail:

- We extend the language by a construct for declaring local variables (Sections 3.1 and 3.2). If \( v \) is a variable (classical or quantum) and \( c \) is a program containing variable \( v \), then \textbf{local} \( v ; c \) is the program where \( v \) is local. That is, the value of \( v \) is saved before executing \( c \) and restored afterwards. (Of course, if \( v \) is quantum, storing does not mean making a copy.)

Based on this, we derive a number of laws for denotational equivalence of programs involving \textbf{local} (such as invariance under \( \alpha \)-renaming, commutativity of nested \textbf{local}-statements, moving of \textbf{local}-statements, adding/removing initializations of local variables, etc.). Closely related, we also introduce some laws concerning the initialization of variables (e.g., when an initialization has no effect because the variable is overwritten). The latter laws are not directly related to local variables but turn out to come up over and over while deriving our theory of local variables. (Section 5)
• Basic reasoning rules for qRHL statements: We provide sound reasoning rules for qRHL for remove local variable declarations and to rename variables. We need to remove local variable declarations to be able to break down a qRHL judgment into judgments about more elementary programs. E.g., we show judgments of the form \( \{A\}c_1; c_2 \sim d_1; d_2\{C\} \) by showing judgments \( \{A\}c_1 \sim d_1\{B\} \) and \( \{B\}c_1 \sim d_1\{C\} \) and then using the Seq rule. To do the same with a goal of the form \( \{A\}\text{local } v; c_1; c_2 \sim \text{local } v; d_1; d_2\{C\} \) we first need to remove the local-declaration, last but not least because we may want to refer to \( v \) in \( B \). Very roughly speaking, the rule says that to prove \( \{A\}\text{local } v; c_1; c_2 \sim \text{local } v; d_1; d_2\{C\} \) it is sufficient to prove \( \{A\}c_1; c_2 \sim d_1; d_2\{C\} \). (Interestingly, the converse does not hold.)

These rules are given in Section 6.

• As explained above, the rules of qRHL from [28] do not allow us to derive that

\[
\{q_1r_1 \equiv_{\text{quant}} q_2r_2\} r \frac{\psi}{\phi} [0] \sim r \frac{\psi}{\phi} [0]\{q_1 \equiv_{\text{quant}} q_2\}.
\]  

(2)

That is, we cannot get rid of variables that occur in a quantum equality, even if these variables are overwritten (which is essentially the same as erasing them). This is because the rules for quantum initialization in [28] (QInit1/2) are one-sided rules. That means they consider only an initialization (e.g., \( r \frac{\psi}{\phi} [0] \)) in the left or the right program but not both simultaneously. To derive (2), though, we need a rule that operates on both initializations simultaneously (intuitively, to make sure the entanglement between \( q \) and \( r \) is handled in a synchronized fashion on the left and right side.5) We prove such a rule (JointQInitEq).

As a consequence, we also prove a two-sided rule for removing local variables from qRHL judgments (JointRemoveLocal). Put simply, we show that to show a judgment such as \( \{q_1 \equiv_{\text{quant}} q_2\}\text{local } r; c \sim \text{local } r; d\{q_1 \equiv_{\text{quant}} q_2\} \), it is sufficient to show \( \{q_1 r_1 \equiv_{\text{quant}} q_2 r_2\} c \sim d\{q_1 r_1 \equiv_{\text{quant}} q_2 r_2\} \). The fact that \( r \) is included in the quantum equality (with the one-sided rules RemoveLocal1/2 it would not be) makes this judgment easier to prove. \( \{q_1 \equiv_{\text{quant}} q_2\} c \sim d\{q_1 \equiv_{\text{quant}} q_2\} \) would only be provable if \( c, d \) do not create any entanglement between \( q \) and \( r \).

The rule JointRemoveLocal in turn is crucial in the derivation of the Adversary rule (see below).

As a simple corollary of JointQInitEq, we also get a strengthening of the QRHLElimEq rule from [28] that allows us to relate qRHL judgments and (in)equalities of probabilities involving programs, we call the new rule QRHLElimEqNew.

(The three new rules are presented in Section 7.)

• Variable changing: The contributions described above already go a long way towards making it possible to work with local variables in qRHL proofs. However, we still cannot have modular proofs (in the sense that one part of the proof does not have to depend on which local variables occur in another part of the proof). Consider the following example: Say, we want to prove a qRHL judgment of the form

\[
\{q_1 \equiv_{\text{quant}} q_2\}\text{local } r; c_0; c \sim \text{local } r; c_0; d\{q_1 \equiv_{\text{quant}} q_2\}.
\]  

(3)

5The need for two-sided rules is not a new observation. Even in the classical pRHL [4], we have a two-sided rule for probabilistic sampling that “synchronizes” the random choices on the left and right side. This rule cannot be emulated using two applications of the one-sided rule for samplings. Similarly, qRHL [28] has a two-sided rule for measurements, synchronizing the measurement outcomes. However, for assignments, there is no two-sided rule in pRHL because there seems to be nothing that this rule could achieve that cannot be achieved with two consecutive applications of the one-sided rule. Thus it comes as a bit of a surprise that the quantum analogue to an assignment does need a two-sided rule.
Say the programs \( \mathbf{c}, \mathbf{d} \) are complex subroutines that we wish to handle in a different subproof. Since \( \sigma_0 \) might entangle \( \mathbf{q} \) and \( \mathbf{r} \), proving (3), we might end up having to prove the subgoal \( X := \{q_1 \mathbf{r}_1 \equiv_{\text{quant}} q_2 \mathbf{r}_2\} \mathbf{c} \sim \mathbf{d}\{q_1 \mathbf{r}_1 \equiv_{\text{quant}} q_2 \mathbf{r}_2\} \). This breaks the modularity of the overall proof because now our analysis of \( \mathbf{c}, \mathbf{d} \) needs to know which local variables (namely, \( \mathbf{r} \)) are used in a different part of the overall proof (namely, the analysis of local \( \mathbf{r}; \sigma_0; \mathbf{c} \) and local \( \mathbf{r}; \sigma_0; \mathbf{d} \)). Even worse, if \( \mathbf{c}, \mathbf{d} \) appear in different place where different local variables are used, we may have to prove several different variants of \( X \), all differing only in which local variable(s) are included in the quantum equality. What we want to do it to prove a single theorem about \( \mathbf{c}, \mathbf{d} \) not mentioning \( \mathbf{r} \), say \( X_0 := \{q_1 \equiv_{\text{quant}} q_2\} \mathbf{c} \sim \mathbf{d}\{q_1 \equiv_{\text{quant}} q_2\} \), and to be able to derive \( X \) from it whenever needed. Unfortunately, we do not know whether \( X_0 \) implies \( X \). However, we do prove a rule (EqVarChange, Section 8) that allows us to derive \( X \) from a theorem of the form \( X_1 := \{q_1\mathbf{q}_{\text{aux},1} \equiv_{\text{quant}} q_2\mathbf{q}_{\text{aux},2}\} \mathbf{c} \sim \mathbf{d}\{q_1\mathbf{q}_{\text{aux},1} \equiv_{\text{quant}} q_2\mathbf{q}_{\text{aux},2}\} \) where \( \mathbf{q}_{\text{aux}} \) is an auxiliary variable that is never used anywhere. (Basically, \( X_1 \) says that equality is preserved even in a larger context.) It might seem as if we can derive \( X \) from \( X_1 \) simply by renaming \( \mathbf{q}_{\text{aux}} \) into \( \mathbf{r} \) (using our rules for renaming variables), but that is not possible because \( \mathbf{q}_{\text{aux}} \) and \( \mathbf{r} \) might not have the same type. Requiring \( \mathbf{q}_{\text{aux}} \) and \( \mathbf{r} \) to have the same type would break the modularity of the proof again, and furthermore there might be more than just one local variable, while our theorem \( X_1 \) always uses the same single auxiliary variable \( \mathbf{q}_{\text{aux}} \).

The rule EqVarChange is also crucial in the derivation of the Adversary rule (see below).

- Adversary rule: Proofs in qRHL (and in other Hoare logics) are often performed by deriving a judgment about the whole program from judgements about the individual statements in that program. However, in a cryptographic context, this is not always possible. We often need to reason about unknown fragments of code, namely whenever we reason about the behavior of an adversary attacking the cryptographic scheme. (From a logical perspective, an adversary is simply a program whose precise code is not known.) Of course, if we do not know the code of a program \( \mathbf{c} \), we cannot say much about the pre- and postconditions. However, what we do now is, informally, that if the same program \( \mathbf{c} \) is used on the left and right side, and the variables of both instances of \( \mathbf{c} \) have the same value, then both instances will behave the same. That is, \( \{Q_1 \equiv_{\text{quant}} Q_2\} \mathbf{c} \sim \mathbf{c}\{Q_1 \equiv_{\text{quant}} Q_2\} \) if \( Q \) contains all free variables of \( \mathbf{c} \). Or, in a more general situation, we have \( \{Q_1 \equiv_{\text{quant}} Q_2\} \mathbf{C}[s] \sim \mathbf{C}[s']\{Q_1 \equiv_{\text{quant}} Q_2\} \) if \( \{Q_1 \equiv_{\text{quant}} Q_2\} \mathbf{s} \sim s'\{Q_1 \equiv_{\text{quant}} Q_2\} \). This would be used in a situation where the adversary is represented by an unknown context \( \mathbf{C} \), and that invokes some known procedure \( s \) (or \( s' \)), e.g., \( s, s' \) might be some real/fake encryption oracle. And since \( s, s' \) are known, we can manually prove \( \{Q_1 \equiv_{\text{quant}} Q_2\} \mathbf{s} \sim s'\{Q_1 \equiv_{\text{quant}} Q_2\} \).

Situations like the examples above (where unknown but identical code occurs on both sides) are handled by an adversary rule. In the classical setting, an adversary rule was already introduced in pRHL [4]. Also in qRHL [28], we have an adversary rule Adversary. However, the rule presented there has several drawbacks in our setting:

- In the presence of local variables, its proof does not apply any more. This is because the proof is by induction over the structure of the adversary/context \( \mathbf{C} \). But the introduction of local variables means that there is another case that would need to be covered in the induction (namely, \( \mathbf{C} = \text{local } \mathbf{v}; \mathbf{C}' \)). Dealing with local variables makes the rule and the induction more complex because we need to make sure the
rule correctly handles cases where a variable of $s$ is local in $C$ (and thus also local in $C[s]$).

- The adversary rule from [28] requires the quantum equality $Q_1 \equiv_{\text{quant}} Q_2$ to be the same in the precondition and postcondition of $\{Q_1 \equiv_{\text{quant}} Q_2\}C[s] \sim C[s']\{Q_1 \equiv_{\text{quant}} Q_2\}$, and in the subgoal $\{Q_1 \equiv_{\text{quant}} Q_2\}s \sim s'\{Q_1 \equiv_{\text{quant}} Q_2\}$. However, this is unnecessarily restrictive. E.g., if $C$ has local variables, those might occur in the subgoal but not in the pre-/postcondition. Or if $C$ initializes certain variables before use, then they can be omitted from the precondition but not from the postcondition.

We present a new rule $\text{Adversary}$ that solves the these problems. Our rule is considerably more fine-grained than the original rule in that allows us to include different variable sets in pre-/postconditions and subgoals, and that it takes into account various kinds of overwritten, local, and read-only variables.

The proof of the adversary rule relies in particular on the rules $\text{JointRemoveLocal}$ and $\text{EqVarChange}$ to maintain the induction hypothesis even below \textbf{local}-statements.

- New/rewritten tactics: In theory, all we need in order to do proofs in qRHL are the rules introduced above and in [28]. In practice, however, manually doing proofs is too cumbersome and error-prone. Instead, [28] introduced the qrhl-tool that allows to develop and check qRHL proofs interactively on the computer. To use the new rules we introduce in this work, we implemented a number of new tactics: $\text{rename}$ for renaming variables (page 32), $\text{local remove}$ for removing local variables (page 32), $\text{local up}$ for moving local variables to the top of a program (page 30), $\text{conseq qrhl}$ for changing variables in a quantum equality using rule $\text{EqVarChange}$ (page 40), $\text{equal}$ implementing the adversary rule (page 45, this tactic existed before but we completely rewrote it based on our new $\text{Adversary}$ rule). We also strengthened the tactic $\text{byqrhl}$ that introduces qRHL subgoals in the first place, using the new rule $\text{QrhlElimEqNew}$ (page 39).

In this paper, we only briefly sketch what those tactics do. For details, see the user manual of qrhl-tool, version 0.5.

Some of the results in this paper are shown in Isabelle/HOL [16]. This concerns especially results which involve inductions with many side conditions (such proofs are particular error prone when done by hand). Those proofs are not proofs from first principles and/or based on the semantics of the language. For this, we would need developments in operator theory that are not yet available in Isabelle/HOL. Instead, we axiomatize the language and semantics, and base all proofs on an explicit list of axioms in the file Assumptions.thy. Those are either facts shown in [28], in manual proofs in this paper, or that are elementary. This approach gives us a good trade-off – avoiding errors in proofs that involve many technical conditions, but at the same time avoiding the extreme effort of formalizing everything in Isabelle/HOL. The Isabelle/HOL formalization consists of 4315 lines of code. The Isabelle theory files for Isabelle/HOL (version Isabelle-2020) are available here [24].

2 Preliminaries

We introduce the notation used in this work. See also the symbol index at the end of this paper.

\footnotetext{6}We have not implemented the two-sided removal via rule $\text{JointRemoveLocal}$, but that rule is implicitly present in the adversary rule.
Variables. A program variable \( x \) (short: variable) is an identifier annotated with a set \( \text{Type}_x \neq \emptyset \), and with a flag that determined whether the variable is quantum or classical. (In our semantics, for classical variables \( x \) the type \( \text{Type}_x \) will be the set of all values a classical variable can store. Quantum variables \( q \) can store superpositions of values in \( \text{Type}_q \).)

We will usually denote classical variables with \( x, y \) and quantum variables with \( q \). Given a set \( V \) of variables, we write \( V^\text{cl} \) for the classical variables in \( V \) and \( V^\text{qu} \) for the quantum variables in \( V \).

Given a set \( V \) of variables, we write \( \text{Type}^\text{set}_V \) for the set of all functions \( f \) on \( V \) with \( f(x) \in \text{Type}_x \) for all \( x \in V \). (I.e., the dependent product \( \text{Type}^\text{set}_V = \prod_{x \in V} \text{Type}_x \).)

Intuitively, \( \text{Type}^\text{set}_V \) is the set of all memories that assign a classical value to each variable in \( V \).

Given a list \( V = (x_1, \ldots, x_n) \) of variables, \( \text{Type}^\text{list}_V := \text{Type}_{x_1} \times \cdots \times \text{Type}_{x_n} \). Note that if \( V \) is a list with distinct elements, and \( V' \) is the set of those elements, then \( \text{Type}^\text{set}_V \) and \( \text{Type}^\text{set}_{V'} \) are not still the same set, but their elements can be identified canonically. Roughly speaking, for a list \( V \), the components of \( m \in \text{Type}^\text{list}_V \) are indexed by natural numbers (and are therefore independent of the names of the variables in \( V \)), while for a set \( V \), the components of \( m \in \text{Type}^\text{set}_V \) are indexed by variable names.

Given disjoint sets \( V, W \) of variables, we write \( VW \) for the union (instead of \( V \cup W \)).

Expressions (i.e., formulas that depend on some classical variables \( X \)) \( e \) are always assumed to have finitely many values to classical variables, we write \( \llbracket e \rrbracket_m \) for \( e \) evaluated on \( m \). We write \( \text{Type}^\text{esp}_e \) for the type of \( e \), i.e., the set of all possible values of \( e \).

An important concept in the formalization of qRHL are indexed variables, i.e., for every variable \( v \) there are two distinct variables \( v_1, v_2 \). In \([28]\), there are explicit operations \( \text{id}_{v_1}, \text{id}_{v_2} \) that replace all variables by indexed variables in a list/set of variables or in an expression. We use a more compact notation and simply index the list/set/expression. I.e., if \( V \) is a list/set of variables, \( v_1 \) refers to \( V \) with every variable \( v \) replaced by \( v_1 \). And \( e_1 \) is the expression \( e \) with every \( v \) substituted by \( v_1 \). (In \([28]\) this would be \( \text{id}_{v_1} V, \text{id}_{v_1} e \).) Similarly, given a quantum predicate \( A \) (defined later in Section \( 4 \)), \( A_1 \) and \( A_2 \) are quantum predicates with all variables \( v \) replaced by \( v_1, v_2 \), respectively.

Let \( V^\text{all} \) be the set of all variables (not including indexed variables).

We make some assumptions about the set \( V^\text{all} \) of all variables. (Those assumptions were not made in \([28]\).) Namely, for any variable \( v \in V^\text{all} \), there exist infinitely many \( w \in V^\text{all} \) that are compatible with \( v \). (I.e. \( v \) and \( w \) are either both quantum or both classical, and \( \text{Type}_v = \text{Type}_w \).) Furthermore, we assume that there is at least one quantum variable \( q \) with \( \| \text{Type}_q \| = \aleph_0 \). (Note, we only assume that those variables exist, not that they are actually used in any given program.)

Linear algebra. We write \( \ell^2(X) \) for the Hilbert space with basis \( \{ |x \rangle \}_{x \in X} \). For a set of quantum variables \( Q \), we write \( \ell^2(Q) \) for \( \ell^2(\text{Type}^\text{set}_Q) \), i.e., the space of all states those quantum variables can take.

Given a vector \( \psi \), we define \( \text{proj}(\psi) := \psi \psi^\ast \). Given a bounded operator \( A \), we define \( \text{toE}(A)(\rho) := A \rho A^\ast \).

A cq-operator is a positive trace-class operator over a set \( V \) of variables of the form \( \sum_m \text{proj}(|m\rangle \langle m|) \otimes \rho_m \) for positive trace-class operators \( \rho_m \) over \( V^\text{qu} \). I.e., a cq-operator is basically a density operator that is classical in the classical variables of \( V^\text{qu} \) (except that we do not require that the trace is \( = 1 \) or \( \leq 1 \)).
A superoperator is a completely positive map $E$ that maps trace-class operators to trace-class operators such that $\exists B \forall \rho. \tr E(\rho) \leq B \tr \rho$.

Subspaces always mean topologically closed subspaces. For a subspace $A$, let $A^\perp$ be the orthogonal complement.

CPTPM means completely positive trace preserving map, while CPTRM means completely positive trace reducing map (i.e., for positive input, the trace of the output is smaller-equal the trace of the input).

For disjoint $R,S \subseteq Q$, let $\text{SWAP}_{R \leftrightarrow S}$ be the unitary operator on $\ell^2[Q]$ that swap the subsystems $R$ and $S$.

