Formalization of Metatheory of the Quipper Quantum Programming Language in a Linear Logic

Mohamed Yousri Mahmoud · Amy P. Felty

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Abstract We develop a linear logical framework within the Hybrid system and use it to reason about the type system of a quantum lambda calculus. In particular, we consider a practical version of the calculus called Proto-Quipper, which contains the core of Quipper. Quipper is a new quantum programming language under active development and recently has gained much popularity among the quantum computing communities. Hybrid is a system that is designed to support the use of higher-order abstract syntax (HOAS) for representing and reasoning about formal systems implemented in the Coq Proof Assistant. In this work, we extend the system with a linear specification logic (SL) in order to reason about the linear type system of Quipper. To this end, we formalize the semantics of Proto-Quipper by encoding the typing and evaluation rules in the SL, and prove type soundness.

Keywords Proto-Quipper \cdot Quantum Programming Languages \cdot Linear Logic \cdot Hybrid \cdot Higher-Order Abstract Syntax \cdot Coq

1 Introduction

Quipper is a functional programming language designed for implementing quantum algorithms [10]. The mathematical foundations of the Proto-Quipper fragment, which retains much of the important expressive power of the full language, is developed in [27]. As the authors themselves have noted [28], there is a great deal of subtlety in the definitions of the syntax and semantics, and many details were fine-tuned during the process of proving the type soundness result. This process certainly would have benefited from formalization and the ability to recheck proofs after each change in the definitions. Quipper is a relatively new language, and additional metatheory will be proved as it

School of Electrical Engineering and Computer Science, University of Ottawa, Ottawa, Canada

 $\hbox{E-mail: myousri@uottawa.ca, afelty@uottawa.ca}\\$

is developed. Providing an environment within a proof assistant that allows the developers to simultaneously develop and formalize this metatheory is a central goal of our work.

The Hybrid system [7] provides support for reasoning about object languages (OLs) such as programming languages and other formal systems using higher-order abstract syntax (HOAS), sometimes referred to as "lambda-tree syntax" [22,23]. It is implemented as a two-level system, an approach first introduced in the $FO\lambda^{\Delta I\!N}$ logic [18]. Using this approach, the specification of the semantics of the OL and the meta-level reasoning about it are done within a single system but at different levels. In the case of Hybrid, an intermediate level is introduced by inductively defining a specification logic (SL) in Coq, and OL judgments are encoded in the SL. The version of Hybrid we use here is implemented as two distinct libraries in the Coq Proof Assistant. The first we adopt without change, while the development of a new version of the second is part of the contributions of this work.

The first Hybrid library provides support for expressing the syntax of OLs. Using HOAS, binding constructs of the OL are encoded using lambda abstraction in Coq. For instance, for Proto-Quipper, type qexp will represent terms or programs, and App of type qexp \rightarrow qexp \rightarrow qexp and Fun of type $(\underline{qexp} \rightarrow qexp) \rightarrow qexp$ will represent application and abstraction, respectively, of the linear lambda calculus, which forms the core of the Proto-Quipper language. Lambda abstraction in Proto-Quipper is a binder because the name of a variable is bound in the body of the abstraction. For example, the term $\lambda x.\lambda y.xy$ can be encoded as (Fun $(\lambda x.\text{Fun }(\lambda y.(\text{App }x\ y)))$). Note that qexp cannot be defined inductively because of the (underlined) negative occurrence of qexp in the type of Fun. Hybrid provides an underlying low-level de Bruijn representation of terms to which the HOAS representation can be mapped internally; the user works directly with the higher level HOAS representation.

Using such a representation, α -conversion at the meta-level directly represents bound variable renaming at the object-level, and meta-level β -conversion can be used to directly implement object-level substitution. As a consequence, we avoid the need to develop large libraries of lemmas devoted to operations dealing with variables, such as capture-avoiding substitution, renaming, and fresh name generation. In proof developments that use a first-order syntax, such libraries are often significantly larger than the formalization of the main metatheory results.

The second Hybrid library defines the SL and provides support for encoding OL judgments and inference rules, and for reasoning about them. The need for different levels arises in Hybrid because there are OL judgments that cannot be encoded as inductive propositions in Coq. As an example, we consider assigning simple types to lambda terms. The standard rule is as follows:

$$\frac{\Gamma, x : T \vdash t : T'}{\Gamma \vdash \lambda x . t : T \to T'}$$

Let qtp be the type of OL types, and let arr be a constant of type qtp \rightarrow qtp \rightarrow qtp for constructing arrow types. Let typeof be a predicate expressing

the relation between a term and its type. If we consider the HOAS encoding of the above rule, using for example, the techniques introduced in the logical framework LF [11], we can encode the above rule as the following formula:

```
\begin{array}{l} \forall T,T': \texttt{qtp.} \ \forall t: \texttt{qexp} \rightarrow \texttt{qexp.} \\ (\forall x: \texttt{qexp.} \ \texttt{typeof} \ x \ T \rightarrow \texttt{typeof} \ (t \ x) \ T') \rightarrow \\ \texttt{typeof} \ (\overline{\texttt{Fun}} \ t) \ (\texttt{arr} \ T \ T') \end{array}
```