Let $\text{supp} A$ denote the support of an operator $A$. (Formally, the image of the smallest projector $P$ such that $PAP = A$.)

For $R \subseteq Q$ and a trace-class operator over $\ell^2[Q]$, let $\tr_n \rho$ denote the partial trace of $\rho$ that traces out $R$. That is, $\tr_n \rho$ is a trace-class operator over $\ell^2[Q \setminus R]$. Sometimes, we annotate $\tr_n$ with the set of remaining variables, i.e., $\tr_n^S$ if $S = Q \setminus R$. If $Q$ consists of indexed variables, we write $\tr 1$ short for $\tr Q^1$ where $Q^1 \subseteq Q$ consists only of the 1-indexed variables. Analogously $\tr 2$.

For a bounded operator $A$, let $A^*$ denote the adjoint of $A$. (i.e., the conjugate transpose, often also written $A^\dagger$.)

[28] also explicitly writes the canonical isomorphisms $U_{\text{vars},Q}$ between different isomorphic spaces related to the variables $Q$. (Namely $\ell^2[Q]$ and $\ell^2(\text{Type}_{Q})$.) We omit those isomorphisms in our notation. In particular, if $\psi \in \ell^2[Q]$, and $A \subseteq \ell^2[Q_1]$, then the expression $\psi \in A$ is well-typed and understood to mean $U^*_{\text{vars},Q_1} U_{\text{vars},Q} \psi \in \ell^2[Q_2]$.

Distributions. Probability distributions are always discrete distributions (i.e., the $\sigma$-algebra of all measurable spaces is the powerset). A subprobability distribution is like a probability distribution except that the total probability may be $\leq 1$. For a (sub)probability distribution $\mu$ over $X$, let $\text{supp} \mu \subseteq X$ be the support of $X$, i.e., the set of values with nonzero probability. For a (sub)probability distribution $\mu$ over $X \times Y$, let $\text{marginal}_1(\mu)$, $\text{marginal}_2(\mu)$ be the first/second marginal (i.e., (sub)probability distributions over $X$ and $Y$, respectively).

3 Language of programs

3.1 Syntax

We recap the syntax from [28], and add one more statement to it, for declaring local variables. Everything else is unchanged.

We will typically denote programs with $c$ or $d$.

Quantum variables are written $q,r$, classical variables $x,y$, an arbitrary variables $v,w$. Sets/lists of variables are $Q,R,S$ or $X,Y$ or $V,W$.
\[ \begin{align*}
c, d & := \text{skip} & \text{(no operation)} \\
X & \leftarrow e & \text{(classical assignment)} \\
X & \leftarrow^\$ e & \text{(classical sampling)} \\
\text{if } e \text{ then } c \text{ else } d & \text{(conditional)} \\
\text{while } e \text{ do } c & \text{(loop)} \\
c; d & \text{(sequential composition)} \\
Q & \leftarrow^\$ e & \text{(initialization of quantum registers)} \\
\text{apply } e \text{ to } Q & \text{(quantum application)} \\
X & \leftarrow \text{measure } Q \text{ with } e & \text{(measurement)} \\
\text{local } v; c & \text{(local variables)}
\end{align*} \]

In the sampling statement, \( e \) evaluates to a distribution. In the initialization of quantum registers, \( e \) evaluates to a pure quantum state, \( q_1 \ldots q_n \) are jointly initialized to that state. In the quantum application, \( e \) evaluates to an isometry that is applied to \( q_1 \ldots q_n \). In the measurement, \( e \) evaluates to a projective measurement, the outcome is stored in \( x \). (Recall that an expression \( e \) can be an arbitrarily complex mathematical formula in the classical variables. So, e.g., an expression that describes an isometry could be something as simple as just \( H \) (here \( H \) denotes the Hadamard transform), or something more complex such as, e.g., \( H^x \), meaning \( H \) is applied if \( x = 1 \).)

The new statement in this syntax (relative to [28]) is \textbf{local} \( v; c \). Intuitively, this means that \( v \) is a local variable in \( c \). More specifically (but still informally), at the beginning of \textbf{local} \( v; c \), the current state of \( v \) is stored (think of a stack), \( v \) is initialized with a default value, \( c \) is executed, and the original state of \( v \) is restored.

Note that \textbf{local} \( v; c \) binds weaker than \( c; d \). I.e., \textbf{local} \( v; c \) means \textbf{local} \( v; (c; d) \), not \( (\text{local} v; d); c \).

A program is \textit{well-typed} according to the following rules:

- \( X \leftarrow e \) is well-typed iff \( \text{Type}^\text{exp}_e \subseteq \text{Type}^\text{list}_X \).
- \( X \leftarrow^\$ e \) is well-typed iff \( \text{Type}^\text{exp}_e \subseteq \text{Type}^\text{list}_X \).
- \text{if } e \text{ then } c \text{ else } d \) is well-typed iff \( \text{Type}^\text{exp}_e \subseteq \{\text{true}, \text{false}\} \) and \( c, d \) are well-typed.
- \text{while } e \text{ do } c \) is well-typed iff \( \text{Type}^\text{exp}_e \subseteq \{\text{true}, \text{false}\} \) and \( c \) is well-typed.
- \( c; d \) is well-typed iff \( c \) and \( d \) are well-typed.
- \( Q \leftarrow^\$ e \) is well-typed iff \( \text{Type}^\text{exp}_e \subseteq \ell^2(\text{Type}^\text{list}_Q) \), and \( \|\psi\| = 1 \) for all \( \psi \in \text{Type}^\text{exp}_e \).
- \text{apply } e \text{ to } Q \) is well-typed iff \( \text{Type}^\text{exp}_e \subseteq \ell^2(\text{Type}^\text{list}_Q) \).
- \( X \leftarrow \text{measure } Q \text{ with } e \) is well-typed iff \( \text{Type}^\text{exp}_e \) is a subset of the set of all projective measurements on \( \text{Type}^\text{list}_Q \) with outcomes in \( \text{Type}^\text{list}_X \).
- \text{local} \( v; c \) is well-typed iff \( c \) is well-typed.

In this paper, we will only consider well-typed programs. That is, “program” implicitly means “well-typed program,” and all derivation rules hold under the implicit assumption that the programs in premises and conclusions are well-typed.

We also consider contexts in this work. A context follows the above grammar, with the additional symbol \( \square_i \) where \( i \) is a natural number. A context \( C \) can be instantiated as \( C[c_1, \ldots, c_n] \). This means that every occurrence of \( \square_i \) is replaced by \( c_i \). (With no special treatment of local-variables. E.g., if \( C = \text{local} \ v; \square_1 \), then \( C[c] = \text{local} \ v; c \) even if \( c \) contains \( v \).)
3.2 Semantics of programs

First, we recap the semantics of the language as defined in [28].

Given a program $c$ (with $\text{fe}(c) \subseteq V$), we define its semantics $\llbracket c \rrbracket$ as a cq-superoperator that maps trace-class cq-operators over $V$ onto trace-class cq-operators over $V$. In the following, let $\rho$ be a trace-class cq-operator over $V$, $m \in \text{Type}_{V}^{cl}$ (i.e., an assignment of values to classical variables), and $\rho_{m}$ a positive trace-class operator over $V^{\text{cu}}$. Note that specifying $\llbracket c \rrbracket$ on operators of the form $\text{proj}(m_{\lambda}) \otimes \rho_{m}$ specifies $\llbracket c \rrbracket$ on all $\rho$, since $\rho$ can be written as an infinite sum of $\text{proj}(m_{\lambda}) \otimes \rho_{m}$.

Then the semantics of the language were defined as follows in [28]:

\[
\llbracket \text{skip} \rrbracket(\rho) := \rho
\]
\[
[x \leftarrow e](\text{proj}(m_{\lambda}) \otimes \rho_{m}) := \text{proj}(m(x := [e]_{m})_{\lambda}) \otimes \rho_{m}
\]
\[
[x \leftarrow e]\text{proj}(m_{\lambda}) \otimes \rho_{m}) := \sum_{z \in \text{Type}_{x}} \llbracket \rho \rrbracket(z) \cdot \text{proj}(m(x := z)_{\lambda}) \otimes \rho_{m}
\]
\[
[\text{if } e \text{ then } c \text{ else } d](\rho) := \llbracket c \rrbracket(\llbracket e \rrbracket(\rho)) + \llbracket d \rrbracket(\neg \llbracket e \rrbracket(\rho))
\]
\[
[\text{while } e \text{ do } c](\rho) := \sum_{i=0}^{\infty} \llbracket e \rrbracket \oplus \llbracket c \rrbracket(\rho)
\]
\[
[\text{local } v; c] := [e_1; e_2] := [e_2] \circ [e_1]
\]
\[
\llbracket Q \text{ to } Q \rrbracket(\text{proj}(m_{\lambda}) \otimes \rho_{m}) := \text{proj}(m_{\lambda}) \otimes \text{tr}_{c} \rho_{m} \otimes \text{proj}(\llbracket e \rrbracket_{m})
\]
\[
[x \leftarrow \text{measure } Q \text{ with } e](\text{proj}(m_{\lambda}) \otimes \rho_{m}) := \sum_{z \in \text{Type}_{x}} \text{proj}(m(x := z)_{\lambda}) \otimes (\llbracket e \rrbracket_{m}(z)) \rho_{m}(\llbracket e \rrbracket_{m}(z))
\]

Here $\llbracket e \rrbracket(\rho)$ is the cq-density operator $\rho$ restricted to the parts where the expression $e$ holds. Formally, $\llbracket e \rrbracket(\rho)$ is the cq-superoperator on $V$ such that

\[
\llbracket e \rrbracket(\text{proj}(m_{\lambda}) \otimes \rho_{m}) := \begin{cases}
\text{proj}(m_{\lambda}) \otimes \rho_{m} & (\llbracket e \rrbracket_{m} = \text{true}) \\
0 & \text{(otherwise)}
\end{cases}
\]

**Local variables.** It remains to give semantics to statements of the form $\text{local } v; c$ as these did not occur in [28].

For every variable $v$, we assume a fixed element $\bullet_{v} \in \text{Type}_{v}$ (the default value). Let $\rho_{v} := \text{proj}(\bullet_{v})$.

In the following definition, for any variable $v$, let $v'$ denote another (so far unused) variable of the same type, with the same default value, and $v'$ is quantum/classical iff $v$ is. Then, for any superoperator $E$,

\[
\text{Local}_{v}[E](\rho) := \text{tr}_{v} \text{ toE}(\text{SWAP}_{v'v}) \circ (E \otimes \text{id}_{v'}) \circ \text{toE}(\text{SWAP}_{v'v}) \rho_{v} (\rho \otimes \rho_{v})
\]

\[
\text{Local}_{v}[E]
\]
Or equivalently:

$$\text{Local}_v[c] := F \otimes \text{id}_v$$

where

$$F(\rho) := \text{tr}_v \mathcal{E}(\rho \otimes \rho_v^*)$$

for all trace-class operators $\rho$ over $V^{\text{all}} \setminus v$.

And then we can define $[\text{local } v; c] = \text{Local}_v[[c]]$.

We write $c \stackrel{d}{=} d$ to denote denotational equivalence, i.e., $[c] = [d]$.

Given the semantics, we can define the probability that a certain condition holds after execution of a program, using the following definition from [28]:

**Definition 1**

Fix a program $c$, an expression $e$ with $\text{Type}^e = \{\text{true, false}\}$, and some trace-class cq-operator $\rho$ over $V^{\text{all}}$. Then $\Pr[e : c(\rho)] := \sum_m \text{s.t. } [e]_m = \text{true} \text{ tr } \rho_m$ where $[c](\rho) =: \sum_m \text{proj}(|m\rangle) \otimes \rho_m$ for trace-class operators $\rho_m$ over $(V^{\text{all}})^{\text{qu}}$.

### 3.3 Variable sets

Given a context (or program) $C$, we define a number of sets of variables such as the set of free variables. These will be used throughout the paper in various rules, most crucially in the **Adversary** rule. Those sets are:

- $\text{fv}(C)$: All free variables in $C$.
- $\text{inner}(C)$: All variables $v$ such that $C$ contains a hole under a $\text{local } v$. (Those are the variables that will be shadowed if we substitute a program into a hole of $C$.)
- $\text{covered}(C)$: All variables $v$ such every hole is under a $\text{local } v$. (Those are the variables which, if a program that is substituted into a hole of $C$ contains them, will still not be visible outside $C$.)
- $\text{overwr}(C)$: All variables that are overwritten in $C$. I.e., written before they are used for the first time. (Thus the content of those variables before execution of $C$ does not matter.)
- $\text{written}(C)$: All variables that are written (i.e., classical variables on the lhs of an assignment or sampling, and all free quantum variables).

The precise recursive definitions follow. All those variables sets are also formally defined in Isabelle/HOL in the theory `Basic_Definitions`. 

13
\[ \begin{align*}
fv(\square_i) & := \emptyset \\
fv(X \leftarrow e) & := X \cup fv(e) \\
fv(X \leftarrow e) & := X \cup fv(e) \\
fv(\text{local } v; C) & := fv(C) \setminus \{v\} \\
fv(\text{apply } Q \text{ to } e) & := Q \cup fv(e) \\
fv(X \leftarrow \text{measure } Q \text{ with } e) & := Q \cup X \cup fv(e) \\
fv(C; C') & := fv(C) \cup fv(C') \\
fv(\text{if } e \text{ then } C \text{ else } C') & := fv(e) \cup fv(C) \cup fv(C') \\
fv(\text{while } e \text{ do } C) & := fv(e) \cup fv(C) \\
fv(\text{skip}) & := \emptyset \\
\end{align*} \]

\[ \begin{align*}
inner(\square_i) & := \emptyset \\
inner(C) & := \emptyset \quad \text{(if } C \text{ is a program)} \\
inner(\text{local } v; C) & := inner(C) \cup \{v\} \quad \text{(if } C \text{ is not a program)} \\
inner(\text{if } e \text{ then } C \text{ else } C') & := inner(C) \cup inner(C') \\
inner(\text{while } e \text{ do } C) & := inner(C) \\
inner(C; C') & := inner(C) \cup inner(C') \\
\end{align*} \]

\[ \begin{align*}
\text{covered}(\square_i) & := \emptyset \\
\text{covered}(C; C') & := \text{covered}(C) \cap \text{covered}(C') \\
\text{covered}(\text{if } e \text{ then } C \text{ else } C') & := \text{covered}(C) \cap \text{covered}(C') \\
\text{covered}(\text{while } e \text{ do } C) & := \text{covered}(C) \\
\text{covered}(\text{local } v; C) & := \text{covered}(C) \cup \{v\} \\
\text{covered}(C) & := \mathcal{V}^{\text{all}} \quad \text{(if } C \text{ is a program)} \\
\end{align*} \]
overwr(□) := ∅
overwr(X ← e) := X \ fv(e)
overwr(X ← e) := X \ fv(e)
overwr(Q ← e) := Q
overwr(apply Q to e) := ∅
overwr(X ← measure Q with e) := X \ fv(e)
overwr(if e then C else C′) := (overwr(C) \ \overwr(C′)) \ \fv(e)
overwr(while e do C) := ∅
overwr(local v; C) := overwr(C) \ \{v\}
overwr(C; C′) := overwr(C) \ \bigcup \ \bigcup :: \overwr(C′) \ \cap \ \covered(C) \bigcup \ \covered(C)
overwr(skip) := ∅

written(□) := ∅
written(X ← e) := X
written(X ← e) := X
written(local v; C) := written(C) \ \{v\}
written(Q ← e) := Q
written(apply Q to e) := Q
written(X ← measure Q with e) := X \ Q
written(if e then C else C′) := written(C) \ \bigcup \ \bigcup :: written(C′)
written(while e do C) := written(C)
written(skip) := ∅
written(C; C′) := written(C) \ \bigcup \ \bigcup :: written(C′)

3.4 Substitutions

A variable substitution σ is a function from variables to variables such that v and σ(v) are compatible, i.e. v and σ(v) are either both quantum or both classical, and Type v = Type σ(v).

Given a variable substitution σ and a program/context c, cσ denotes the result of replacing every non-local variable v in c by σ(v). In contrast, cσ replaces every variable v by σ(v). (E.g., if σ(v) = w, then (v ← 1; local v; v ← 1)v = (w ← 1; local w; w ← 1)v but (v ← 1; local v; v ← 1)v = (w ← 1; local w; w ← 1).)

Renaming variables using a substitution may lead to conflicts with existing local variables. The following inductive predicate noconflict(·, ·) ensures that this does not happen.

\[
\begin{array}{llll}
\text{noconflict}(\sigma, c) & \text{noconflict}(\sigma, d) & \text{noconflict}(\sigma, c) & \text{noconflict}(\sigma, d) \\
\text{noconflict}(\sigma, \text{if } e \text{ then } c \text{ else } d) & \text{noconflict}(\sigma, c) & \text{noconflict}(\sigma, c; d) & \\
\text{noconflict}(\sigma, \text{while } e \text{ do } c) & \text{noconflict}(\sigma, X ← e) & \text{noconflict}(\sigma, X ← e) \end{array}
\]
\[ \begin{array}{ll}
\text{noconflict}(\sigma, Q \triangleq \epsilon) & \text{noconflict}(\sigma, \text{apply } Q \text{ to } \epsilon) \\
\text{noconflict}(\sigma, X \leftarrow \text{measure } Q \text{ with } \epsilon) & \text{noconflict}(\sigma, \text{skip}) \\
\text{noconflict}(\sigma, v := v), c & v \notin \sigma(fv(c) \cap \text{dom } \sigma) \\
\text{noconflict}(\sigma, \text{local } v; c) & \\
\end{array} \]

Here \( \text{dom } \sigma := \{ v : \sigma(v) \neq v \} \).

In the Isabelle theories, the substitution \( c\sigma \) is formalized as `Basic_Definitions.subst_vars`, the substitution \( c'\sigma \) as `Basic_Definitions.full_subst_vars`, and `noconflict(\sigma, c)` as `Basic_Definitions.no_conflict`.

## 4 Quantum relational Hoare logic

In this section, we recap the relevant definitions of qRHL from [28]. We slightly rewrite the definitions to make them compatible with our notational conventions.

A quantum predicate \( A \) over variables \( V \) is, formally, an expression with variables in \( V^d \) that evaluates to a subspace of \( \ell^2[V^\omega] \). Intuitively, a memory (with classical and quantum variables) satisfies \( A \) iff the quantum part of the memory lies in \( A \), when we instantiate the variables of \( A \) with the classical variables of the memory. For pre-/postconditions in qRHL we use quantum predicates over \( V^{\omega_1}V^{\omega_2} \). If such a memory is represented as a density operator \( \rho \), we say “\( \rho \) satisfies \( A \)” if this holds. A formal definition is given in [27, Definition 14]. Following [26], we only consider quantum predicates that depend on a finite number of variables, then \( fv(A) \), the set of free classical and quantum variables of \( A \), is well-defined (see [26] for details).

For detailed discussion of quantum predicates, we refer to [28]. Here we only recall the most important constructions of quantum predicates:

- Intersection \( \cap \) of quantum predicates is the analogue of conjunction \( \land \) of classical predicates. Sum \( + \) of spaces is the analogue to disjunction \( \lor \). \( A \subseteq B \) intuitively means that \( A \) implies \( B \). (Note that \( A \subseteq B \) is not a quantum predicate, just a mathematical proposition.)

- Given a classical predicate \( P \) (i.e., a Boolean formula depending only on classical variables), we can construct a quantum predicate \( \mathcal{C}[P] \). \( \mathcal{C}[P] \) is defined to be the whole space if \( P \) is true, and to be the 0-space if \( P \) is false. This way, a state \( \rho \) satisfies \( \mathcal{C}[P] \) if the classical variables of \( \rho \) satisfy \( P \).

- Furthermore, [28] introduces the notation \( S \cdot Q \) to denote the predicate that encodes the fact that \( Q \) has a value in \( S \) (\( S \) must be a subspace of \( \ell^2[Q] \)). \( A \cdot Q \) can also be used for operators \( A \) to emphasize that \( A \) operates on \( \ell^2[Q] \). And \( A \cdot \psi \) is an operation specific to the QINIT rule, we omit the definition here. See [28] for details. We write \( Q =_{q} \psi \) to mean \( \text{span} \{ \psi \} \subseteq Q \), i.e., the quantum predicate that says that \( Q \) is in state \( \psi \).

**Quantum equality.** One very important quantum predicate (that can be combined with other predicates, e.g., using \( \cap \) and \( + \)) is the quantum equality. If \( Q, R \) are disjoint lists of quantum variables, then \( Q \equiv_{\text{quant}} R \) intuitively means that \( Q \) and \( R \) have the same content. Formally, \( Q \equiv_{\text{quant}} R \) is the space of all vectors that are invariant under \( \text{SWAP}_{Q \leftrightarrow R} \), i.e., the unitary that swaps registers \( Q \) and \( R \) in a quantum state. Intuitively, this makes sense: two variables have the same content if exchanging them does not change the overall state of the system. Though not formally required, \( Q \) will always contain 1-indexed variables, and \( R \) will contain 2-indexed...
variables (or vice versa). That way, we can use a quantum equality in a pre-/postcondition in a qRHL judgment (to state that the quantum variables of two programs are “equal”). For example \( q_1 r_1 \equiv_{\text{quant}} q_2 r_2 \) means that \( q, r \) jointly have the same content in the left and right memory.

There is an extended form of the quantum equality, \( UQ \equiv_{\text{quant}} VR \) where \( U, V \) are unitaries (or more generally, bounded operators, but then the intuitive meaning of the quantum equality gets lost). Intuitively, \( UQ \equiv_{\text{quant}} VR \) means that the variables in \( Q \), when we apply \( U \) have the same content as the variables in \( R \), when we apply \( V \). For example \( \text{id} q_1 r_1 \equiv_{\text{quant}} \text{CNOT} q_2 r_2 \) means that \( qr \) on the left is what you get from \( qr \) on the right after a CNOT. We refer to [27, Definition 27] for the formal definition.

An important fact about the quantum equality is that \( QQ' \equiv_{\text{quant}} RR' \) is not equivalent to \( Q \equiv_{\text{quant}} R \cap Q' \equiv_{\text{quant}} R' \), we merely have \( Q \equiv_{\text{quant}} R \cap Q' \equiv_{\text{quant}} R' \subseteq Q \equiv_{\text{quant}} R \cap Q' \equiv_{\text{quant}} R' \). This makes it harder to work with the quantum equality than the classical equality. For useful laws about the quantum equality, see [28].

**qRHL judgments.** In qRHL, we want to express that given a precondition \( A \) (on a pair of memories, i.e., a quantum predicate on \( V_1^{\text{all}}V_2^{\text{all}} \)), when executing the programs \( c, d \), the postcondition \( B \) holds, in short \( \{ A \} c \sim d \{ B \} \). However, this simplified description is somewhat misleading. We do not simply execute \( c, d \) in parallel on an initial state consisting of two memories satisfying \( A \) and look whether the final state satisfies \( B \). The reason is that if we did that, even simple fact such as \( \{ \text{CNOT} \} x \sim \mathcal{U} \mathcal{U} x \sim \mathcal{U} \{ \text{CNOT} \} x = x \) would not hold (where \( \mathcal{U} \) is the uniform distribution on \( \{0, 1\} \)).

In Figures 1, 2, 3, we state the rules from [28] that still hold, using our more compact notation (in particular, we omit the types of the various variables and expressions, and we omit explicitly stated canonical isomorphisms between various spaces). We omit the rather lengthy rules \text{Trans} and \text{JointMeasure} that also still hold for brevity, see [28].

---

\[ \text{Definition 2: Quantum relational Hoare judgments} \]

Let \( c, d \) be programs. Let \( A, B \) be quantum predicates over \( V_1^{\text{all}}V_2^{\text{all}} \).

Then \( \{ A \} c \sim d \{ B \} \) holds iff for all separable \( \rho \) that satisfy \( A \), we have that there exists a separable \( \rho' \) that satisfies \( B \) such that \( \text{tr}_2 \rho' = [c](\text{tr}_2 \rho) \) and \( \text{tr}_1 \rho' = [d](\text{tr}_1 \rho) \).

---

4.1 Rules of qRHL

Most rules proven in [28] still hold (with the same proof) in our setting (even though the definition of the language has changed). This is because the proof of these rules are “semantic”. By this, we mean that, if a program \( c \) is all-quantified in a rule, the proof makes no assumptions about the code of \( c \), and instead only refers to its semantics \( [c] \). Thus the exactly same proofs work when more statements are added to the language. (But not if the definition of existing statements is changed.) A notable exception is the \textbf{Adversary} rule from [28] which does not apply any more since it is proven by induction of the structure of programs.

In Figures 1, 2, and 3, we state the rules from [28] that still hold, using our more compact notation (in particular, we omit the types of the various variables and expressions, and we omit explicitly stated canonical isomorphisms between various spaces). We omit the rather lengthy rules \text{Trans} and \text{JointMeasure} that also still hold for brevity, see [28].

---

\[ ^7 \text{We also use Lemma 1 to justify replacing assumptions of the form “c is V-local” by “fv(c) \subseteq V”} \].
\[ \begin{array}{ll}
\text{SYM} & \{A \sigma\} d \sim c (B \sigma) \quad \forall v. \sigma(v_1) := v_2, \sigma(v_2) := v_1 \\
& \{A\} c \sim d (B) \\
\text{SEQ} & \{A\} c_1 \sim c_2 (B) \quad \{B\} d_1 \sim d_2 (C) \\
& \{A\} c_1; d_1 \sim c_2; d_2 (C) \\
\text{EQUAL} & f v(c) \subseteq X Q \\
& \{\text{Cl}a[X_1 = X_2] \cap (Q_1 \equiv_{\text{quant}} Q_2)\} c \sim c \{\text{Cl}a[X_1 = X_2] \cap (Q_1 \equiv_{\text{quant}} Q_2)\} \\
\text{FRAME} & f v(R) \subseteq V_1 V_2' \quad f v(c) \cap V \text{ and } f v(d) \cap V' \text{ are classical} \\
& c \text{ is } (f v(c) \cap V)\text{-readonly} \quad d \text{ is } (f v(d) \cap V')\text{-readonly} \\
& \{A\} c \sim d (B) \\
\text{QRHLElim} & \rho \text{ is separable} \quad \rho \text{ satisfies } A \quad \rho_1 := tr^{v_1} \rho \quad \rho_2 := tr^{v_2} \rho \\
& \{A\} c \sim d \{\text{Cl}a[e_{\rho_1} \Rightarrow f_2]\} \\
& \Pr[e : c(\rho_1)] \leq \Pr[f : d(\rho_2)] \quad \text{(also holds for } =, \iff \text{ and } \geq, \leq \text{ instead of } \leq, \Rightarrow) \\
\text{QRHLElimEq} & f v(A)^{\text{eq}} \subseteq Q \quad \{\text{Cl}a[X_1 = X_2] \cap (Q_1 \equiv_{\text{quant}} Q_2) \cap A_1 \cap A_2\} c \sim d \{\text{Cl}a[e_{\rho_1} \Rightarrow f_2]\} \\
& \Pr[e : c(\rho)] \leq \Pr[f : d(\rho)] \quad \text{(also holds for } =, \iff \text{ and } \geq, \leq \text{ instead of } \leq, \Rightarrow) \\
\text{TransSimple} & X_p := f v(p)^d, \quad Q_p := f v(p)^{\text{eq}} \text{ for } p = c, d, e \\
& \{\text{Cl}a[X_{c1} = X_{c2}] \cap (Q_{c1} \equiv_{\text{quant}} Q_{c2})\} c \sim d \{\text{Cl}a[X_{d1} = X_{d2}] \cap (Q_{d1} \equiv_{\text{quant}} Q_{d2})\} \\
& \{\text{Cl}a[X_{d1} = X_{d2}] \cap (Q_{d1} \equiv_{\text{quant}} Q_{d2})\} d \sim e \{\text{Cl}a[X_{c1} = X_{c2}] \cap (Q_{c1} \equiv_{\text{quant}} Q_{c2})\} \\
& \{\text{Cl}a[X_{c1} = X_{c2}] \cap (Q_{c1} \equiv_{\text{quant}} Q_{c2})\} c \sim e \{\text{Cl}a[X_{c1} = X_{c2}] \cap (Q_{c1} \equiv_{\text{quant}} Q_{c2})\} \\
\end{array} \]

Figure 1: Rules for qRHL (general rules).
Skip

\(\{ A \} \text{skip} \sim \text{skip}\{ A \}\)

Assign1

\(\{ B( e_1/x_1) \} x \leftarrow e \sim \text{skip}\{ B \}\)

Sample1

\[
A := (\text{Cla}[ e_1 \text{ is total}] \cap \bigcap_{z \in \text{supp} e_1} B\{ z/x_1 \})
\]

\(\{ A \} x \leftarrow e \sim \text{skip}\{ B \}\)

JointSample

\[
A := (\text{Cla}[\text{ marginal}_1( f) = e_1 \land \text{ marginal}_2( f) = e_2'] \cap \bigcap_{(z,z') \in \text{supp} f} B\{ z/x_1, z'/y_2 \})
\]

\(\{ A \} x \leftarrow e \sim \text{skip}\{ B \}\)

If1

\[
\{ \text{Cla}[ e_1] \cap A \} c \sim \text{skip}\{ B \} \quad \{ \text{Cla}[\neg e_1] \cap A \} d \sim \text{skip}\{ B \}
\]

\(\{ A \} \text{if } e \text{ then } c \text{ else } d \sim \text{skip}\{ B \}\)

JointIf

\[
A \subseteq \text{Cla}[ e_1 = e_2'] \quad \{ \text{Cla}[ e_1 \land e_2'] \cap A \} c \sim c' \{ B \} \quad \{ \text{Cla}[\neg e_1 \land \neg e_2'] \cap A \} d \sim d' \{ B \}
\]

\(\{ A \} \text{if } e \text{ then } c \text{ else } d \sim \text{if } e' \text{ then } c' \text{ else } d' \{ B \}\)

While1

\[
\{ \text{Cla}[ e_1] \cap A \} c \sim \text{skip}\{ A \} \quad A \subseteq B_1 \quad (\text{while } e \text{ do } c) \text{ is total on } B
\]

\(\{ A \} \text{while } e \text{ do } c \sim \text{skip}\{ \text{Cla}[\neg e_1] \cap A \}\)

JointWhile

\[
A \subseteq \text{Cla}[ e_1 = e_2'] \quad \{ \text{Cla}[ e_1 \land e_2'] \cap A \} c \sim d \{ A \}
\]

\(\{ A \} \text{while } e \text{ do } c \sim \text{while } e' \text{ do } d \{ \text{Cla}[\neg e_1 \land \neg e_2'] \cap A \}\)

Figure 2: Rules for qRHL (related to individual classical statements). For the rules Assign1, Sample1, If1, and While1, there is also an analogous symmetric rule that we do not list explicitly.

5 Semantics-related lemmas

Lemma 1

If \( fv( c) \subseteq V \), then there is a \( E \) on \( V \) such that \( \llbracket c \rrbracket = E \otimes \text{id}_V \setminus \langle V \rangle \).

(This lemma was already stated in [28] but the proof was not “semantic”.)

Proof. We show this by induction on \( c \). Each case is elementary to check, we only show the case \( c = \text{local } v; c' \) here:

Since \( fv( c) = fc( c') \setminus \{ v \} \), we have \( fv( c') \subseteq V \cup \{ v \} \). By induction hypothesis, there is an \( E' \) on \( V \cup \{ v \} \) with \( \llbracket c' \rrbracket = E' \otimes \text{id}_V \setminus \langle V \rangle \setminus \{ v \} \).
Figure 3: Rules for qRHL (related to individual quantum statements). For the rules \textbf{Measure1}, \textbf{QApply1}, and \textbf{QInit1}, there is also an analogous symmetric rule that we do not list explicitly.

We have (expressing the various superoperators as circuits for readability):

\[
\begin{array}{c}
\begin{array}{c}
\begin{array}{c}
[\mathbf{c}] \\
\text{\textsuperscript{\text{\textasteriskcentered}}} \\
\text{\textsuperscript{\text{\textasteriskcentered}}} \\
\text{\textsuperscript{\text{\textasteriskcentered}}} \\
\end{array}
\end{array}
\end{array}
\end{array}
\]

Here (\textsuperscript{\text{\textasteriskcentered}}) is by the semantics of the language, and (\textsuperscript{\text{\textasteriskcentered}}} since \([\mathbf{c}'] = \mathcal{E}' \otimes \text{id}_{\mathbf{V}' \setminus \mathbf{V}} \). If \(\mathbf{v} \notin \mathbf{V} \), let \(\mathcal{E} \) be the dotted box in the rhs. If \(\mathbf{v} \in \mathbf{V} \), let \(\mathcal{E} \) be the dotted box together with the \(\mathbf{v}\)-wire. Then \(\mathcal{E} \) is a superoperator on \(\mathbf{V} \), and \([\mathbf{c}] = \mathcal{E} \otimes \text{id}_{\mathbf{V}' \setminus \mathbf{V}} \).

\textbf{Lemma 2}

If \(\mathbf{f}(\mathbf{c}) \cap \mathbf{f}(\mathbf{d}) = \emptyset \), then \(\mathbf{c}, \mathbf{d} \equiv \mathbf{d}, \mathbf{c} \).

\textbf{Proof.} Let \(\mathbf{V} := \mathbf{f}(\mathbf{c})\) and \(\mathbf{W} := \mathbf{V}' \setminus \mathbf{f}(\mathbf{d}) \). By \textbf{Lemma 1}, there exists \(\mathcal{E}_c\) on \(\mathbf{V}\) such that \([\mathbf{c}] = \mathcal{E}_c \otimes \text{id}_W\). And there exists \(\mathcal{E}_d\) on \(\mathbf{W}\) such that \([\mathbf{d}] = \text{id}_V \otimes \mathcal{E}_d\). Thus

\[
[c; d] = [d] \circ [c] = (id_V \otimes E_d) \circ (E_c \otimes id_W) = E_c \otimes E_d = (E_c \otimes id_W) \circ (id_V \otimes E_d) = [c] \circ [d] = [d; c].
\]

\textbf{Lemma 3}

(i) local v; local v; c \(\equiv\) local v; c. (And \(\text{Local}_v [\text{Local}_v \mathcal{E}] = \text{Local}_v \mathcal{E}\).)

(ii) local v; local w; c \(\equiv\) local w; local v; c. (And \(\text{Local}_v [\text{Local}_w \mathcal{E}] = \text{Local}_w [\text{Local}_v \mathcal{E}]\).)
Proof. In this proof, we show the claims in parentheses, involving $\text{Local}_v[E]$ etc. The claims involving local $v$ etc. are an immediate consequence.

(We show only the claims in terms of local $v$; ... The claims in terms of Local, etc. are shown analogously.)

By definition of Local$[\ldots]$, Local$[\ldots]$, the lhs and rhs of (i) are described by the following circuits:

The only difference is the third wire in the lhs which is initialized with $\bullet$ and then discarded again, is the same as the identity. Thus the lhs and rhs are equal, (i) follows.

By definition of the semantics of the language, the lhs and rhs of (ii) are described by the following circuits:

The only difference is the order in which the last two wires are drawn which has no semantic meaning. Thus the lhs and rhs are equal, (ii) follows. □

This lemma implies that the order in which variables are declared local does not matter. This motivates the following shorthand: For a finite $V$ we introduce the following shorthand:

\[(\text{local } V; c) := (\text{local } v_1; \ldots; \text{local } v_n; c)\]

where $v_1, \ldots, v_n$ are the elements of $V$ in arbitrary order.

Similarly, we define $\text{Local}_V[E] := \text{Local}_v[\ldots \text{Local}_v[E]]$.

As an immediate consequence of the definition and Lemma 3(ii), we get

**Lemma 4**

(i) local $\emptyset; c = c$. (Also Local$[\emptyset][E] = E$.)

(ii) local $V; \text{local } V'; c \equiv \text{local } V \cup V'; c$. (Also Local$[\emptyset][E] = \text{Local}_{V \cup V'}[E]$.)

(iii) [local $V; c] = \text{Local}_V[[c]]$.

**Lemma 5**

Let $I$ be a set and $E_i (i \in I)$ be superoperators. Assume that $\sum_{i \in I} E_i$ converges. Then

$\sum_{i \in I} \text{Local}_V[E_i] = \text{Local}_V[\sum_{i \in I} E_i]$ (and the lhs converges).\(^a\) Here convergence is pointwise convergence with respect to the trace-norm.

\(^a\) Note that the converse does not hold: If $\sum_{i \in I} \text{Local}_V[E_i]$ converges, $\sum_{i \in I} E_i$ does not necessarily converge. For example, let $E_i(\rho) := \text{proj}_i(\psi)\rho\text{proj}_i(\psi)$ where $\psi$ is a normalized vector orthogonal to $\bullet\rangle$. Then
Proof. In this proof, unless mentioned otherwise, convergence of trace-class operators is with respect to trace-norm, and convergence of superoperators is pointwise with respect to trace-norm. Whenever we write an equality, we mean that equality holds whenever the sums in lhs and rhs converge, and that the lhs converges if the rhs does.