The second line contains a formula with embedded implication and universal quantification (known as hypothetical and parametric judgments), in particular universal quantification over variable x of type qexp and an internal assumption (underlined) about the type of this x. We note that the typeof predicate cannot be expressed inductively because this underlined occurrence is negative. A two-level system solves this problem by encoding OL predicates inside the SL, where negative occurrences are allowed. We will see how this is done in Section 5.1, where we encode rules such as the typing rule for lambda abstraction in the quantum lambda calculus.

The linear SL we implement here is an extension of the ordered linear SL implemented in [7] and the ordered and linear SLs presented in [17]. We extend and adapt this previous work to the much larger case study considered here, and we design the new SL to be general so that it can be adopted directly for reasoning about a variety of other OLs with linear features.

We formalize the key property of type soundness (also called subject reduction) of Proto-Quipper, which requires several important lemmas about context subtyping.

The issue of the adequacy of HOAS representations is important (see [11]), which here means that we must prove that the encoding in Hybrid does indeed represent the intended language. The work described here includes extending previous work on adequacy to our setting, where both the OL (Proto-Quipper) and the SL (a linear logic) are more complex than those considered previously.

We begin in the next section with background material on Proto-Quipper. Then in Section 3, we present the encoding of types and of the subtyping relation in Coq. Proto-Quipper types and subtyping can be encoded directly using inductive types. There are no binders and no substitution. One of the strengths of Hybrid as implemented in Coq is that it is straightforward to combine such direct encodings of OL syntax with encodings that use the HOAS and SL facilities provided by Hybrid. In Section 4, we present the Hybrid system including both background information on the first Coq library, as well as our new implementation of the second library, which encodes our linear SL in Coq and develops some important general meta-theoretic properties that help in reasoning about OLs.

The encoding of Proto-Quipper terms and of the typing rules, along with some properties about them appear in Section 5. The encoding of reduction rules is presented in Section 6, along with the statement of type soundness and a discussion of its formal proof.

We discuss adequacy of our encoding in Section 7, and finally, we conclude and discuss related and future work in Section 8.

The files of our formalization are publicly available [15].

2 Proto-Quipper

We give a brief background of the Proto-Quipper language, focusing on the aspects that are required for understanding the formalization in later sections. Proto-Quipper is based on the quantum lambda calculus and focuses on Quipper's abilities to generate and manipulate quantum circuits [27]. The types and terms of Proto-Quipper are defined by the following grammars:

```
\begin{array}{ll} T,U & ::= & \mathbf{qubit} \mid 1 \mid T \otimes U \\ A,B & ::= & \mathbf{qubit} \mid 1 \mid !1 \mid \mathbf{bool} \mid ! \, \mathbf{bool} \mid A \otimes B \mid !(A \otimes B) \mid \\ & A \multimap B \mid !(A \multimap B) \mid \mathrm{Circ}(T,U) \mid !(\mathrm{Circ}(T,U)) \\ t & ::= & q \mid * \mid \langle t_1,t_2 \rangle \\ a,b,c & ::= & x \mid q \mid (t,C,a) \mid \mathsf{True} \mid \mathsf{False} \mid \langle a,b \rangle \mid * \mid ab \mid \lambda x.a \mid \\ & rev \mid unbox \mid box^T \mid \mathsf{if} \ a \ \mathsf{then} \ b \ \mathsf{else} \ c \mid \\ & \mathsf{let} \ * = & a \ \mathsf{in} \ b \mid \mathsf{let} \ \langle x,y \rangle = a \ \mathsf{in} \ b \end{array}
```

Proto-Quipper distinguishes between quantum data types (T, U) and types (A, B) where the former is a subset of the latter, and similarly between quantum data terms (t) and terms (a, b, c). Here x and y are term variables from a set \mathcal{V} , q is a quantum variable from a set \mathcal{Q} , and \mathcal{C} is a circuit constant from a set \mathcal{C} . The sets \mathcal{V} , \mathcal{Q} , and \mathcal{C} are all assumed to be countably infinite.