**Claim 1** \( \sum_i (E_i \otimes id) = (\sum_i E_i) \otimes id \).

**Proof of claim.** Let \( \mathcal{L}' := \sum_{i \in I} E_i \). By assumption, \( \mathcal{L}' \) exists and is trace bounded. Let \( B \) such that \( tr \mathcal{L}'(\rho) \leq B tr \rho \) for all positive \( \rho \). For finite \( F \) and positive \( \rho \), we have \( \sum_{i \in F} tr(E_i \otimes id)(\rho) = \sum_{i \in F} E_i(tr(\rho)) \leq \mathcal{L}'(tr(\rho)) \). Thus the sum \( \sum_{i \in F} tr(E_i \otimes id)(\rho) \) is bounded (as a function of finite \( F \)). Furthermore, since \( E_i \) is completely positive, \( (E_i \otimes id)(\rho) \) is positive. Thus \( \sum_{i \in F} (E_i \otimes id)(\rho) \) is bounded and increasing, hence it converges. Thus the limit \( \mathcal{L}'(\rho) := \sum_{i \in I} E_i(\otimes id)(\rho) \) exists for positive \( \rho \). Since every trace class \( \rho \) is a linear combination of four positive \( \rho \), the limit also exists for arbitrary \( \rho \).

We are left to show that \( (\mathcal{L}' \otimes id) = \mathcal{L}' \). Assume this is not the case. Since the set of all trace class operators is spanned by operators \( \sigma \otimes \tau \) with unit trace, this implies that there are \( \sigma, \tau \) with unit trace such that \( (\mathcal{L}' \otimes id)(\sigma \otimes \tau) \neq \mathcal{L}'(\sigma \otimes \tau) \). Let \( \delta := \| (\mathcal{L}' \otimes id)(\sigma \otimes \tau) - \mathcal{L}'(\sigma \otimes \tau) \| \). Since \( \mathcal{L}'(\sigma) \) is the limit of \( \sum_i E_i(\sigma) \), for sufficiently large finite \( F \),

\[
\left\| \sum_{i \in F} E_i(\sigma) - \mathcal{L}'(\sigma) \right\| \leq \frac{\delta}{3}. \tag{5}
\]

And since \( \mathcal{L}'(\sigma \otimes \tau) \) is the limit of \( \sum_i (E_i \otimes id)(\sigma \otimes \tau) \), for sufficiently large finite \( F \),

\[
\left\| \sum_{i \in F} (E_i \otimes id)(\sigma \otimes \tau) - \mathcal{L}'(\sigma \otimes \tau) \right\| \leq \frac{\delta}{3}. \tag{6}
\]

Fix an \( F \) such that both (5) and (6) hold. Furthermore,

\[
\left\| \sum_{i \in F} E_i(\sigma) - \mathcal{L}'(\sigma) \right\| = \left\| \left( \sum_{i \in F} E_i(\sigma) - \mathcal{L}'(\sigma) \right) \otimes \tau \right\| \leq \left\| \sum_{i \in F} (E_i \otimes id)(\sigma \otimes \tau) - (\mathcal{L}' \otimes id)(\sigma \otimes \tau) \right\|.
\]

With (5), this implies

\[
\left\| \sum_{i \in F} (E_i \otimes id)(\sigma \otimes \tau) - (\mathcal{L}' \otimes id)(\sigma \otimes \tau) \right\| \leq \frac{\delta}{3}.
\]

With (6) and the triangle inequality, we get \( \| (\mathcal{L}' \otimes id)(\sigma \otimes \tau) - \mathcal{L}'(\sigma \otimes \tau) \| \leq 2\delta/3 \), in contradiction to the definition of \( \delta \). Thus \( (\mathcal{L}' \otimes id) = \mathcal{L}' \).

**Claim 2** \( \sum_i \text{Local}_\nu [E_i] = \text{Local}_\nu [\sum_i E_i] \).

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Proof of claim. We have:

\[
\sum_i \text{Local}_v [\mathcal{E}_i](\rho) \overset{(4)}{=} \sum_i \text{tr}_v \left( \text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'})(\mathcal{E}_i \otimes \text{id}_{\mathcal{V}'})\left(\text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'})(\rho \otimes \rho_i^*)\right)\right)
\]

\[
\overset{(\prime)}{=} \text{tr}_v \left( \text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'})(\sum_i (\mathcal{E}_i \otimes \text{id}_{\mathcal{V}'})\left(\text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'})(\rho \otimes \rho_i^*)\right))\right)
\]

\[
\overset{(\prime\prime)}{=} \text{tr}_v \left( \text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'})(\left(\sum_i (\mathcal{E}_i) \otimes \text{id}_{\mathcal{V}'})\right)\left(\text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'})(\rho \otimes \rho_i^*)\right))\right)
\]

\[
\overset{\bullet}{=} \text{tr}_v \left( \text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'})(\left(\sum_i (\mathcal{E}_i) \otimes \text{id}_{\mathcal{V}'})\right)\left(\text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'})(\rho \otimes \rho_i^*)\right))\right)
\]

Here each equality means that the lhs converges if the rhs converges. And (\prime) follows because \text{tr}_v and \text{toE}(\text{SWAP}_{\mathcal{V} \leftrightarrow \mathcal{V}'}) are trace-preserving. And (\prime\prime) follows by definition of pointwise convergence. \hfill \Diamond

The lemma follows by induction over \mathcal{V} with Claim 2. \hfill \Box

For simpler notation, we write \text{init}_\mathcal{V} for v \xleftarrow{\diamond} |\_\rangle_v or v \leftarrow \_\_\_v, depending on whether v is quantum or classical. For a finite set \mathcal{V}, let \text{init}_\mathcal{V} denote \text{init} v_1; \ldots; \text{init} v_n where v_1, \ldots, v_n are the elements of \mathcal{V} in some arbitrary order. (The order does not matter due to Lemma 2.)

**Lemma 6**

For finite \mathcal{V} = \{v_1, \ldots, v_n\}, let \mathcal{E}^{\text{init}}\mathcal{V} be the superoperator \rho \mapsto \text{proj}(\_\rangle_{v_1} \otimes \ldots \otimes \_\rangle_{v_n}) \otimes \text{tr} \rho, where \_\rangle_v := \_\rangle_{v_1} \otimes \cdots \otimes \_\rangle_{v_n}.

Then [\text{init} \mathcal{V}] = \mathcal{E}^{\text{init}}\mathcal{V} \otimes \text{id}_{\mathcal{V} \setminus \mathcal{V}}.

**Proof.** For \mathcal{V} = \{q\} or \mathcal{V} = \{x\}, this follows from the definition of \text{init} q and \text{init} x, as well as the semantics of assignment and quantum initialization. By definition of \mathcal{E}^{\text{init}}\mathcal{V}, \mathcal{E}^{\text{init}}\mathcal{V} \otimes \text{id}_{\mathcal{V} \setminus \mathcal{V}} \otimes \mathcal{E}^{\text{init}}\mathcal{W} \otimes \text{id}_{\mathcal{V} \setminus \mathcal{W}} = \mathcal{E}^{\text{init}}\mathcal{VW} \otimes \text{id}_{\mathcal{V} \setminus \mathcal{VW}}. The lemma then follows by induction. \hfill \Box

**Lemma 7**

(i) local \mathcal{V}; c \xleftarrow{\diamond} c if \mathcal{V} \cap \text{fv}(c) = \emptyset.

(ii) local \mathcal{V}; c \xleftarrow{\diamond} local \mathcal{V}; (\text{init} \mathcal{V}'; c) if \mathcal{V}' \subseteq \mathcal{V}.

(iii) local \mathcal{V}; c \xleftarrow{\diamond} local \mathcal{V}; (c; \text{init} \mathcal{V}') if \mathcal{V}' \subseteq \mathcal{V}.

**Proof.** We first show (i). By Lemma 1, there is an \mathcal{E} on \text{fv}(c) such that \[c] = \mathcal{E} \otimes \text{id}_{\mathcal{V} \setminus \text{fv}(c)}.\]
Thus we can represent $[c]$ and $[\text{local } V; c]$ by the following circuits:

![Diagram](attachment:diagram.png)

The only difference is the third wire that is created and discarded on the rhs. This is equal to the identity, thus the two circuits are identical and we have $c \equiv \text{local } V; c$. This shows (i).

We now show (ii). We show the special case $\text{local } v; c \equiv \text{local } v; (\text{init } v; c)$. The general case follows by induction. The lhs and rhs, as circuits are, respectively:

![Diagram](attachment:diagram2.png)

Here we used Lemma 6 for expressing $[\text{init } v]$ in terms of $\mathcal{E}^\text{init}_v$.

It follows immediately from the definition of $\mathcal{E}^\text{init}_v$ that $\mathcal{E}^\text{init}_v(\text{proj}(\bullet)) = \text{proj}(\bullet)$. Thus the two circuits compute the same function. Hence $\text{local } v; c \equiv \text{local } v; (\text{init } v; c)$. (ii) follows.

We now show (iii). We show the special case $\text{local } v; c \equiv \text{local } v; (c; \text{init } v)$. The general case follows by induction. The lhs and rhs, as circuits are, respectively:

![Diagram](attachment:diagram3.png)

Here we used Lemma 6 for expressing $[\text{init } v]$ in terms of $\mathcal{E}^\text{init}_v$.

Since $\mathcal{E}^\text{init}_v$ is trace-preserving, $\text{tr} \circ \mathcal{E}^\text{init}_v = \text{tr}$. I.e., $\mathcal{E}^\text{init}_v$ and $\mathcal{E}^\text{init}_v$ compute the same function. Thus the lhs and rhs compute the same function, i.e., $\text{local } c; d \equiv \text{local } v; (c; \text{init } v)$. (iii) follows.

\[\square\]

**Lemma 8**

Let $\sigma$ be a bijective variable substitution. Assume $\text{dom } \sigma \cap \text{fv}(c) = \varnothing$. Then $c \sigma \equiv d$.

**Proof.** Let $U_\sigma$ be the unitary on $\ell^2(\mathcal{V}^{\text{all}})$ defined by $U_\sigma |m\rangle = |m \circ \sigma\rangle$. That is $U_\sigma$ reorders the subsystems corresponding to the variables in $\mathcal{V}^{\text{all}}$. Let $\mathcal{E}_\sigma(\rho) := U_\sigma \rho U_\sigma^\dagger$.

Since $c \sigma$ simply renames all variables (even the local ones), $[c] \sigma$ simply operates on the reordered variables, formally $[c] \sigma(\rho) = \mathcal{E}_\sigma^{-1} \circ [c] \circ \mathcal{E}_\sigma$.

Since $\sigma$ is the identity on $\text{dom } \sigma$, $\mathcal{E}_\sigma = \mathcal{E}_0 \circ \text{id}$ for some $\mathcal{E}_0$ on $\text{dom } \sigma$. And $[c] = \mathcal{E}_0 \circ \text{id}$ for some $\mathcal{E}_0$ on $\text{fv}(c)$. Since $\text{dom } \sigma$ and $\text{fv}(c)$ are disjoint, this implies that $\mathcal{E}_\sigma$ and $[c]$ commute.

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Thus
\[
[c^\sigma](\rho) = \mathcal{E}_{\sigma^{-1}} \circ [c] \circ \mathcal{E}_\sigma = \mathcal{E}_{\sigma^{-1}} \circ \mathcal{E}_\sigma \circ [c] = \mathcal{E}_{\sigma \circ \sigma^{-1}} \circ [c] = \mathcal{E}_{\text{id}} \circ [c] = [c]. \quad \square
\]

**Lemma 9**

Let \( \sigma \) be a variable substitution that is injective on \( V \) and let \( W := \sigma(V) \). Assume that \( \sigma = \text{id} \) outside \( V \) and that \( (fv(c) \setminus V) \cap W = \emptyset \). Assume noconflict(\( \sigma, c \)).

Then local \( V; c \triangleq \text{local } W; (c[W/V]) \).

This is shown in Isabelle/HOL, as rename_locals in theory Rename_Locals.thy. See Section 1.1 for remarks about our Isabelle/HOL development.

**Lemma 10**

(i) \((\text{local } V; c); (\text{local } V; d) \triangleq \text{local } V; (c; \text{init } V; d)\).

(ii) If \( V \cap fv(c) = \emptyset \), then \( c; (\text{local } V; d) \triangleq \text{local } V; (c; d)\).

**Proof.** We first show (i) in the special case \( V = v \). The lhs and rhs are depicted by the following circuits (using Lemma 6 for the semantics of init \( v \)): 

By definition (Lemma 6), \( \mathcal{E}^{\text{init}}_\psi : \rho \mapsto \text{proj}(\cdot) \otimes \text{tr } \rho \). Or, as a circuit, \( \bullet \otimes \xrightarrow{V} \cdot \). Thus the two circuits are identical, hence (i) follows.

We prove (ii) in the special case \( V = v \):

\[
c; (\text{local } v; d) \overset{(\ast)}{=} (\text{local } v; c); (\text{local } v; d) \overset{(\ast\ast)}{=} \text{local } v; (c; \text{init } v; d)\]

\[
\overset{(\ast\ast\ast)}{=} \text{local } v; (\text{init } v; c; d) \overset{(\ast\ast\ast)}{=} \text{local } v; (c; d)\]

Here (\( \ast \)) uses Lemma 7 (i), (\( \ast\ast \)) uses Lemma 2, and (\( \ast\ast\ast \)) uses Lemma 7 (ii).

This shows (ii).

The general case of (ii) is a straightforward induction over \( V \), using the special case for the induction step. We did the proof of the general case in Isabelle/HOL (Helping_Lemmas.locals_seq2), using the special of (ii) as an axiom.

The general case of (i) is proven by a simple induction over \( V \), using the special case of (i) and the general case of (i) for the base case. We did the proof of the general case in Isabelle/HOL (Helping_Lemmas.locals_seq_merge), using the special of (i) as an axiom. \( \square \)
Lemma 11

(i) If $X \subseteq \text{overwr}(c)$, then $X \leftarrow e; c \equiv c$.

(ii) If $Q \subseteq \text{overwr}(c)$, then $Q \triangleleft\triangledown e; c \equiv c$.

(iii) If $V \subseteq \text{overwr}(c)$, then $\text{init } V; c \equiv c$.

Proof. We first show a special case of (iii), namely that $\text{init } v; c \equiv c$ if $v \in \text{overwr}(c)$. We show this by induction over the structure of $c$.

We distinguish the following cases:

- Cases $c = \text{skip}$, $c = \text{while } e \text{ do } c'$, $c = \text{apply } e \text{ to } Q$:
  
  In these cases, $\text{overwr}(c) = \emptyset$. By assumption, $v \in \text{overwr}(c)$. Thus this case cannot arise.

- Case $c = X \leftarrow e$:
  
  In this case, $v \in \text{overwr}(c) = X \setminus \text{fv}(e)$. Thus $v$ is a classical variable, $v \in X$, and $v \notin \text{fv}(e)$.
  
  We have for all $m, \rho$:

  \[
  [\text{init } v; c](\text{proj}(m)_{\text{val}}) \otimes \rho
  = [X \leftarrow e] \circ [v \leftarrow \bullet_v](\text{proj}(m)_{\text{val}}) \otimes \rho \quad \text{(sem. of ;, def. of init)}
  = [X \leftarrow e](\text{proj}(m(v := \bullet_v))_{\text{val}}) \otimes \rho \quad \text{(sem. of assignment)}
  = \text{proj}(m(v := \bullet_v)(X := [e]_m)_{\text{val}}) \otimes \rho \quad \text{(sem. of assignment)}
  \]

  Here $(\ast)$ follows since $v \notin \text{fv}(e)$ and thus $[e]_{m(v := \bullet_v)} = [e]_m$. And $(\ast\ast)$ follows since $v \in X$ and thus $m(v := \bullet_v)(X := [e]_m) = m(X := [e]_m)$.
  
  Thus $[\text{init } v; c] = [c]$. On all states of the form $\text{proj}(m)_{\text{val}} \otimes \rho$. Since states of this form span all cq-states, by linearity, $\text{init } v; c \equiv c$.

- Case $c = X \triangleleft\triangledown e$:
  
  In this case, $v \in \text{overwr}(c) = X \setminus \text{fv}(e)$. Thus $v$ is a classical variable, $v \in X$, and $v \notin \text{fv}(e)$.
We have for all $m, \rho$

\[
\begin{align*}
[\text{init } v; c] &\cdot (\text{proj}(m)_{\text{blind}}) \otimes \rho \\
&= [X \triangleleft e] \cdot [v \leftarrow \bullet_v] (\text{proj}(m)_{\text{blind}}) \otimes \rho & (\text{sem. of } ; \text{ def. of init}) \\
&= [X \triangleleft e] (\text{proj}(m(v := \bullet_v))_{\text{blind}}) \otimes \rho & (\text{sem. of assignment}) \\
&= \sum_z [e]_{m(v := \bullet_v)}(z) \cdot \text{proj}(m(v := \bullet_v)(X := z))_{\text{blind}} \otimes \rho & \text{(sem. of sample)} \\
&\leq \sum_z [e]_{m}(z) \cdot \text{proj}(m(X := z))_{\text{blind}} \otimes \rho \\
&= [X \triangleleft e] (\text{proj}(m)_{\text{blind}}) \otimes \rho = [e] (\text{proj}(m)_{\text{blind}}) \otimes \rho & \text{(sem. of assignment)}
\end{align*}
\]

Here $(\ast)$ follows since $v \notin \text{fv}(e)$ and thus $[e]_{m(v := \bullet_v)} = [e]_{m}$. And $(\ast\ast)$ follows since $v \in X$ and thus $m(v := \bullet_v)(X := [e]_{m}) = m(X := [e]_{m})$.

Thus $[\text{init } v; c] = [e]$ on all states of the form $\text{proj}(m)_{\text{blind}} \otimes \rho$. By linearity, $\text{init } v; c \triangleleft c$.

- Case $c = Q \triangleleft e$:

In this case, $v \in \text{overwr}(c) = Q$. Thus $v$ is a quantum variable and $v \in Q$. We have for all $m, \rho$

\[
\begin{align*}
[\text{init } v; c] &\cdot (\text{proj}(m)) \otimes \rho \\
&= [Q \triangleleft e] \cdot [\text{init } v] (\text{proj}(m)) \otimes \rho & (\text{def. of } c, \text{ semantics of } ;) \\
&= [Q \triangleleft e] (\text{proj}(m)) \otimes \text{tr}^m \rho \otimes \text{proj}(\bullet) & (\text{Lemma 6}) \\
&= \text{proj}(m) \otimes \text{tr}_m \rho \otimes \text{proj}(\bullet) \otimes [e]_m & \text{(sem. of quant. init.)} \\
&= \text{proj}(m) \otimes \text{tr}_m \rho \otimes [e]_m & (v \in Q) \\
&= [Q \triangleleft e] (\text{proj}(m)) \otimes [c] & \text{(sem. of quant. init.)} \\
&= [c] (\text{proj}(m)) \otimes [c] & \text{(definition of } c)
\end{align*}
\]

Thus $[\text{init } v; c] = [c]$ on all states of the form $\text{proj}(m)_{\text{blind}} \otimes \rho$. By linearity, $\text{init } v; c \triangleleft c$.