Most types and term constructs come directly from the quantum lambda calculus, e.g., [29]. The type $\mathrm{Circ}(T_1,T_2)$ represents the set of all circuits having an input interface of type T_1 and an output interface of type T_2 . A circuit constant C represents a low-level quantum circuit, and a term (t,C,a) represents a circuit as Proto-Quipper data, where t is a structure representing a finite set of inputs to C, and similarly a represents a finite set of outputs. In Proto-Quipper, it is assumed that two functions exists, In and Out, from C to the set of all subsets of Q, where In(C) and Out(C) are a superset of the set of input and output quantum variables, respectively, of circuit C. The terms rev, unbox, and box^T represent functions on circuits. We refer the reader to [27] for further description of these types and terms.

In quantum computing, variable cloning is prohibited. This features is reflected in Proto-Quipper by using the modal operator !, where variables having type !A are called duplicable and can be cloned whereas variables of types that do not follow this pattern are called linear and cannot be cloned or copied. Note that instead of introducing a general ! operator on types, we restrict it to prohibit more than one consecutive occurrence of the bang operator !. This presentation of types differs from the one in [27].

¹ In general, when we stray from the original presentation, our intention is to simplify formalization, and we only do so when there is a clear equivalence to the original. In this case, we simplify the formalization of the subtyping relation without changing the semantics of types. As we will discuss in the next section, making this kind of change also led to the discovery of a small mistake in the original presentation.

 \dagger Note that the last two rules have the proviso that A and B do not have a leading!.

Fig. 1 Subtyping rules for Proto-Quipper

The use of the bang operator ! introduces a subtyping relation among types: A variable of type !A obviously is also of type A. The subtyping rules of Proto-Quipper are shown in Figure 1. The subtyping relation <: is the smallest relation on types satisfying these rules.

The Proto-Quipper typing judgment has the form Φ ; $Q \vdash a : A$. In this sequent, Φ is a finite set of typing declarations of the form x:A where x is a variable and A is a type (A may have the form !C or not). In the presentation of the rules, Φ always appears in two parts Φ' ,! Ψ where the types in the latter all follow the pattern ! A, while those in the former never contain a leading! Q is a quantum context containing a finite set of quantum variables, typically the free quantum variables in a. Also a is a term and A is a type. The typing rules are shown in Figure 2. We write \cdot to represent an empty context. The ";" is used to separate the typing context from the quantum context whereas the "," is used to append two contexts. The rules containing !ⁿ abbreviate two distinct rules, one where n=0, i.e., there is no leading!, and one where n = 1. These rules are taken from [27], with some modifications that do not change the semantics. For example, when $!^n$ appears in the rules there, n can be any natural number. The restriction here takes into account our modification to the syntax of types discussed above. Also, the ax_x and ax_c rules replace a single rule for subtyping in [27]. Here, we give an initial rule for term variables (ax_x) , similar to the one for quantum variables (ax_q) . When using LF-style hypothetical and parametric judgments, such rules for variables are implicit; they do not appear in the encoding of the inference rules in the SL. In general, we avoid explicit treatment of variables whenever possible to get the full advantage of HOAS encodings. In addition, the subtyping rule in [27] is restricted only to term variables. Again to avoid specific reasoning about variables, our ax_c rule is valid for any valid expression of Proto-Quipper.

In the (cst) rule c ranges over the set $\{box, unbox, rev\}$, and we write box(T, U) as $box^{T}(U)$ to make explicit that the constant box is always annotated with its type (see the grammar).

 A_{box^T} , A_{unbox} , and A_{rev} are defined as follows:

$$\begin{array}{l} A_{box^T}(U) := !(T \multimap U) \multimap !\operatorname{Circ}(T,U) \\ A_{unbox}(T,U) := \operatorname{Circ}(T,U) \multimap !(T \multimap U) \\ A_{rev}(T,U) := \operatorname{Circ}(T,U) \multimap !\operatorname{Circ}(U,T) \end{array}$$

Fig. 2 Typing rules for Proto-Quipper

3 Proto-Quipper Types

In the previous section, the types supported in Proto-Quipper were presented using a context free grammar, where there are two classes of types. Here, we consider a single "universal" class of types, and then define predicates that discriminate between the two classes. We start the formalization of the Proto-Quipper types (file ProtoQuipperTypes.v) by defining an inductive type of the universal class:

```
Inductive qtp: Type :=
  qubit: qtp | one: qtp | bool: qtp
| tensor: qtp -> qtp -> qtp | arrow: qtp -> qtp -> qtp
| circ: qtp -> qtp -> qtp | bang: qtp -> qtp.
```