- Case $c = \text{if } e \text{ then } c' \text{ else } d'$:

Since $v \in \text{overwr}(c) = (\text{overwr}(c') \cap \text{overwr}(d')) \setminus \text{fv}(e)$ we have: $v \in \text{overwr}(c')$, $v \in \text{overwr}(d')$, $v \notin \text{fv}(e)$.

We will show that $[\text{init } v; c] (\text{proj}(m)_{\text{blind}}) \otimes \rho = [c] (\text{proj}(m)_{\text{blind}}) \otimes \rho$ for all $m, \rho$. By linearity, this then shows $\text{init } v; c \triangleleft c$. Fix $m, \rho$. We assume $[e]_m = \text{true}$. The case $[e]_m = \text{false}$ is shown analogously.

We distinguish two cases, depending on whether $v$ is a classical or a quantum variable:

- Case $v$ is classical:
Since $v \notin fu(e)$, we have

$$[c]_{m(v := \bullet_v)} = [e]_m = \text{true} \quad (7)$$

And

$$[[\text{init } v; c] (\text{proj}(|m|_{\text{Val}}) \otimes \rho)) = [[e] (\text{proj}(|m|_{\text{Val}}) \otimes \rho)) \quad \text{(sem. of ;, def. of init)}$$

$$[[\text{init } v; c] (\text{proj}(|m|_{\text{Val}}) \otimes \rho)) = [[e] (\text{proj}(|m|_{\text{Val}}) \otimes \rho)) \quad \text{(sem. of qu. init.)}$$

Case $v$ is quantum:
Let $\rho' := \text{tr}_Q \rho \otimes \text{proj}([e]_m)$. We have

$$[[\text{init } v; c] (\text{proj}(|m|_{\text{Val}}) \otimes \rho)) = [[e] (\text{proj}(|m|_{\text{Val}}) \otimes \rho)) \quad \text{sem., def. of init)}$$

$$[[\text{init } v; c] (\text{proj}(|m|_{\text{Val}}) \otimes \rho)) = [[e] (\text{proj}(|m|_{\text{Val}}) \otimes \rho)) \quad \text{(induction hypothesis)$$

• Case $c = c'; d'$:
We have $v \in \text{overwr}(c) = \text{overwr}(c') \cup \left(\text{overwr}(d') \setminus \text{fu}(c')\right) \cap \text{covered}(c')$. We thus distinguish the following cases:

  – Case $v \in \text{overwr}(c')$:
  
  By induction hypothesis, $\text{init } v; c' \models d'$. Thus $\text{init } v; c \models \text{init } v; c'; d' \models c'$. $d' = c$.

  – Case $v \in \text{overwr}(d') \setminus \text{fu}(c')$:
  
  Since $v \notin \text{fu}(c')$ and $\text{fu}(\text{init } v) = \{v\}$, we have $\text{init } v; c' \models c'$; $\text{init } v$ by Lemma 2. And since $v \in \text{overwr}(d')$, by induction hypothesis, we have $\text{init } v; d' \models d'$. Thus $\text{init } v; c \models \text{init } v; c'; d' \models c'$; $\text{init } v; d' \models c'$; $d' = c$.

• Case $c = X \leftarrow \text{measure } Q$ with $e$:
Since $v \in \text{overwr}(c) = X \setminus \text{fu}(e)$, we have that $v$ is classical, $v \in X$, but $v \notin \text{fu}(e)$.  

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Thus this shows (iii).

Finally, we show (ii). It is easy to check from the semantics that \( X \leftarrow e ; \text{init } X \leftarrow e; \text{init } X; c \stackrel{\text{def}}{=} c \) for all \( m, \rho \).

We have for all \( m, \rho \):

\[
\begin{align*}
\text{init } v; c \left[ \text{proj}(z) \otimes \rho \right] &= \text{init } v; c \left[ \text{proj}(z) \otimes \rho \right] \\
&= [X \leftarrow \text{measure } Q \text{ with } e] \circ [v \leftarrow \bullet v][\text{proj}(z) \otimes \rho] \quad \text{(sem. of ;, def. of init)} \\
&= [X \leftarrow \text{measure } Q \text{ with } e][\text{proj}(z) \otimes \rho] \quad \text{(sem. of assignment)} \\
&= \sum_{z} \text{proj}(z) \circ P_{\rho}P_{z} \\
&= [X \leftarrow \text{measure } Q \text{ with } e][\text{proj}(z) \otimes \rho] \quad \text{(sem. of measurement)} \\
&= [c][\text{proj}(z) \otimes \rho]
\end{align*}
\]

Here \((*)\) follows since \( v \in X \) and thus \( m(v := \bullet_v)(X := z) = m(X := z) \).

- Case \( c = \text{local } w; c' \):

Since \( v \in \text{overwr}(c) = \text{overwr}(c') \setminus \{w\} \), we have \( v \in \text{overwr}(c') \) but \( v \neq w \). By induction hypothesis, we have \( \text{init } v; c \stackrel{\text{def}}{=} c' \). By Lemma 10 (ii), we have \( \text{init } v; \text{local } w; c' \stackrel{\text{def}}{=} \text{local } w; \text{init } v; c' \). Thus \( \text{init } v; c \stackrel{\text{def}}{=} \text{init } v; \text{local } w; c' \stackrel{\text{def}}{=} \text{local } w; \text{init } v; c' \).

Thus we have shown:

\[
\text{init } v; c \stackrel{\text{def}}{=} c \quad \text{if } v \in \text{overwr}(c). \tag{8}
\]

From this we can conclude (iii): Let \( \{v_1, \ldots, v_n\} := V \subseteq \text{overwr}(c) \).

\[
\text{init } v_1; \ldots; \text{init } v_n; c \stackrel{\text{def}}{=} \text{init } v_1; \ldots; \text{init } v_n; c \stackrel{\text{def}}{=} \ldots \stackrel{\text{def}}{=} c.
\]

This shows (iii).

We show (i). It is easy to check from the semantics that \( X \leftarrow e; \text{init } X \leftarrow e; \text{init } X; c \stackrel{\text{def}}{=} c \).

Finally, we show (ii). It is easy to check from the semantics that \( Q \leftarrow e; \text{init } Q \leftarrow e; \text{init } Q; c \stackrel{\text{def}}{=} c \).

Thus

\[
Q, e; c \stackrel{\text{def}}{=} Q, e; \text{init } Q; c \stackrel{\text{def}}{=} \text{init } Q; c \stackrel{\text{def}}{=} c.
\]

\hfill \Box

\begin{lemma}
\end{lemma}

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(i) For \( c := (\text{local } V_1; c_1); \ldots; (\text{local } V_n; c_n) \), we have \( c \overset{d}{=} \text{local } V^1; (c'_1; \ldots; c'_n) \) where \( c'_i := \text{init } V^i; \text{local } V^i; c_i \), \( W_i := V_i \cup V^i \setminus (fv(c_i) - V^i) \), \( V_i - V^i \setminus W_i \subseteq V^i \subseteq V_i \cup V^i \subseteq V_i \subseteq V^i \cup V^i \), \( V^i \setminus (fv(c_i) \setminus V^i) \cup V^i \setminus (fv(c_i) \setminus V^i) \subseteq \emptyset \). Applying Lemma 12 repeatedly as long as possible. In the footnotes in Lemma 12, we describe how to move all or selected local variables upwards as far as possible. This is done by repeatedly changing its semantics. We have implemented a tactic \( \text{locals_up_block} \) in Isabelle/HOL, as \( \text{locals_up_block} \) in theory Locals_Up_Block.thy. See Section 1.1 for remarks about our Isabelle/HOL development.

(ii) Assume \( V^i \cup V^i \setminus V^i \subseteq V^i \), \( V^i \cup V^i \setminus V^i \subseteq V^i \). Then

\[
\text{if } e \text{ then } \{ \text{local } V^i \text{; } c \text{then} \} \text{ else } \{ \text{local } V^i \text{; } c \text{else} \} \overset{d}{=} \text{local } V^i \text{; if } e \text{ then } \{ \text{local } V^i \text{; } c \text{then} \} \text{ else } \{ \text{local } V^i \text{; } c \text{else} \}.
\]

We now show (ii). By definition, \([e \text{; } c \text{then} \text{ else } d \text{else}] = [c \text{then}] \circ \downarrow = \downarrow \circ [d \text{else}] \circ \downarrow \circ e \). Let \( d_e, d_{\neg e} \) be arbitrary programs with \([d_e] = \downarrow = \downarrow = \downarrow = \downarrow = \text{if } e \text{ then } c \text{then} \text{ else } d \text{else} = \downarrow = \). Then

\[
([e \text{; } c \text{then} \text{ else } d \text{else}] = [d_e; c \text{then}] + [d_{\neg e}; c \text{else}] \quad \text{ for any } c \text{then}, c \text{else}. \quad (9)
\]

Thus

\[
[e \text{; } c \text{then} \text{ else } d \text{else}] = [d_e; c \text{then}] + [d_{\neg e}; c \text{else}]
\]

\( \overset{(3)}{=} \text{Local}_V^i \left[ [d_e; c \text{then}] ; (c \text{then}) \right] + \text{Local}_V^i \left[ [d_{\neg e}; c \text{else}] ; (c \text{else}) \right]
\]

\( \overset{(2)}{=} \text{Local}_V^i \left[ [d_e; c \text{then}] ; (c \text{then}) \right] + \text{Local}_V^i \left[ [d_{\neg e}; c \text{else}] ; (c \text{else}) \right]
\]

This lemma allows us to move local variable declarations upwards in a program without changing its semantics. We have implemented a tactic \text{local up} in qrhl-tool that allows us to move all or selected local variables upwards as far as possible. This is done by repeatedly applying Lemma 12 repeatedly as long as possible. In the footnotes in Lemma 12, we describe how the tactic instantiates the lemma (we call this the “greedy instantiation”) in order to move as many variables as possible.

Proof. (i) is shown in Isabelle/HOL, as \text{locals_up_block} in theory Locals_Up_Block.thy. See Section 1.1 for remarks about our Isabelle/HOL development.
\( V_2 := V_{\text{then}}, V_1^i := \emptyset, V_2^i := V_{\text{then}}^i, V_1^\dagger, V_2^\dagger := \emptyset, W_1 := V^\dagger, W_2 := V^\dagger \setminus f\varepsilon(\epsilon). \)

The premises of (i) then follow from the premises of (ii) (using also that \( f\varepsilon(d_i) = f\varepsilon(\epsilon) \) and \( f\varepsilon(d_i; \text{local } V_{\text{then}}; c_{\text{then}}) = f\varepsilon(\epsilon) \cup (f\varepsilon(c_{\text{then}}) \setminus V_{\text{then}}) \)). The second invocation is instantiated analogously, with \textit{else} instead of \textit{then}, and with \( c_1 := d_{\text{-}e} \).

This shows (ii).

We now show (iii).

By definition, \( \text{while } \epsilon \text{ do } c = \sum_{i=0}^{\infty} \downarrow_{\text{-}e} \circ (\llbracket c \rrbracket \circ \downarrow_{\text{-}e})^i. \) (Convergence is pointwise with respect to the trace-norm.) Let \( d_e, d_{\text{-}e} \) be arbitrary programs with \( \llbracket d_e \rrbracket = \downarrow_{\epsilon}, \llbracket d_{\text{-}e} \rrbracket = \downarrow_{\text{-}e} \) and \( f\varepsilon(d_e), f\varepsilon(d_{\text{-}e}) = f\varepsilon(\epsilon). \) Then

\[
\text{while } \epsilon \text{ do } c = \sum_{i=0}^{\infty} \llbracket d_i ; c ; \ldots ; d_i ; c ; d_{\text{-}e} \rrbracket \text{ for any } c \tag{10}
\]

From (i), we have

\[
d_e ; (\text{local } V^i; c) ; \ldots ; d_e ; (\text{local } V^i; c) ; d_{\text{-}e} \triangleq \text{local } V^i ; (\text{init } V^i ; \text{local } V^i ; c) ; \ldots ; d_e ; (\text{init } V^i ; \text{local } V^i ; c) ; d_{\text{-}e} \tag{11}
\]

Specifically, we instantiate (i) as follows:

\[
c_1, \ldots, c_{2n+1} := d_e, c, d_e, c, \ldots, d_e, c, d_{\text{-}e} \]

\[
c'_1, \ldots, c'_{2n+1} := d_e, (\text{init } V^i ; \text{local } V^i ; c), d_e, (\text{init } V^i ; \text{local } V^i ; c), \ldots, d_e, (\text{init } V^i ; \text{local } V^i ; c), d_{\text{-}e} \]

\[
V_1, \ldots, V_{2n+1} := \emptyset, V, \emptyset, V, \ldots, \emptyset, V, \emptyset \]

\[
V_1^i, \ldots, V_{2n+1}^i := \emptyset, V^i, \emptyset, V^i, \ldots, \emptyset, V^i, \emptyset \]

As well as \( V^\dagger := V^i. \) (The values of \( W_i \) do not matter in this application of (i).) Then the premises of (i) are elementary to check (using also \( f\varepsilon(d_e; (\text{local } V^i; c) ; \ldots ; d_e; (\text{local } V^i; c); d_{\text{-}e}) = f\varepsilon(\epsilon) \cup (f\varepsilon(c) \setminus V) \) and the premises \( V^\dagger \subseteq V \setminus f\varepsilon(\epsilon) \) and \( V^i = V \setminus V^\dagger \)). (11) follows.

And from (10), we have

\[
\text{while } \epsilon \text{ do (init } V^i; \text{local } V^i; c) \triangleq \sum_{i=0}^{\infty} \llbracket c^*_i \rrbracket. \tag{12}
\]
This implies:
\[
\llbracket \text{while } e \text{ do (local } V; c) \rrbracket \overset{10/11}{=} \sum_{i=0}^{\infty} \llbracket \text{local } V^\uparrow; c^\uparrow_i \rrbracket = \sum_{i=0}^{\infty} \text{Local}_{V^\uparrow} \llbracket c^\uparrow_i \rrbracket \\
\overset{\text{lem. 10 (ii)}}{=} \text{Local}_{V^\uparrow} \left( \sum_{i=0}^{\infty} [c^\uparrow_i] \right) = \text{Local}_{V^\uparrow} \left( \llbracket \text{while } e \text{ do (init } V^\uparrow; \text{local } V^\downarrow; c) \rrbracket \right) \\
= \llbracket \text{local } V^\uparrow; \text{while } e \text{ do (init } V^\uparrow; \text{local } V^\downarrow; c) \rrbracket \\
\overset{\text{lem. 10 (ii)}}{=} \llbracket \text{local } V^\uparrow; \text{while } e \text{ do (local } V^\downarrow; \text{init } V^\uparrow; c) \rrbracket .
\]

This shows (iii). \(\square\)

\(^*\)E.g., \(d_e := \text{if } e \text{ then halt else skip, } d_{\text{no}} := \text{if } e \text{ then skip else halt, } \text{halt := while true do skip.}\)

6 Basic rules for variable renaming/removal

\begin{align*}
\quad & \begin{array}{c}
\text{RENAMEQRHL1} \\
\text{noconflict}(\sigma, c) & \quad \sigma \text{ injective on } f(v(c)) \cup \{v : v_1 \in f(v(A)) \cup f(v(B))\}
\end{array} \\
& \quad \{A_1 \text{ c } \sim \text{ c}\{B_1\}} \\
& \quad \{A\text{ c } \sim \text{ d}\{B\}}
\end{align*}

Here \(\sigma(v_1) := w_1\) whenever \(\sigma(v) = w\) (and \(\sigma(v_2) := v_2\) for all \(v\)).

Analogously RenameQRhl2 for renaming in \(d\).

This is shown in Isabelle/HOL, as rename_qrhl_left and rename_qrhl_right in theory Rename_Locals.thy. See Section 1.1 for remarks about our Isabelle/HOL development.

We have implemented a tactic rename in qrhl-tool that implements this rule.

\begin{align*}
\quad & \begin{array}{c}
\text{REMOVELocal1} \\
f(v(A)), f(v(B)) \cap V_1 = \emptyset & \quad \{A \cap (V_1 = \text{ q } \bullet\nu)\} \text{ c } \sim \text{ d}\{B\}
\end{array} \\
& \quad \{A\text{ local } V; c \sim \text{ d}\{B\}}
\end{align*}

Analogously RemoveLocal2 for removing on the right side.

Note that the converse of this rule does not hold: If \(\{A\text{ local } V; c \sim \text{ d}\{B\}\}\), then we do not necessarily have \(\{A \cap (V_1 = q \bullet\nu)\} \text{ c } \sim \text{ d}\{B\}\) \(^*\)

We have implemented this rule as the tactic local remove in qrhl-tool which allows us to remove selected (or all) local variable declarations from the top of the left or right program. The tactic is a little weaker in that it does not include \(V_1 = q \bullet\nu\) in the precondition of the new subgoal.

Proof. We show the rule for \(V = v\) (only one variable). The general case follows by induction.

Let \(w \in V^{\text{all}}\) be an arbitrary variable such that \(w_1 \notin f(v(A), B), w \notin f(v(c), |\text{Type}_w| \geq |\text{Type}_v|, |\text{Type}_w| = \infty.\) Then \(|\text{Type}_{\text{set}}^w| = |\text{Type}_{\text{set}}^v| = |\text{Type}_w|\). Hence there is a bijection \(\phi : \text{Type}_w \rightarrow \text{Type}_{\text{set}}^w\). Thus \(U : |x|_w \rightarrow |\phi(x)|_w\) is a unitary from \(\ell^2[w]\) to \(\ell^2[vw]\).

Since \(w \notin f(v(c))\), by Lemma 1, \([c] = E \otimes |d|_w\) for some \(E\) on \(V^{all} \setminus w\). In slight abuse of

\(^*\)Counterexample: Let \(c := \langle q \in \mathbb{R} : \frac{1}{\sqrt{2}}(00) + \frac{1}{\sqrt{2}}(11) \rangle\), \(d := \langle x \in \mathbb{R} : \{0, 1\}\rangle\) (here \(\{0, 1\}\) stands for the uniform distribution on \(\{0, 1\}\)). Then \(\{A \cap (q_1 = q |x|_2)\} \sim \text{ d}\{B\}\). Yet \(\text{local } r\; c\) is equivalent to assigning randomly \(|0\) or \(|1\) to \(q\), thus \(\{A\text{ local } y; c \sim \text{ d}\{B\}\) holds.

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Two-sided initialization

Consider the following circuit (but ignore the wavy lines with boxes on the bottom for now):

\[
\begin{array}{c}
\begin{tikzpicture}
\node (A) at (0,0) {$v$};
\node (B) at (4,0) {$w$};
\node (C) at (2,1) {$\mathcal{U}$};
\node (D) at (6,1) {$\mathcal{U}$};
\node (E) at (4,2) {$\mathcal{A}$};
\node (F) at (6,2) {$\mathcal{B}$};
\node (G) at (8,0) {$v^\mathit{all}_w$};
\node (H) at (0,0) {$v^\mathit{all}_v$};
\draw[->] (A) -- (B);
\draw[->] (B) -- (C);
\draw[->] (C) -- (D);
\draw[->] (D) -- (E);
\draw[->] (E) -- (F);
\draw[->] (F) -- (G);
\end{tikzpicture}
\end{array}
\]

\[
\begin{array}{c}
A = \mathcal{A} \otimes \ell^2[\nu_1 w_1], \quad A' = \text{span}\{\bullet \nu_1 \}\otimes \ell^2[\nu'_1 w_1], \quad B = \mathcal{B} \otimes \ell^2[\nu_2 w_1], \quad B' = \text{span}\{\bullet \nu_2 \} \otimes \ell^2[\nu'_2 w_1].
\end{array}
\]

First, note that \( \mathcal{U} \) commutes with \([\mathcal{C}]\). And since \( \mathcal{U} \) is unitary, \( \mathcal{U}^* \) and \( \mathcal{U} \) are inverses. Thus \( \mathcal{U}^* \) and \( \mathcal{U} \) cancel out in this circuit. The remaining circuit is by definition \([\text{local } v; c] \) (see (4)).

Abbreviating, we say “\( \rho_1, \rho_2 \) satisfy \( \mathcal{A} \)” if there exists a separable \( \rho \) (the “coupling”) such that \( \text{tr}_1 \rho = \rho_1, \text{tr}_2 \rho = \rho_2 \), and \( \rho \) satisfies \( \mathcal{A} \).

We need to show \([A] \text{local } v; c \sim d \{B\} \). For this, fix cq-operators \( \rho_1, \rho_2 \) on \( V^\mathit{all} \) satisfying \( \mathcal{A} \). We need to show that \([\text{local } v; c] (\rho_1), [d] (\rho_2) \) satisfy \( \mathcal{B} \).

Let \( \rho^{(1)}, \ldots, \rho^{(2)} \) be the states at the corresponding wavy lines when executing the above circuit with initial state \( \rho_1 \). In particular, \( \rho^{(2)} = \rho_2 \) and \( \rho^{(2)} = [\text{local } v; c] (\rho_1) \). Let \( \mathcal{C}^{(i)} \) denote the predicate given in the box under the wavy line for \( \rho^{(i)} \).

Since \( \rho_1, \rho_2 \) satisfy \( \mathcal{A} \), we have that \( \rho^{(1)}, \rho^{(2)} \) satisfy \( \mathcal{C}^{(2)} \). Then \( \rho^{(2)}, \rho_2 \) satisfy \( \mathcal{C}^{(2)} \). (The coupling is \( \rho \otimes \text{proj}(\bullet \nu_1) \) if the previous coupling was \( \rho \).)

Then \( \rho^{(2)}, \rho_2 \) satisfy \( \mathcal{C}^{(2)} \). (The coupling is \( \text{(toE(SWAP)}_{v,v'v'}) \otimes \text{id}) \rho \) if the previous coupling was \( \rho \).)

Then \( \rho^{(1)}, \rho_2 \) satisfy \( \mathcal{C}^{(2)} \) since \( U^* \) maps \( \ell^2[\nu'_1 w_1] \) to \( \ell^2[\nu_2 w_1] \). (The coupling is \( \text{(toE}(U^*) \otimes \text{id}) \rho \) if the previous coupling was \( \rho \).)

By assumption, \( \{ \mathcal{A} \cap (v_1 = q, \bullet \nu_1) \} \text{~dist~} d \{B\} \). And since \( \rho^{(1)}, \rho_2 \) satisfy \( \mathcal{C}^{(2)} = \mathcal{A} \cap (v_1 = q, \bullet \nu_1) \), we have that \([\mathcal{C}] (\rho^{(1)}), [d] (\rho_2) \) satisfy \( \mathcal{B} = \mathcal{C}^{(2)} \). Since \( \rho^{(1)} = [\mathcal{C}] (\rho^{(1)}), [d] (\rho_2) \) satisfy \( \mathcal{C}^{(2)} \).

Then \( \rho^{(2)}, [d] (\rho_2) \) satisfy \( \mathcal{C}^{(2)} \) since \( U \) maps \( \ell^2[\nu_1 w_1] \) to \( \ell^2[\nu'_2 w_1] \). (The coupling is \( \text{(toE}(U) \otimes \text{id}) \rho \) if the previous coupling was \( \rho \).)

Then \( \rho^{(2)}, [d] (\rho_2) \) satisfy \( \mathcal{C}^{(2)} \). (The coupling is \( \text{(toE}(\text{SWAP}_{v,v'v'}) \otimes \text{id}) \rho \) if the previous coupling was \( \rho \).)

Then \( \rho^{(2)}, [d] (\rho_2) \) satisfy \( \mathcal{C}^{(2)} \). (The coupling is \( \text{tr}_{v,v'} \rho \) if the previous coupling was \( \rho \).)

As mentioned above, \( \rho^{(2)} = [\text{local } v; c] (\rho_1) \). And \( \mathcal{C}^{(2)} = B \). Thus \([\text{local } v; c] (\rho_1), [d] (\rho_2) \) satisfy \( \mathcal{B} \).

This shows \([A] \text{local } v; c \sim d \{B\} \).
The following simple case is probably easier to understand at first reading. We obtain it by setting $U, U', V, V' := id$ and weakening the postcondition.

**Proof of JointQInitEq.** By [27, Lemma 36], it is sufficient to show that for all $m_1, m_2, \psi_1, \psi_2$ with normalized $\psi_1 \otimes \psi_2 \in [A']_{m_1 m_2}$, there is a separable state $\rho'$ with $\text{tr}(\rho') = [Q \otimes e](\text{proj}(|m_1 \rangle \otimes \psi_1))$ and $\text{tr}(\rho') = [Q' \otimes e'](\text{proj}(|m_2 \rangle \otimes \psi_2))$ and $\rho'$ satisfies $B'$.

Since in the following proof, we will use the same $m_1, m_2$ throughout, for ease of notation, we will simply write $A'$ instead of $[A']_{m_1 m_2}$, and analogously for all other expressions (e.g., $B, U, V, e, e'$, etc.).

Since $(V \otimes U)R_1Q_1 \equiv_{\text{quant}} (V' \otimes U')R_2Q_2 \supseteq A'$, we have $\psi_1 \otimes \psi_2 \in (V \otimes U)R_1Q_1 \equiv_{\text{quant}} (V' \otimes U')R_2Q_2$. Since $\text{Cfa}[U, U', V, V'$ are isometries] $\supseteq A'$, we have that that $U, U', V, V'$ are isometries.

By [27, Lemma 29], this implies that there are normalized $\psi_1^{QR}, \psi_1^E, \psi_2^{QR}, \psi_2^E$ on $Q_1R_1, V_{\text{all}} \setminus Q_1R_1, Q_2R_2', V_{\text{all}} \setminus Q_2'R_2'$ such that: $\psi_1 = \psi_1^{QR} \otimes \psi_1^E$ and $\psi_2 = \psi_2^{QR} \otimes \psi_2^E$ and $(U \otimes V)\psi_1^{QR} = (U' \otimes V')\psi_2^{QR}$. Let $\{ \phi_z \}_{z \in \Sigma}$ be an orthonormal basis of $\text{im} U \cap \text{im} U'$. Then $U^*\phi_z$ are orthonormal, and $U'^*\phi_z$ are orthonormal.

Let $\psi_{12} := (\text{proj}(U^*\phi_z) \otimes id)\psi_1^{QR} \otimes \psi_1^E$ and $\psi_{22} := (\text{proj}(U'^*\phi_z) \otimes id)\psi_2^{QR} \otimes \psi_2^E$.

Note that $(\text{proj}(U^*\phi_z) \otimes id)\psi_1^{QR}$ is of the form $U^*\phi_z \otimes \psi_1^{QR}$ for some (not necessarily normalized) $\psi_1^{QR}$. And similarly $(\text{proj}(U'^*\phi_z) \otimes id)\psi_2^{QR}$ is of the form $U'^*\phi_z \otimes \psi_2^{QR}$ for some $\psi_2^{QR}$. We fix those $\psi_1^{QR}$ and $\psi_2^{QR}$.

Let

$$\psi_z := e_1 \otimes e_2 \otimes \phi_z \otimes \psi_1^E \otimes \psi_2^E \otimes \psi_2^{QR} \otimes \psi_2^E \frac{1}{\|\psi_z\|^2},$$

and

$$\rho := \sum_z \text{proj}(|m_1 \rangle \otimes |m_2 \rangle \otimes \psi_z).$$

(Note that $e_1, e_2$ are normalized vectors on $Q_1, Q_2$, respectively because we assume that the programs in the rule are well-typed.)

**Claim 3** For all $z$, $\|\psi_z\| = \|\psi_z^{QR}\|$ and $V\psi_z = U\psi_z^{QR}$.
Claim 4 Let \( \rho \). Claim 5 Thus \( (U \otimes V)(\text{proj}(U^* \phi_z) \otimes id)\psi_1^{QR} \cong (U \otimes V)(\text{proj}(U^* \phi_z) \otimes id)(U^*U \otimes id)\psi_1^{QR} \)

\[ = (\text{proj}(U^* \phi_z) \otimes id)(U \otimes V)\psi_1^{QR} \cong (\text{proj}(U^* \phi_z) \otimes id)(U \otimes V)\psi_1^{QR} \]

\[ = (U^* \otimes V^*)(\text{proj}(U^* \phi_z) \otimes id)(U^*U' \otimes id)\psi_1^{QR} \cong (U^* \otimes V')\text{proj}(U^* \phi_z) \otimes id)\psi_2^{QR} . \]

(14)

Here \( (\ast) \) uses that \( U, U' \) are isometries. And \( (\ast\ast) \) uses that \( \psi_z \in \text{im} \cap \text{im} U' \). And \( (\ast\ast\ast) \) uses that \( U, V \) are isometries. Analogously, \( \|\psi_1^R\| = \|\psi_1^{QR}\| \) (this was shown above). Then

\[ \|\psi_1^R\| \overset{\ast}{=} \|U^* \phi_z \otimes \psi_1^R\| \overset{\ast\ast}{=} \|\text{proj}(U^* \phi_z) \otimes id)\psi_1^{QR}\| \overset{\ast\ast\ast}{=} \|(U \otimes V)(\text{proj}(U^* \phi_z) \otimes id)\psi_1^{QR}\| \]

Here \( \ast \) uses that \( U^* \phi_z \) is normalized. And \( \ast\ast \) is by definition of \( \psi_1^R \). And \( \ast\ast\ast \) uses that \( U, V \) are isometries. By (14), this implies \( \|\psi_1^R\| = \|\psi_2^{QR}\| \).

Furthermore,

\[ \phi_z \otimes V\psi_1^R \overset{\ast}{=} UU^* \phi_z \otimes V\psi_1^R \overset{\ast\ast}{=} (U \otimes V)(\text{proj}(U^* \phi_z) \otimes id)\psi_1^{QR} \]

\[ \overset{\ast\ast\ast}{=} (U' \otimes V')\text{proj}(U^* \phi_z) \otimes id)\psi_2^{QR} \overset{\ast\ast\ast}{=} U'U^* \phi_z \otimes V'\psi_2^R \overset{\ast}{=} \phi_z \otimes V'\psi_2^R . \]

Here \( \ast \) holds since \( \phi_z \in \text{im} \cap \text{im} U' \). Here \( \ast\ast \) holds by definition of \( \psi_1^R, \psi_2^R \). Thus \( \phi_z \otimes V\psi_1^R = \phi_z \otimes V'\psi_2^R \). Since \( \phi_z \neq 0 \), this implies \( V\psi_1^R = V'\psi_2^R \). \( \diamond \)

Claim 4 Let \( \gamma \in \ell^2[Q] \) be orthogonal to all \( U^* \phi_z \). Then \( (\text{proj}(\gamma) \otimes id)\psi_1 = 0 \).

Let \( \gamma' \in \ell^2[Q'] \) be orthogonal to all \( U^* \phi_z \). Then \( (\text{proj}(\gamma') \otimes id)\psi_2 = 0 \).

Proof of Claim. We have \( (U \otimes V)\psi_1^{QR} \in \text{im} U \otimes \mathcal{H} \) where \( \mathcal{H} \) is the range of \( V, V' \).

We also have \( \psi_2^{QR} \in \text{im} U' \otimes \mathcal{H} \). Since \( (U \otimes V)\psi_1^{QR} = (U' \otimes V')\psi_2^{QR} \), we have \( (U \otimes V)\psi_1^{QR} \in (\text{im} U \otimes \mathcal{H}) \cap (\text{im} U' \otimes \mathcal{H}) = (\text{im} U \cap \text{im} U') \otimes \mathcal{H} \). Since \( \phi_z \) are a basis of \( \text{im} U \cap \text{im} U' \), this implies that \( (U \otimes V)\psi_1^{QR} \in \text{span}\{\phi_z\}_z \otimes \mathcal{H} \), and thus \( \psi_1^{QR} = (U^* \otimes V^*)(U \otimes V)\psi_1^{QR} \in \text{span}(U^* \phi_z) \otimes \ell^2[Q] \). Since \( \gamma \) is orthogonal to \( U^* \phi_z \), we then have \( (\text{proj}(\gamma) \otimes id)\psi_1^{QR} = 0 \). And since \( \psi_1 = \psi_1^{QR} \), \( (\text{proj}(\gamma') \otimes id)\psi_2 = 0 \).

This shows the first half of the claim. The second half is shown analogously. \( \diamond \)

Claim 5 \( \rho' \) satisfies B'.

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Proof of claim. We have that $\psi_1 \otimes \psi_2 \in A' \subseteq B$. Since $fu(B) \cap Q_1Q_2' = \emptyset$, and $\text{proj}(U^* \phi_z), \text{proj}(U'^* \phi_z)$ operate on $Q_1, Q_2'$ respectively, we have that $\psi_{1z} \otimes \psi_{2z} = (\text{proj}(U^* \phi_z) \otimes \text{id} \otimes \text{proj}(U'^* \phi_z) \otimes \text{id})(\psi_1 \otimes \psi_2) \in B$.

We thus have $\psi_{1z} \otimes \psi_{2z} = U^* \phi_z \otimes \psi_{1z}' \otimes \psi_{2z}' \otimes U'^* \phi_z \otimes \psi_{1z}' \otimes \psi_{2z}' \in B$. Since $fu(B) \cap Q_1Q_2' = \emptyset$ and $U^* \phi_z, U'^* \phi_z$ are on $Q_1, Q_2'$ and nonzero, it follows that also $\psi'_{1z} e_1 \otimes \psi_{1z}' \otimes \psi_{2z}' \otimes \psi_{2z}' = \frac{1}{\|\psi_{1z}\|} \in B$. And obviously $\psi'_{2z} \in \text{span}|e_1\rangle_{Q_1} \cap \text{span}|e_2\rangle_{Q_2'}$.

(Because the only difference is in the tensor factors in $Q_1Q_2'$.) Furthermore, by Claim 3, $V\psi_{1z}' = V'\psi'_{2z}$. Thus by [27, Lemma 29], $\psi_{1z} \otimes \psi_{2z} \in \text{span}|e_1\rangle_{Q_1} \cap \text{span}|e_2\rangle_{Q_2'}$.

Hence altogether $\psi'_2 \in B'$. Thus $\rho' = \sum_z \text{proj}(\psi'_z)$ satisfies $B'$.

Claim 6 $\text{tr}^{[1]}\rho' = [Q, e]([\text{proj}(m_1) \otimes \psi_1])$ and $\text{tr}^{[2]}\rho' = [Q', e']([\text{proj}(m_2) \otimes \psi_2])$. 

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Proof of claim. Let $\mathcal{E}(\rho) := \text{tr}_A \rho \otimes \text{proj}(e_1)$, the operation of initializing $Q$ with the state $e$. With that definition, $[Q \triangleright \epsilon](\text{proj}([m_1]) \otimes \rho) = \text{proj}([m_1]) \otimes \mathcal{E}(\rho)$.

Let $\mathcal{M}_z(\rho) := \text{proj}(U^* \phi_z) \rho \text{proj}(U^* \phi_z)^*$. Since $\{\phi_z\}_{z \in Z}$ are an orthonormal basis of $\text{im} U \cap \text{im} U'$, and $U$ is an isometry, $U^* \phi_z$, $z \in Z$ are orthonormal. We can thus extend that set to an orthonormal basis $\{U^* \phi_z\}_{z \in Z} \cup \{\gamma_y\}_{y \in Y}$. Let $\mathcal{M}_y(\rho) := \text{proj}(\gamma_y) \rho \text{proj}(\gamma_y)^*$. Then $\mathcal{M}(\rho) := \sum_y \mathcal{M}_y(\rho) + \sum_y \mathcal{M}_y(\rho)$ is a CPTPM on $Q$.

We have

$$\text{tr}^{(1)} \rho \oplus \text{tr}^{(1)} \rho = \sum_z \text{proj}([m_1]) \otimes \text{proj}(\psi_z) \equiv \sum_z \text{proj}([m_1]) \otimes \mathcal{E}(\text{proj}([m_1]) \otimes \mathcal{E}(\rho)) \equiv \mathcal{E}(\rho) \oplus \mathcal{E}(\rho)$$

Here $(\ast)$ follows because the fraction is 1 by Claim 3. And $(\ast\ast)$ uses that $||U^* \phi_z|| = 1$ since $\phi_z$ is normalized and $U$ is an isometry and $\phi_z \in \text{im} U \cap \text{im} U'$. And $(\ast\ast\ast)$ by definition of $\psi_z$ and $(\ast\ast\ast\ast)$ by definition of $\psi_z \oplus \psi_z$.

Since $\mathcal{M}$ is a CPTPM on $Q$, and by definition of $\mathcal{E}$, we have $\mathcal{E} \circ (\mathcal{M} \otimes \text{id}) = \mathcal{E}$. Then

$$\text{tr}^{(1)} \rho \oplus \text{tr}^{(1)} \rho \equiv \sum_z \text{proj}([m_1]) \otimes \mathcal{E}(\sum_z (\mathcal{M}_z \otimes \text{id})(\text{proj}(\psi_z)))$$

Here $(\ast)$ follows from Claim 4. And $(\ast\ast)$ is because $\mathcal{E} \circ (\mathcal{M} \otimes \text{id}) = \mathcal{E}$. And $(\ast\ast\ast)$ was explained after the definition of $\mathcal{E}$.