Certainly, the above definition does not model Proto-Quipper types. For instance, it does allow for the parameters of the circuit type constructor to be of the general class, whereas the argument expressions are supposed to be of the quantum data type. Accordingly, we define the inductive predicate valid that captures the notion of quantum data types (grammar T, U):

```
Inductive valid: qtp -> Prop :=
  Qubit: valid qubit
```

```
| One: valid one
| Tensor: forall A1 A2, valid A1 -> valid A2 ->
  valid (tensor A1 A2).
Then, we define the general validT predicate to identify the general types
(grammar A, B):
Inductive validT: qtp -> Prop :=
 vQubit: validT qubit
| bQubit: validT (bang qubit)
| vTensor: forall A B, validT A -> validT B ->
 validT (tensor A B)
| bTensor: forall A B, validT A -> validT B ->
 validT (bang (tensor A B))
| vCirc: forall A B, valid A -> valid B ->
 validT (circ A B)
| bCirc: forall A B, valid A -> valid B ->
  validT (bang (circ A B)).
```

In longer definitions such as this one, we often omit parts when it is clear how to fill in the complete idea of the definition. We have proved that (valid A) implies (valid A), confirming that class T, U is a subclass of A, B.

The last step in the formalization of the Proto-Quipper types is the development of the subtyping relation. The following inductive proposition directly encodes the rules of Figure 1.

```
Inductive Subtyping: qtp -> qtp -> Prop :=
   QubitSub: Subtyping qubit qubit
| OneSub: Subtyping one one
:
| CircSub: forall A1 A2 B1 B2,
   Subtyping A2 A1 -> Subtyping B1 B2 ->
   validT (circ A1 B1) -> validT (circ A2 B2)->
   Subtyping (circ A1 B1) (circ A2 B2)
| BangSub1: forall A B, Subtyping A B ->
   validT (bang A) -> Subtyping (bang A) B
| BangSub2: forall A B, Subtyping A B ->
   validT (bang A) -> Subtyping (bang A) (bang B).
```

The main difference between this definition and the original subtyping rules in [27] are the last two rules. As mentioned in Section 2, they are stated so that they prevent consecutive applications of the ! operator. The first of these rules (BangSub1) is concerned with the weakening of subtype A by adding the bang operator. The second rule concerns weakening both sides of the subtyping relation. The use of the predicate validT throughout the definition ensures

that non-Quipper types are ruled out. This presentation of the subtyping rules for the bang operator make the formal proof of the transitivity of the subtyping relation much easier; in particular it avoids a lot of unneeded induction cases. An important theorem, which states that the subtyping relation implies the validity of its arguments, is stated below.

```
Theorem SubAreVal: forall A B, Subtyping A B -> validT A /\ validT B.
```

Given the above definition of Proto-Quipper subtyping, we successfully verified all the required specifications reported in [27], which ensures that the implemented definition follows the intended behavior. In the following, we list examples of the formally proven properties:

```
Theorem Subtyping_Prop1: forall B,
   Subtyping qubit B -> B = qubit.
```

Similar theorems have been proven for the other base types one and bool. The following specification ensures that whenever the top-level type constructor of the super-type is the bang operator, then the subtype should be too.

```
Theorem Subtyping_Prop6: forall A B1,
  Subtyping A (bang B1) ->
  exists A1, A = (bang A1) /\ Subtyping A1 B1.
```

The second conjunct of this theorem can be concluded by inversion using the Bang_Sub2 rule. It is important to know that this property cannot be proven for the original subtyping relation reported in [27]. Let us consider the case of (Subtyping !one !!one), from which one cannot conclude that (Subtyping one !one). Thanks to the formal proof, we were able to spot this ill-formed condition. The author has been contacted and confirmed the mistake.

Similar to the bang constructor, we prove that if the outermost type constructor of the subtype (not the super-type) is arrow then the super-type should be too:

```
Theorem Subtyping_Prop2: forall A1 A2 B,
Subtyping (arrow A1 A2) B ->
exists B1 B2,
B = arrow B1 B2 /\ Subtyping B1 A1 /\ Subtyping A2 B2.
```

Similar theorems have been developed for the other type constructors tensor and circ. Finally, we provide two important properties of the subtyping relation: reflexivity and transitivity:

```
Theorem sub_ref: forall A, validT A -> Subtyping A A.
```

Note that reflexivity is subject to the validity of A, i.e., it belongs to the Proto-Quipper types.

```
Theorem sub_trans: forall A B C,
Subtyping A B -> Subtyping B C -> Subtyping A C.
```

Note that transitivity does not require that validity of A, B, and C since it is implicitly imposed from the subtyping antecedents (see Theorem SubAreVal).

This concludes the Proto-Quipper types formalization, where we considered the formal development of valid Proto-Quipper types and the subtyping relation on them.