Thus we have shown $\text{tr}^{(1)} \rho = [Q \triangleright \epsilon](\text{proj}([m_1]) \otimes \psi_1)$.

$\text{tr}^{(1)} \rho = [Q \triangleright \epsilon][\text{proj}([m_2] \otimes \psi_2)]$ is shown analogously. (With the sole exception that we do not need Claim 3 to simplify the fraction in (15) because the nominator and denominator are the same term in this case.)

As mentioned in the first paragraph of this proof, Claim 5 and Claim 6 implies the conclusion of the rule. ($\rho'$ is separable by definition.)

---

**JointRemoveLocal**

$$\begin{align*}
\text{fo}(A, B) \cap Q_1 Q'_2 X_1 X'_2 = \emptyset & \quad Q := A \cap (Q_1 = q \{\bullet\} \cap (Q'_2 = q \{\bullet\})) \cap \mathcal{C}[X_1 = \bullet \land X'_2 = \bullet] \\
B' := B \cap \mathcal{C}[U, U', V, V'] \text{ are unitaries} & \quad \cap (U \otimes V) \mathcal{Q}_1 \mathcal{R}_1 \equiv_{\text{quant}} (U' \otimes V') \mathcal{Q}'_2 \mathcal{R}'_2 \\
\{A\} \text{ local } Q \times X; c \sim \text{ local } Q' \times X'; d \{B \cap (V \mathcal{R}_1 \equiv_{\text{quant}} V' \mathcal{R}'_2)\} \\
\end{align*}$$

A simpler variant of this rule (that probably illustrates the core ideas better) is the following:

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We have not implemented a tactic for either of these rules in qrhl-tool. During the case study [25], we first implemented and used a preliminary version\(^9\) of a local remove joint tactic. However, after further improvements of the equal tactic (which is essentially an application of the Adversary rule, see Section 9), we first implemented and used a preliminary version of the rule JointRemoveLocal. However, the rule JointRemoveLocal is still important because it is used to prove the improved Adversary rule which made it possible to remove the local remove joint tactic in the first place.

**Proof of JointRemoveLocal.** By rule JointQInitEq, we have

\[
\{B'\} \text{init } \tilde{Q} \sim \text{init } \tilde{Q}' \{B \cap (VR_1 \equiv_\text{quant} V'R_2')\}.
\]

(The rule needs the premise \(f(v(B) \cap \tilde{Q}_1\tilde{Q}'_2) = \emptyset\) which follows from the premises of rule JointRemoveLocal.)

With the premise \(\{A'\}c \sim d\{B'\}\) and rule Seq, we get

\[
\{A'\}c; \text{init } \tilde{Q} \sim d; \text{init } \tilde{Q}' \{B \cap (VR_1 \equiv_\text{quant} V'R_2')\}.
\]

By consecutive application of rule RemoveLocal1 and RemoveLocal2, we get

\[
\{A\} \text{local } QX; c \sim \text{local } QX; d; \text{init } \tilde{Q}' \{B \cap (VR_1 \equiv_\text{quant} V'R_2')\}.
\]

(This requires \(f(v(A,B) \cap \tilde{Q}_1\tilde{Q}'_2) = \emptyset\) which is provided in the premises of this proof.)

By Lemma 7 (iii), local \(QX; c \sim \text{local } QX; d; \text{init } \tilde{Q}' \equiv \text{local } QX; d; \text{init } \tilde{Q}' \equiv \text{local } QX; d\). (Using the premises \(Q \subseteq Q, Q' \subseteq Q'\).)

Thus

\[
\{A\} \text{local } QX; c \sim \text{local } QX; d; \{B \cap (VR_1 \equiv_\text{quant} V'R_2')\}.
\]

\(\square\)

**Proof of JointRemoveLocal0.** We have \((Q_1 =_q \bullet) \cap (Q_2 =_q \bullet) \subseteq (Q_1 \equiv_\text{quant} Q_2)\) by [27, Lemma 33]. And \((Q_1 \equiv_\text{quant} Q_2) \cap (R_1 \equiv_\text{quant} R_2) \subseteq (Q_1R_1 \equiv_\text{quant} Q_2R_2)\) since the lhs consists of states invariant under swapping \(Q_1\) and \(Q_2\) and invariant under swapping \(R_1\) and \(R_2\), while the rhs consists of states invariant doing both those swaps. And \(\text{Cla}[X_1 = \bullet \land X_1 = \bullet] \subseteq \text{Cla}[X_1 = X_2]\).

Thus

\[
A' := A \cap (Q_1 =_q \bullet) \cap (Q_2' =_q \bullet) \cap \text{Cla}[X_1 = \bullet \land X_1' = \bullet] \subseteq A \cap (Q_1R_1 \equiv_\text{quant} Q_2R_2) \cap \text{Cla}[X_1 = X_2].
\]

\(^9\)Preliminary means that it was not based on the proven rule but instead was based on intuition and thus not necessarily sound.
we get with the qRHL judgment from the premise and rule Seq:

\[ \{ A' \} c \sim d \{ B \cap (Q_1 R_1 \equiv_{quant} Q_2 R_2) \} \]

By setting \( U, U', V, V' := id, \, Q', \, \tilde{Q}, \, \tilde{Q}' := Q, \, R' := R \) in rule \textsf{JointRemoveLocal}, this implies the conclusion of rule \textsf{JointRemoveLocalQ}.

The rule \textsf{JointQInitEq} also gives us the opportunity to easily strengthen the \textsf{QrhlElimEq} rule from [28]. The rule \textsf{QrhlElimEq} allows us to derive a relationship between probabilities (which is what we eventually care about in cryptographic proofs) from a qRHL judgment. The new rule gives us more flexibility in terms of the variables that have to be involved in the (quantum) equalities in the pre-/postconditions of that qRHL judgment.

\[ \textsf{QrhlElimEqNEW} \]

\[ \begin{array}{l}
\rho \text{satisfies } A & \Rightarrow Q \supseteq fe(c) \setminus overw(c) \quad Q \supseteq fe(d) \setminus overw(d) \\
Q \supseteq fe(A) & \Rightarrow \{\text{fail}[X_1 = X_2] \cap (Q_1 \equiv_{quant} Q_2) \cap A_1 \cap A_2 \} \, e \sim d \{\text{fail}[e_1 \implies f_2] \}
\end{array} \]

\[ \text{Pr}[e : c(\rho)] \leq \text{Pr}[f : d(\rho)] \]

The same holds with \( \iff / \implies \) instead of \( \implies / \leq \).

We rewrote the tactic by \texttt{qrhl} in the \texttt{qrhl-tool} that implements the rule \textsf{QrhlElimEq} to require the more liberal variable conditions from \textsf{QrhlElimEqNEW}.

**Proof.** We first show an auxiliary claim:

**Claim 7** For any program \( c \) and expression \( e \) and finite set of quantum variables \( Q \), \( \text{Pr}[e : (c; \text{init } Q)(\rho)] = \text{Pr}[e : c(\rho)] \).

**Proof of claim.** We show that \( \text{Pr}[e : (c; \text{init } q)(\rho)] = \text{Pr}[e : c(\rho)] \). The general case \( \text{Pr}[e : (c; \text{init } Q)(\rho)] = \text{Pr}[e : c(\rho)] \) follows by induction over \( Q \).

Let \( \rho' := \llbracket c \rrbracket(\rho) \). If we write \( \rho' \) as \( \rho' := \sum_m \text{proj}(m) \otimes \rho_m^\prime \) (here \( V^d \) is the set of all classical variables), by definition of \( \text{Pr}[e : c(\rho)] \) [27, Definition 9], we have

\[ \text{Pr}[e : c(\rho)] = \sum_m \text{s.t. } \llbracket e \rrbracket = \text{true } \text{tr } \rho_m^\prime. \]

Let \( \rho'' := \llbracket c; \text{init } q \rrbracket(\rho) \). Since \init q = q \uplus_{\bullet} \bullet_\lambda by definition, \( \rho'' := \llbracket q \uplus_{\bullet} \bullet_\lambda \rrbracket(\rho) \). By the semantics of the language, \( \rho'' = \sum_m \text{proj}(m) \otimes \rho_m^\prime \) where \( \rho_m^\prime = \text{tr}_2 \rho_m^\prime \otimes \text{proj}(\bullet_\lambda) \).

Note that \( \text{tr} \rho_m^\prime = \text{tr} \rho_m^\prime \) since \( \llbracket \bullet_\lambda \rrbracket = 1 \).

Again by definition of \( \text{Pr}[[...]] \), we have \( \text{Pr}[e : (c; \text{init } q)(\rho)] = \sum_m \text{s.t. } \llbracket e \rrbracket = \text{true } \text{tr } \rho_m^\prime. \)

Since \( \text{tr} \rho_m^\prime = \text{tr} \rho_m^\prime \), it follows that \( \text{Pr}[e : (c; \text{init } q)(\rho)] = \text{Pr}[e : c(\rho)] \).

\( \square \)

Let \( \tilde{X} := X \cup fe(c)^d \cup fe(d)^d \) and \( \tilde{Q} := Q \cup fe(c)^q \cup fe(d)^q \) and \( \tilde{c} := \text{init } \tilde{Q} \setminus Q; \, c. \)

\( \tilde{d} := \text{init } \tilde{Q} \setminus Q; \, d. \)

We have

\[ \{\text{fail}[X_1 = X_2] \cap (Q_1 \equiv_{quant} Q_2) \cap A_1 \cap A_2 \} \]

\( \subseteq \{\text{fail}[X_1 = X_2] \cap (Q_1 \equiv_{quant} Q_2) \cap A_1 \cap A_2 \} \)

\( \quad (\text{since } X \subseteq \tilde{X}) \)

\( \text{init } (Q \setminus \tilde{Q}) \sim \text{init } (Q \setminus Q) \quad \{\text{fail}[X_1 = X_2] \cap (Q_1 \equiv_{quant} Q_2) \cap A_1 \cap A_2 \} \)

\( (\text{JointQInitEq0}) \)

\( c \sim d \{e_1 \implies f_1\} \)

(by assumption)

The application of rule \textsf{JointQInitEq0} uses that \( fe(A) \subseteq Q \) by assumption and therefore \( fe(A_1 \cap A_2) \cap (Q \setminus Q)_1(Q \setminus Q)_2 = \emptyset. \)

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Thus with rules \text{Conseq} and \text{Seq}, and by definition of \( \tilde{e}, \tilde{d} \), we have

\[
\{ \tilde{c}\a[\tilde{X}_1 = \tilde{X}_2] \cap (\tilde{Q}_1 \equiv_{\text{quant}} \tilde{Q}_2) \cap A_1 \cap A_2 \} \tilde{e} \sim \tilde{d}(e_1 \implies f_1) \].
\]

Furthermore, we have that \( \rho \) satisfies \( A \) (by assumption) and \( fv(\tilde{e}), fv(\tilde{d}) \subseteq \tilde{X} \tilde{Q} \) and \( fv(A)^{\text{qu}} \subseteq Q \) (by definition of \( \tilde{c}, \tilde{d}, \tilde{X}, \tilde{Q} \)). Thus, by rule \text{QRHLELIMEq} from \cite{28}, we have

\[
\Pr[e : \tilde{c}(\rho)] \leq \Pr[f : \tilde{d}(\rho)]. \tag{16}
\]

Furthermore,

\[
\tilde{c} \overset{d}{=} \text{init} (\tilde{Q} \setminus Q) \cap \text{overwr}(c); \text{init} (\tilde{Q} \setminus Q) \setminus fv(c); c
\]

\[
\overset{d}{=} \text{init} (\tilde{Q} \setminus Q) \cap \text{overwr}(c); c; \text{init} (\tilde{Q} \setminus Q) \setminus fv(c) \overset{d}{=} c; \text{init} I \tag{17}
\]

The first \( \overset{d}{=} \) follows since \( (\tilde{Q} \setminus Q) \cap \text{overwr}(c) \cup (\tilde{Q} \setminus Q) \setminus fv(c) = \tilde{Q} \setminus Q \). The second \( \overset{d}{=} \) follows by \text{Lemma 2} (and using that \( (\tilde{Q} \setminus Q) \setminus fv(c) \) and \( fv(c) \) are disjoint). The third \( \overset{d}{=} \) follows by \text{item iii} (using that \( fv(\tilde{Q} \setminus Q) \cap \text{overwr}(c)) \subseteq \text{overwr}(c) \)).

From (17), we get \( \Pr[e : \tilde{c}(\rho)] = \Pr[e : \{c; \text{init} I\}(\rho)] \). Furthermore, by \text{Claim 7}, \( \Pr[e : \{c; \text{init} I\}(\rho)] = \Pr[e : \{c; \text{init} \}(\rho)] \).

Thus \( \Pr[e : \tilde{c}(\rho)] = \Pr[e : c(\rho)] \). Analogously, we have \( \Pr[f : \tilde{d}(\rho)] = \Pr[f : d(\rho)] \).

With (16), this implies \( \Pr[e : \tilde{c}(\rho)] \leq \Pr[f : \tilde{d}(\rho)] \) and concludes the proof.

(The case using \( \iff \) instead of \( \implies \) \( \iff \) \leq \) is shown analogously, using the corresponding variant of rule \text{QRHLELIMEq}.)

\( ^{\ast} \)The latter is shown in Isabelle/HOL, \text{Helping_Lemmas.qrhlseqaux}.

8 Variable change in quantum equality

\[
\text{EqVarChange}
\]

\[
\begin{align*}
\text{Type}_{\mathbf{Q}}^\text{list} &= \text{Type}_{\mathbf{Q}}^\text{list} & \text{Type}_{\mathbf{Q}}^\text{list} &= \text{Type}_{\mathbf{Q}}^\text{list} & |\text{Type}_{\mathbf{Q}}^\text{list}| & \leq |\text{Type}_{\mathbf{Q}}^\text{list}| \text{ or } |\text{Type}_{\mathbf{Q}}^\text{list}| = \infty \\
fv(A), fv(B) \cap Q, Q_1 \equiv_{\text{quant}} Q_2 & = \emptyset & fv(c) \cap Q & = \emptyset & \text{Type}_{\mathbf{Q}}^\text{list} & = \emptyset & fv(d) \cap Q' & = \emptyset \\
\{A \cap (U_S \otimes id)S_1Q_1 \equiv_{\text{quant}} (U'_S \otimes id)S'_1Q'_1\}c \sim d\{B \cap (U_R \otimes id)R_1Q_1 \equiv_{\text{quant}} (U'_R \otimes id)R'_1Q'_1\} & \\
\{A \cap (U_S \otimes id)S_1Q_1 \equiv_{\text{quant}} (U'_S \otimes id)S'_1Q'_1\}c \sim d\{B \cap (U_R \otimes id)R_1Q_1 \equiv_{\text{quant}} (U'_R \otimes id)R'_1Q'_1\} & \\
\end{align*}
\]

The above rule is implemented in \text{qrhl-tool} by the \text{conseq qrhl} tactic, which combines the rule \text{Seq} with rule \text{EqVarChange}. That is, it allows to take a given, already proven qRHL judgment, (optionally) replaces specified variables in the quantum equality in the pre/postcondition by new variables, and then uses the resulting qRHL judgment \( X \) to solve the current subgoal \( Y \) using the \text{Seq} rule. (This means the current subgoal \( Y \) must be a qRHL judgment as well with the same programs as \( X \), and new subgoals are created to show the relationship between the pre/postconditions of \( X \) and \( Y \).)

\textbf{Proof.} Let \( A^*, B^* \) denote the pre-/postcondition of the conclusion, and \( \tilde{A}, \tilde{B} \) denote the pre-/postcondition of the premise.

Fix \( \psi_1 \otimes \psi_2 \in A^* \). We need to show that there is a separable \( \rho' \) such that \( tr_2 \rho' = \)

40
\[
\begin{align*}
\langle U_S \otimes \text{id} \rangle S_1 \tilde{Q}_1 & \equiv \text{quant} \left( \langle U_S' \otimes \text{id} \rangle S_1' \tilde{Q}_1' \right) \\
U_1 \otimes U_2 & = \langle U_S \otimes \text{id} \rangle S_1 \tilde{Q}_1 \equiv \text{quant} \left( \langle U_S' \otimes \text{id} \rangle S_1' \tilde{Q}_1' \right)
\end{align*}
\]

Figure 4: Circuit: Quantum equality swap and \( U_1 \otimes U_2 \)

\[
\begin{align*}
\langle U_S \otimes \text{id} \rangle S_1 \tilde{Q}_1 & \equiv \text{quant} \left( \langle U_S' \otimes \text{id} \rangle S_1' \tilde{Q}_1' \right) \\
U_1 \otimes U_2 & = \langle U_S \otimes \text{id} \rangle S_1 \tilde{Q}_1 \equiv \text{quant} \left( \langle U_S' \otimes \text{id} \rangle S_1' \tilde{Q}_1' \right)
\end{align*}
\]

Figure 5: Circuit: \( U_1 \otimes U_2 \) and quantum equality swap

\[
\begin{align*}
|c] (\text{proj}(\psi_1)) \text{ and } \text{tr}_1 \rho' & = [d] (\text{proj}(\psi_2)) \text{ and } \text{supp} \rho' \subseteq B^*. \\
\text{Let } S_1 := \text{supp} \text{tr}^\alpha \text{proj}(\psi_1) \subseteq \ell^2[Q] \text{ and } S_2 := \text{supp} \text{tr}^\alpha \text{proj}(\psi_1) \subseteq \ell^2[Q'] \text{ and } S := S_1 + S_2. \text{(} S_1 + S_2 \text{ is meaningful because } |\text{Type}^{\text{list}}_Q| = |\text{Type}^{\text{list}}_{\tilde{Q}}| \text{ and hence } \ell^2[Q] = \ell^2[Q']. \text{) Since every density operator has countably dimensional support, dim } S_1, \text{ dim } S_2 \leq N_0 \text{ and thus dim } S \leq N_0. \text{ Furthermore, dim } S \leq \dim \ell^2[Q] \leq |\text{Type}^{\text{list}}_Q|. \text{ Since } |\text{Type}^{\text{list}}_Q| \leq |\text{Type}^{\text{list}}_{\tilde{Q}}| \text{ or } N_0 \leq |\text{Type}^{\text{list}}_{\tilde{Q}}| \text{ by assumption of the rule, we have dim } S \leq |\text{Type}^{\text{list}}_{\tilde{Q}}|. \text{ (Dimensions are Hilbert space dimensions, not vector space dimensions.)}
\end{align*}
\]

Let \((\beta_i)_{i \in I}\) be an orthonormal basis of \( S \), and let \((\beta_i)_{i \in B}\) be an extension of that basis to the whole space \( \ell^2[Q] \). We have \(|I| = \dim S \leq |\text{Type}^{\text{list}}_Q| \). Thus there exists an injection \( \iota : I \rightarrow |\text{Type}^{\text{list}}_Q| \). Fix such an \( \iota \).