4 Two-Level Hybrid

As mentioned, the purpose of the first Hybrid library (implemented as Hybrid.v) is to provide support for expressing the higher-order abstract syntax of OLs. This file is described in Section 4.1, focusing on the aspects that are required for understanding the formalization in later sections. The second library (implemented as LSL.v) is described in Section 4.2 and contains the encoding of the specification logic (SL), which provides the two-level reasoning capabilities as described earlier. Hybrid allows the use of different SLs, and as mentioned, one of the contributions of this paper is to present a new one. In fact, our goal is to provide a general framework for reasoning about a large class of OLs that have linear features, and preliminary work toward this goal is discussed in [16]. This aspect of our work follows the tradition of a variety of linear logical frameworks that have been introduced in the literature (though none that we know of is maintained in a such a way that we could easily adopt it for our work). In addition, there is growing body of OLs with linear features that would benefit from such a framework. Examples of such frameworks and applications are discussed in Section 8.

4.1 Expressing Syntax of Object Languages in Hybrid

At the core is a type expr that encodes a de Bruijn representation of lambda terms. It is defined inductively in Coq as follows:

```
Inductive expr: Set :=
| CON: con -> expr
| VAR: var -> expr
| BND: bnd -> expr
| APP: expr -> expr -> expr
| ABS: expr -> expr.
```

Here, VAR and BND represent bound and free variables, respectively, and var and bnd are defined to be the natural numbers. The type con is a parameter to be filled in when defining the constants used to represent an OL. The library then includes a series of definitions used to define the operator lambda of type $(\exp r \to \exp r) \to \exp r$, which provides the capability to express OL syntax using HOAS, including negative occurrences in the types of binders. Expanding its definition fully down to primitives gives the low-level de Bruijn representation, which is hidden from the user when reasoning about metatheory. In

fact, the user only needs CON, VAR, APP, and lambda to define operators for OL syntax. Two other predicates from the Hybrid library will appear in the proof development, proper: $\exp r \to \operatorname{Prop}$ and $\operatorname{abstr}: (\exp r \to \exp r) \to \operatorname{Prop}$. The proper predicate rules out terms that have occurrences of bound variables that do not have a corresponding binder (dangling indices). The abstr predicate is applied to arguments of lambda and rules out functions of type ($\exp r \to \exp r$) that do not encode object-level syntax, discussed further in Section 7.

As mentioned, the type con is actually a parameter in the Hybrid library. This will become explicit when presenting Coq definitions, where we write (expr con) as the type used to express OL terms. The constants for Proto-Quipper will be introduced later as an inductive type called Econ and the type qexp mentioned earlier is an abbreviation for (expr Econ).

Before describing our SL in the next section, we include here a summary of the steps of the implementation of any SL. Formulas of the SL are implemented as an inductive type oo. This definition introduces constants for the connectives of the SL and their Coq types. The rules of the SL are defined as a Coq inductive proposition, where each clause represents one rule. This definition is called seq and has one argument for each of the elements of a sequent, which includes the context(s) of assumptions and the conclusion of the sequent. It may also include a natural number used to keep track of the height of a deriviation.

The rules of the OL are also defined as an inductive propostion called prog. In our case, prog defines the inference rules for well-formedness of Proto-Quipper terms, typing of Proto-Quipper terms, and the reduction relation for evaluating Proto-Quipper terms. Its definition uses the capability to express hypothetical and parametric judgments. In the library file defining the SL, prog is a parameter to the definition of seq.

When encoding an OL, the file Hybrid.v must be imported since it is (usually) required to represent the syntax of the OL, while the file containing the SL must be imported when defining prog. When an element of the syntax can be defined directly as an inductive type, however, there is no need to import any Hybrid files. This is the case for the syntax of types of Proto-Quipper as we have seen. The terms of Proto-Quipper, however, cannot be defined inductively; instead we will define a HOAS representation, which uses the lambda operator and other constructors of type expr. As mentioned, using Hybrid provides the flexibility to mix both kinds of representations.

4.2 A Linear Specification Logic

In this section, we will give a brief account of linear logic, highlighting differences with minimal intuitionistic logic, which is the main SL used in Hybrid historically. Then we present the sequent calculus of our selected version of linear logic, namely an intuitionistic linear logic. It has both an intuitionistic

and a linear context of assumptions. The latter is important for modeling the type system of Proto-Quipper.