Let \( q \) be a fresh variable (i.e., \( q \notin \text{fv}(c, d, A^*, B^*, \tilde{A}, \tilde{B}) \)) with \( |\text{Type}^{\text{list}}_Q| \). Define
the bounded operator $U : \ell^2[Q\hat{Q}q] \to \ell^2[Q\hat{Q}q]$ with
\[
U(\beta_a \otimes |b\rangle_q \otimes |c\rangle_{q'^*}) = \begin{cases} 
\beta_0 \otimes |\iota(a)\rangle_q \otimes |b\rangle_a & (a \in I, \ b \in \text{Type}_Q^\text{list}) \\
0 & (a \notin I, \ b \in \text{Type}_Q^\text{list}).
\end{cases}
\]
(Here $0$ in the index of $\beta_0$ refers to an arbitrary but fixed element of $I$.) Note that $U$ is also an operator $\ell^2[Q\hat{Q}q] \to \ell^2[Q\hat{Q}q]$. In slight abuse of notation, we will also write $U$ for $U \otimes id_{Q\hat{Q}q'^*}$ or $U \otimes id_{Q\hat{Q}q'^*}$. We write $U_1, U_2$ if $U$ is applied to the left/right memory, respectively.

Claim 8 \(U_1\psi_1 \otimes U_2\psi_2 \in \bar{A}\).
**Proof of claim.** Since $\psi_1 \otimes \psi_2 \in A^*$, we have $\psi_1 \otimes \psi_2 \in A$. Since $fv(A) \cap Q, Q_1, Q_2, Q_3, Q_4, Q_5 = \emptyset$ (by assumption of the rule ad definition of $q$), and $U_1, U_2$ operate on $Q, Q_1, Q_2, Q_3, Q_4, Q_5$, we have $U_1 \psi_1 \otimes U_2 \psi_2 \in A$.

Since $\psi_1 \otimes \psi_2 \in A^*$, we have $\psi_1 \otimes \psi_2 \in (U_S \otimes id)S_1 Q, Q_1 \equiv_{\text{quant}} (U_S \otimes id)S_2 Q_2$. By definition of the quantum equality, this means that $\psi_1 \otimes \psi_2$ is invariant under the quantum circuit depicted in the black (left) part of Figure 4.

Furthermore, the blue (right) part of Figure 4 is an application of $U_1 \otimes U_2$ if we define $V, W$ as follows: $V \beta_a := |a\rangle$ for $a \in T$, $V \beta_a := 0$ otherwise. $W (|b\rangle \otimes |c\rangle) := |b\rangle |c\rangle$.

Thus the result of applying Figure 4 to $\psi_1 \otimes \psi_2$ is $U_1 \psi_1 \otimes U_2 \psi_2$.

Furthermore, the blue (left) part of Figure 5 is $U_1 \otimes U_2$. And by definition of quantum equality, a state is in $(U_S \otimes id)S_1 Q, Q_1 \equiv_{\text{quant}} (U_S \otimes id)S_2 Q_2$ iff it is invariant under the quantum (right) part of Figure 5.

Thus, $U_1 \psi_1 \otimes U_2 \psi_2 \in (U_S \otimes id)S_1 Q, Q_1 \equiv_{\text{quant}} (U_S \otimes id)S_2 Q_2$ iff the result of applying Figure 5 to $\psi_1 \otimes \psi_2$ is $U_1 \psi_1 \otimes U_2 \psi_2$.

Furthermore, note that the circuits in Figures 4 and 5 compute the same function (they are identical as networks of linear operations). Since the result of Figure 4 is $U_1 \psi_1 \otimes U_2 \psi_2$, so is that of Figure 5. Thus $U_1 \psi_1 \otimes U_2 \psi_2 \in (U_S \otimes id)S_1 Q, Q_1 \equiv_{\text{quant}} (U_S \otimes id)S_2 Q_2$ and hence $U_1 \psi_1 \otimes U_2 \psi_2 \in A$.

---

"Strictly speaking, we only require $|\text{Type}_q| = |\text{Type}'_{\mathcal{Q}}|$, then we can identify $\text{Type}_q$ with $(\text{Type}'_{\mathcal{Q}})^*$.

Such a $q$ always exists for the following reason: If $\text{Type}'_{\mathcal{Q}}$ is infinite, then $|\text{Type}'_{\mathcal{Q}}| = |\text{Type}_{q'}|$ for some $q' \in \mathcal{Q}$.

And $|\text{Type}'_{\mathcal{Q}}| = |\text{Type}_{\mathcal{Q}}|$. Thus we need $q$ with $\text{Type}_q = \text{Type}_{q'}$. Since we assume that there are infinitely many variables of each type (see preliminaries), and since $fe(c, d, A^*, B^*, \tilde{A}, \tilde{B})$ is finite (see preliminaries), $q$ exists.

If $\text{Type}'_{\mathcal{Q}}$ is finite, then $|\text{Type}'_{\mathcal{Q}}| = |\text{Type}_{\mathcal{Q}}|$. Since we assume that there is a quantum variable of cardinality $\aleph_0$ (see preliminaries), and of each type there are infinitely variables, and $fe(c, d, A^*, B^*, \tilde{A}, \tilde{B})$ is finite, $q$ exists.

Since $\{A\} c \sim d (B)$ by assumption, Claim 8 implies that there is a separable state $\rho''$ such that $tr^{(1)} \rho'' = [c](\text{proj}(U_1 \psi_1))$ and $tr^{(2)} \rho'' = [d](\text{proj}(U_2 \psi_2))$ and $\text{supp} \rho'' \subseteq \tilde{B}$. Let $\rho' := \text{toE}(U_1^* \otimes U_2^*)(\rho'')$. (Here $*$ denotes an arbitrary but fixed element of $\text{Type}_{\mathcal{Q}}$.)

**Claim 9** $\rho'$ is separable.

**Proof of claim.** $\rho''$ is separable by definition. Thus $\rho' = \text{toE}(U_1^* \otimes U_2^*)(\rho'')$ is separable.

---

**Claim 10** $tr^{(1)} \rho' = [c](\text{proj}(\psi_1))$ and $tr^{(2)} \rho' = [d](\text{proj}(\psi_2))$.\"
Proof of claim. Since $f_U(c) \cap \mathbb{QQ}q = \emptyset$ (by assumption of the rule ad definition of $q$), $[c]$ and $\text{toE}(U_1)$ commute. Thus
\[ \text{tr}^{[i]} \rho'' = [c] \circ \text{toE}(U_1)(\text{proj}(\psi_1)) = \text{toE}(U_1) \circ [c](\text{proj}(\psi_1)). \] (18)
Thus $\text{supp} \text{tr}^{[i]} \rho'' \subseteq \text{im} U_1$. Thus $\text{supp} \rho'' \subseteq \text{im} U_1 \otimes \ell^2(\mathbb{V}^{\text{all}}_2)$.

Analogously, $\text{supp} \rho'' \subseteq \text{im} \ell^2(\mathbb{V}^{\text{all}}_1) \otimes \text{im} U_2$.
Let $\tilde{\rho} := \text{toE}(id \otimes U_2') \rho''$. Since $\text{supp} \rho'' \subseteq \ell^2(\mathbb{V}^{\text{all}}_1) \otimes \text{im} U_2$, and $U_2'$ is an isometry on $\text{im} U_2$ (since $U_2'$ is an isometry), $\text{tr}^{[i]} \tilde{\rho} = \text{tr}^{[i]} \rho''$. Then
\[ \text{tr}^{[i]} \rho' = \text{tr}^{[i]} \text{toE}(U_1^* \otimes id)(\tilde{\rho}) = \text{toE}(U_1^*) \circ \text{tr}^{[i]} \tilde{\rho} = \text{toE}(U_1^*) \circ \text{tr}^{[i]} \rho'' \]
$\overset{(*)}{=} \text{toE}(U_1^*) \circ \text{toE}(U_1) \circ [c](\text{proj}(\psi_1)) \overset{(*)}{=} [c](\text{proj}(\psi_1))$.

Here $(*)$ uses that $U_1$ is an isometry.

$U_2'$, restricted to $\ell^2(\mathbb{V}^{\text{all}}_1 \otimes \text{span} |\psi\rangle_{a_2})$, is an isometry. Thus $\text{tr}^{[i]} \tilde{\rho} = \text{tr}^{[i]} \rho'' \otimes \text{proj}(\text{span} |\psi\rangle_{a_2})$. By definition of $\rho''$, we have $\text{tr}^{[i]} \rho'' = [c] \text{proj}(U_1 \psi_1)$. Thus $\text{tr}^{[i]} \tilde{\rho} = [c] \text{proj}(U_1 \psi_1) \otimes \text{proj}(\text{span} |\psi\rangle_{a_2})$.

$\text{tr}^{[i]} \rho' = [d](\text{proj}(\psi_2))$ is shown analogously. $\diamond$

Claim 11 $(U_1^* \otimes U_2^*) \hat{B} \subseteq B^*$.

Proof of claim. Fix $\psi \in \hat{B}$. Then $\psi \in B$. Since $f_U(B) \cap \mathbb{QQ}Q_1 \mathbb{Q} Q_2 = \emptyset$ (by assumption of the rule ad definition of $q$), $U_1, U_2$ operate on $Q_1 Q_2 Q_1 q_1 Q_2 q_1 q_2$, we have $(U_1^* \otimes U_2^*) \psi \in B$.

Since $\psi \in B$, we have $\psi \in (U_R \otimes id)R_1 \mathbb{Q}_1 \equiv_{\text{quant}} (U_R' \otimes id)R_2 \mathbb{Q}_2$. By definition of the quantum equality, this means that $\psi$ is invariant under the quantum circuit depicted in the black (left) part of Figure 6.

Furthermore, the blue (right) part of Figure 6 is an application of $U_1^* \otimes U_2^*$ if we define $V, W$ as in the proof of Claim 8.

Thus the result of applying Figure 6 to $\psi$ is $(U_1^* \otimes U_2^*) \psi$.

Furthermore, the blue (left) part of Figure 5 is $U_1^* \otimes U_2^*$. And by definition of quantum equality, a state is in $(U_R \otimes id)R_1 Q_1 \equiv_{\text{quant}} (U_R' \otimes id)R_2 Q_2$ if it is invariant under the black (right) part of Figure 7.

Thus, $(U_1^* \otimes U_2^*) \psi \in (U_R \otimes id)R_1 Q_1 \equiv_{\text{quant}} (U_R' \otimes id)R_2 Q_2$ if it is invariant under the blue (right) part of Figure 7.

Thus, $(U_1^* \otimes U_2^*) \psi \in (U_R \otimes id)R_1 Q_1 \equiv_{\text{quant}} (U_R' \otimes id)R_2 Q_2$ if it is invariant under the blue (right) part of Figure 7. Thus $(U_1^* \otimes U_2^*) \psi \in (U_R \otimes id)R_1 Q_1 \equiv_{\text{quant}} (U_R' \otimes id)R_2 Q_2$ and hence $(U_1^* \otimes U_2^*) \psi \in B^*$. $\diamond$

Claim 12 $\text{supp} \rho' \subseteq B^*$.  

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9 Adversary rule

Auxiliary notation: \( \equiv \) V stands for \( V^\equiv_1 \equiv V^\equiv_2 \cap \text{Clau}[V^\equiv_1 = V^\equiv_2] \).

\[\begin{array}{l}
\text{If } r \text{ is a predicate } s_i, s'_i \text{ are programs} \\
\text{C is a multi-hole context } V_{in}, V_{mid}, V_{out} \text{ are finite sets of variables} \\
Q_{aux} \text{ is a quantum variable} \\
\left[\text{Type}_{Q_{aux}}\right] = \infty \\
Q_{aux} \notin V_{mid} \\
\exists i. Q_{aux} \notin fv(s_i) \\
\forall i. Q_{aux} \notin fv(s'_i) \\
(V_{out} \setminus V_{in}) \cap V_R = \emptyset \\
V_{mid} \cap V_R \subseteq V_{in} \cup \text{covered}(C) \\
\forall i. V_{mid} \cap (fv(s_i) \cup fv(s'_i)) \subseteq V_{in} \cup \text{covered}(C) \\
V_{R} \cap \text{inner}(C) = \emptyset \\
V_{R} \cap \text{written}(C) = \emptyset \\
\forall i. \{ R \cap \equiv V_{mid} \} s_i \sim s'_i \{ R \cap \equiv V_{mid} \} \\
\{ R \cap \equiv V_{in} \} C[s_1, \ldots, s_n] \sim \{ R \cap \equiv V_{out} \} C[s'_1, \ldots, s'_n] \\
\end{array}\]

This is shown in Isabelle/HOL, as adversary_rule in theory Adversary_Rule.thy. See Section 1.1 for remarks about our Isabelle/HOL development.

We have implemented this rule in the \texttt{equal} tactic in qrhl-tool.\footnote{The tactic is called \texttt{equal} because in its most basic form, it reasons about two programs that are identical (e.g., the same adversary invocation in the left and right program). In more advanced situations, the two programs can differ but the idea is still that this tactic can be applied when the last statement on the left/right side are “mostly equal”.} The tactic allows to apply this rule to the last statement on the left/right side (or suffix consisting of several statements, if the user chooses). The sets \( V_{in}, V_{mid}, V_{out} \) can be used specified but the tactic makes a best effort attempt to find the minimum sets \( V_{in}, V_{mid}, V_{out} \) that make all the premises of the rule true. The tactic also automatically rewrites the postcondition into the form \( R \cap \equiv V_{out} \) in a way that makes \( R \) as weak as possible. For more details about the \texttt{equal} tactic, see the manual of [23].

In many situations, the tactic makes it very easy to apply the \texttt{adversary} rule. A manual application would be very inconvenient because there are many technical conditions that need to be checked. Yet, in our case study [25], in many situations no arguments to \texttt{equal} are needed at all, and when they were needed, it was only to specify the quantum variables in \( V_{mid} \) to control which variables occur (and in what order) in the subgoals \( \{ R \cap \equiv V_{mid} \} s_i \sim s'_i \{ R \cap \equiv V_{mid} \} \) for the mismatches \( s_i, s'_i \).

---

Proof of claim. By definition of \( \rho'' \), we have \( \text{supp} \rho'' \subseteq \hat{B} \). Furthermore, \( \rho = \text{toE}(U_1 \otimes U_2)(\rho'') \) by definition. Thus

\[\begin{array}{l}
\text{supp} \rho' \subseteq (U_1 \otimes U_2)\text{supp} \rho'' \subseteq (U_1 \otimes U_2)\hat{B}^{(*)} \subseteq B^*. \\
\end{array}\]

Here \( (*) \) is by Claim 11.

Since \( \psi_1 \otimes \psi_2 \in A^* \) was arbitrary, from Claims 9, 10 and 12, we immediately get \( \{ A^* \} c \sim d \{ B^* \} \). \( \square \)
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Symbol index

$S^\perp$ Orthogonal complement of subspace $S$  

$\text{supp } M$ Support of an operator $M$  

$\text{toE}(U)$ Superoperator corresponding to $U$. I.e. $\text{toE}(U)(\rho) := U\rho U^\dagger$.  

A quantum program variable
Probability that e holds after running c on initial state ρ
List/set of program variables
Default value for variable v
Density operator with default value for variable v
Unitary swapping v, v’
Program: Initialize v with default value
Probability that e holds after running c on initial state ρ
List/set of program variables
Default value for variable v
Density operator with default value for variable v
Unitary swapping v, v’
Program: Initialize v with default value
Function update, i.e., (f(x := y))(x) = y
i-th hole in a context
Set of all program variables that can be used in the execution of a program
Variables written by c
Inner variables of context C
Program: assigns expression e to x
Support of distribution μ
Truth value “true”
Truth value “false”
Lifts operator or subspace to variables Q
A superoperator
Hilbert space with basis Type_v
Tensor product of vectors/operators A and B
Restrict state/distribution ρ to the case e = true holds
A program variable (classical or quantum)
A classical program variable
Apply variable substitution σ to expression e
Substitute f for variable x in e
Identity over variables V
Identity
Equality of quantum variables X_1 and X_2
Projector onto x. More precisely, xx^∗
Absolute value of x / cardinality of set x
Classical variables in V
Quantum variables in V
Type of variable v
Free variables in an expression e (or program)
Type of a list V of variables
Type of a set V of variables
Denotation of a classical expression e, evaluated on classical memory m
Type of an expression e
Superoperator E with variable v made local
Span, smallest subspace containing A
| Symbol | Description |
|--------|-------------|
| A, B, C | (Quantum) predicates |
| noconflict(σ,c) | Renaming c with σ leads to no free variable conflict |
| c,σ | Full substitution (incl. local variables) |
| ċ|a[e] | Classical predicate meaning e = true |
| c, d | Denotational equivalence |
| V =_ψψ | Predicate: V is in state ψ |
| overw(c) | Overwritten variables of c |
| covered(C) | Covered variables of context C |
| Q, R, S | List/set of quantum program variables |
| X, Y | List/set of classical program variables |
| [c] | Denotation of a program c |
| c, d | A program |
| if c then c₁ else c₂ | Statement: If (conditional) |
| skip | Program that does nothing |
| x ← e | Statement: Sample x according to distribution e |
| while e do c | Statement: While loop |
| apply q₁...qₙ to U | Statement: Apply unitary/isometry U to quantum registers q₁...qₙ |
| q₁...qₙ, e | Statement: Initialize q₁,...,qₙ with quantum state e |
| ℓ²(B) | Hilbert space with basis indexed by B |
| x ← measure q₁...qₙ with e | Statement: Measure quantum variables q₁...qₙ with measurement e |
| | Basis vector in Hilbert space ℓ²[V] |
| A* | Adjoint of the operator A |
| tr M | Trace of matrix/operator M |
| ||x|| | ℓ²-norm of vector x, or operator-norm |
| dom f | Domain of f |
| im A | Image of A |
| tr²(V)(ρ) | Partial trace, keeping variables V, dropping variables W |
| marginal₁(μ) | i-th marginal distribution of μ |
| ĉ, v | Superoperator initializing v |
| {F}c ~ c'{G} | Quantum relational Hoare judgment |
| A ⊢ ψ | Part of A containing ψ |
| local V; c | Program: c with local variables V |
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