In minimal intuitionistic logic, there are three logical connectives (\land, \lor) and \Rightarrow), in addition to the logical constants True and False. A sequent in this logic has the form $\Gamma \vdash C$ where Γ is a logical context (a set of formulas) and C is a formula. If a sequent $\Gamma \vdash C$ is valid in intuitionistic logic, then the sequent obtained by adding a hypothesis B to the context, i.e., $\Gamma, B \vdash C$, is also valid. This is called context weakening. If a sequent of the form $\Gamma, B, B \vdash C$ is valid in intuitionistic logic, then the sequent $\Gamma, B \vdash C$ is also valid. This is called context contraction. These two key structural properties of intuitionistic logic are primarily prohibited in linear logic, where we deal with the context as a collection of resources, i.e., the hypotheses are considered as resources that can be used one time and they must be consumed (or used). Accordingly, $\Gamma \vdash C$ does not guarantee the linear validity of $\Gamma, B \vdash C$, and $\Gamma, B, B \vdash C$ does not guarantee the linear validity of Γ , $B \vdash C$. In addition, linear logic has two types of logical connectives: the multiplicative connectives (\otimes, \mathcal{R}) and $-\circ$, and the additive connectives $\&, \oplus$ and \Rightarrow . In addition to the intuitionistic constants, there is the universal consumer constant \top , which can consume any linear resource (i.e., hypothesis). Our choice for SL is a slightly different version of the standard linear logic, namely intuitionistic multiplicative linear logic, with the two kinds of contexts mentioned above: the intuitionistic context Γ (a set of formulas) and the linear context Δ (a multiset of formulas). The contraction and weakening rules are permitted for the intuitionistic context Γ . The logic has two classes of formulas—goals and program clauses—whose syntax is:

Goals
$$G ::= A \mid \top \mid \forall x : \tau \ G \mid A \Rightarrow G \mid G_1 \& G_2 \mid G_1 \otimes G_2 \mid A \multimap G$$

Clauses $P ::= \forall (A \longleftarrow [G_1, \dots, G_m][G'_1, \dots, G'_n])$

In the above grammar, A is an atomic formula. Note that this logic includes universal quantification over typed variables. Here, τ is a primitive type. It will be instantiated with qexp in our case study. A clause in the form above consists of two lists, the first one of intuitionistic goals, the other of linear ones. It is an abbreviation for the formula:

$$\forall (G_1 \Rightarrow \cdots \Rightarrow G_m \Rightarrow G_1' \multimap \cdots \multimap G_n' \multimap A)$$

where the outer \forall represents quantification over all free variables in $G_1, \ldots, G_m, G'_1, \ldots, G'_n, A$, whose types may be τ or $\tau \to \tau$, where τ is primitive. Thus, our logic is second-order in the sense that it is possible to quantify over functions (of type qexp -> qexp in our case).

Sequents of this logic have the form Γ ; $\Delta \vdash_{\Pi} G$, where G is a goal formula, Γ is an intuitionistic context of formulas, Δ is a linear context, and Γ and Δ contain only atomic formulas. Π is a set of program clauses, which we omit when presenting the rules because it is fixed and does not change within a proof. This format emphasizes the view of this calculus as a non-deterministic logic programming interpreter, which is a feature of most SLs implemented in the two-level style. See e.g., [7] and [21]. The sequent rules of such a logic are

Fig. 3 Intuitionistic Linear Logic Sequent Rules

shown in Figure 3. There are two initialization rules. The linear rule (l_init) strictly prohibits the existence of any hypothesis inside Δ except A, and it does not care about the contents of Γ . The intuitionistic rule (i_init) strictly requires an empty Δ whereas A should be part of Γ . We can use & if its operands can be proven linearly at the same time, i.e., all the required linear resources are available in the contexts of both premises (&-R). Recall that a linear resource can be used only once. On the other hand, additive conjunction requires that the resources be split and used in the proof of only one premise (\otimes -R). This connective is suitable when the operands are sharing the linear resources. The implication rules (\Rightarrow -R and \multimap -R) vary based on which context the antecedent A comes from. The \forall -R rule has the usual proviso that y does not appear in Γ , Δ , or B.

In the bc rule, $[\Pi]$ represents all possible instances of clauses in Π (clauses with instantiations for all variables quantified at the outermost level). Applying this rule in a backward direction corresponds to backchaining on a clause in Π , instantiating the universal quantifiers so that the head of the clause matches A. There is one hypothesis for each subgoal, both linear and intuitionistic.

The first step towards the formalization of the linear specification logic in Coq is defining an inductive type oo for formulas given by the G and P grammars:

```
Inductive oo: Set :=
| atom: atm -> oo
| T: oo
| Conj: oo -> oo -> oo
| And: oo -> oo -> oo
| Imp: atm -> oo -> oo
| limp: atm -> oo -> oo
| All: (expr con -> oo) -> oo.
```

where the atom constructor accepts an atomic formula of type atm and casts it into the formula type oo. The type atm is defined for each OL and typically includes the atomic relations or predicates of the OL, e.g., typeof for Proto-Quipper typing (see Section 5.2). The constructor T corresponds to the universal consumer, Conj corresponds to multiplicative conjunction and And to additive conjunction. The type constructors Imp and 1Imp corresponds to intuitionistic and linear implication, respectively, where in both cases, the formula on the left must be an atom. The All constructor takes a function as an argument, and thus the bound variable in the quantified formula is encoded using lambda abstraction in Coq.

The next step is defining the sequent rules themselves. This step is done using an inductive predicate definition as follows:

```
Inductive seq: nat -> list atm -> list atm -> oo -> Prop :=
| s_bc: forall (i:nat) (A:atm) (IL LL:list atm)
  (lL iL:list oo), prog A iL lL ->
    splitseq i L [] iL -> splitseq i IL LL lL ->
    seq (i+1) IL LL (atom A)
:
| s_all: forall (i:nat) (B:expr con -> oo) (IL LL:list atm),
    (forall x:expr con, proper x -> seq i IL LL (B x)) ->
    seq (i+1) IL LL (All B)
with
splitseq: nat -> list atm -> list atm -> list oo -> Prop :=
| ss_init: forall (i:nat) (IL:list atm), splitseq i IL [] []
| ss_general: forall (i:nat) (IL lL1 lL2 lL3:list atm)
    (G:oo) (Gs:list oo),
    split lL1 lL2 lL3 -> seq i IL lL2 G ->
    splitseq i IL lL3 Gs -> splitseq i IL lL1 (G::Gs).
```

where we use the variables IL to represent the intuitionistic context, and LL for the linear one. The definition of seq follows the standard rules described earlier. Only a representative set of the inference rules of the formal definition is shown above. The natural number argument allows proofs by induction over the height of a sequent derivation, which we often use. This argument can be ignored when doing proofs by structural induction. The reader is referred to [15] for the full definition. In the s_bc rule the predicate splitseq is used to check the provability of a list of subgoals. The predicate splitseq is used twice; once for the intuitionistic subgoals iL under the empty linear context, and once for the linear subgoals 1L. When we discuss the rules for prog later, we will say that we must intuitionistically prove the goals in iL and linearly prove the goals in 1L. The predicates seq and splitseq are defined using Coq's mutual induction. The inductive definition of splitseq is at the very end of the definition. In the case when the list of goals is non-empty, the head subgoal G is proven under the linear context 1L2 and the remaining list of subgoals Gs is proven under the context 1L3 if and only if there exists a context 1L1 such that split 1L1 1L2 1L3. We describe the split predicate by example (and omit its definition here): the split of [A;B;C] can be [A;B] and [C], [C] and [A;B], [A] and [C;B], or [B] and [C;A]. The idea of the split is that the two sublists divide the big list, regardless of the order of elements inside the sublist. This is to ensure that there are no shared linear resources between 1L2 and 1L3. Finally, (prog A iL 1L) represents a formula from the program context defining the rules of the OL (i.e., Π). Later (in Section 5.2), we will see the implementation of prog for Proto-Quipper.

The rule for All has an argument of function type $expr con \rightarrow oo$, unlike the other rules, since quantification is over terms of the OL. Recall that con is a parameter to the type expr, and must be implemented for each OL. Note that we restrict x to terms satisfying the proper predicate (terms without dangling indices).

The implemented specification logic has been validated by proving a number of essential properties. We show two here. The first property is a cutelimination rule for the intuitionistic context:

Lemma seq_cut_aux:

```
forall (i j:nat) (a:atm) (b:oo) (il ll:list atm),
seq i il ll b -> In a il ->
seq j (remove eq_dec a il) [] (atom a) ->
seq (i+j) (remove eq_dec a il) ll b).
```

The theorem states that if we remove all instances of the hypothesis a from the list of intuitionistic hypotheses il, and a is found to be provable under the new list of hypotheses, then eliminating a does not affect the provability of b. Note that the remove function takes a proof that equality at type atm is decidable. Since atm is a parameter to the SL, so is eq_dec. The second property is the weakening property for the intuitionistic context:

Theorem seq_weakening_cor:

```
forall (i:nat) (b:oo) (il il' ll:list atm),
(forall (a:atm), In a il -> In a il') ->
seq i il ll b -> seq i il' ll b.
```

This concludes the formalization of the linear specification language and some of its metatheory. In the following sections, we will present Proto-Quipper as an OL that benefits from this logic, where will give a concrete implementation for the parameters presented in this section, in particular, atm, con, and prog, as well as prove decidability of equality for our instantiation of atm.

5 Encoding Proto-Quipper Programs and Semantics in Hybrid

In this section, we discuss a key aspect of this work, where we present the encoding of Proto-Quipper in the Hybrid framework. This includes the formalization of Proto-Quipper syntax as a concrete implementation of the types con and atm, and the main parts of the program context prog, which includes the typing rules in Figure 2. We then present a number of theorems that are important for proving type soundness of Proto-Quipper.

5.1 Encoding Proto-Quipper Terms

Recall that in Hybrid, con is a parameter to the type expr. The implementation of con for an OL typically includes all constants that appear in the language. This includes the names of the operations supported by the OL, e.g., if and let. The implementation of con for Proto-Quipper is as follows:

```
Inductive Econ: Set :=
| qABS: Econ | qAPP: Econ | qPROD: Econ
| qLET: Econ | sLET: Econ | qCIRC: Econ | qIF: Econ
| BOX: qtp -> Econ | UNBOX: Econ | REV: Econ
| TRUE: Econ | FALSE: Econ | STAR: Econ
| Qvar: nat -> Econ | Crcons: nat -> Econ.
```

This definition might cause some confusion since it does not differentiate between constants like TRUE and FALSE, and operations like lambda abstraction qABS and the let statement qLET. Actually, these are just constants and this definition does not include any semantics or functionality by itself. The functionality of these operations will be addressed next. In our formalization, we encode all quantum variables of Proto-Quipper as constants using the constant Qvar, which maps natural numbers to quantum variables. Similarly, the constant C (see Section 2). The argument of type qtp to the BOX operator encodes the type superscript in box^T . As mentioned earlier, qexp is an abbreviation for (expr Econ).

```
Definition qexp: Set := expr Econ.
```

As stated earlier, all OL constructs are encoded using CON, VAR, APP and lambda. These definitions are the only place where the constructors of the expr type and the lambda operator are seen explicitly. Once the new constants are defined, we use only these. We start with the simplest item in the language, namely variables:

```
Definition Var: var -> qexp := VAR Econ
```

The definition is simple as it just uses the Hybrid VAR parameterized with the Proto-Quipper constants Econ. Another simple example of encoding Proto-Quipper operations in Hybrid is function application:

```
Definition App (e1 e2:qexp) : qexp := APP (APP (CON qAPP) e1) e2.
```

To help the reader to understand the above definition, it is better to view the Hybrid constructor APP as a concatenation operator. Another possible definition is (APP (CON qAPP) (APP e1 e2)). One might wonder if it is useless to add the constant qAPP. Remember that the APP constructor is used to represent other program statements, e.g., the if statement. Therefore, we need to add such constants for each type of expression so we can identify statements with different meanings. Similarly, we formally define the product and circuit statements as follows:

```
Definition Prod (e1 e2:qexp) : qexp :=
  APP (APP (CON qPROD) e1) e2.

Definition Circ (e1:qexp) (i:nat) (e2:qexp) : qexp :=
  APP (APP (APP (CON qCIRC) e1) (CON (Crcons i))) e2.
```

Now, let us turn to a Proto-Quipper construct that is a bit more difficult, namely function abstraction.

```
Definition Fun (f:qexp -> qexp) : qexp :=
APP (CON qABS) (lambda f).
```

This expression has an argument that is a function of type (qexp -> qexp). To better understand this construct, we give some examples. Let f be the function fun x => App (Var 0) x. Consider the term (lambda f). If definitions are expanded, the Hybrid operator lambda disappears and the result is the de Bruijn format of this term which replaces the bound variable x by the correct de Bruijn index. For the above example, (lambda f) unfolds to ABS (APP (VAR ECON 0) (BND 0)). As stated, we never need to expand such definitions. Now that we have the full encoding of Proto-Quipper terms, we can return to the example term from the introduction, $\lambda x.\lambda y.xy$, which is encoded as (Fun (fun x:qexp => (Fun (fun y:qexp => (App x y))))).

Similarly, we handle the more difficult case of the Let expression.

```
Definition Let (f:qexp \rightarrow qexp \rightarrow qexp) (e1:qexp): qexp:= APP (CON qLET) (APP (lambda (fun x => (lambda (f x)))) e1).
```

Recall that the let statement in Proto-Quipper is restricted to product expressions, i.e., it always takes the form let $\langle x,y\rangle=a$ in b. Therefore, we have two function abstractions, e.g., fun x => fun y => App y x. Since the lambda is only defined for functions of type exp -> exp (not exp -> exp -> exp), we have to make two applications of lambda in the way presented in the above definition in order to satisfy the typing condition of lambda. This is the first case study using Hybrid that requires a function of more than one argument to represent OL syntax.

We note that terms in Hybrid are equivalent up to η -conversion, so the body of the definition of Fun and Let operators, respectively, could also be written:

```
(APP (CON qABS) (lambda (fun x => (f x)))). 

(APP (CON qLET) 

(APP (lambda (fun x => (lambda (fun y => (f x y)))) b)).
```

The formal encoding of the other Proto-Quipper expressions is similar to the definitions presented above [15].

We also define the following predicate that holds for expressions that only involve quantum variables, the star constant, and the product constructor Prod.

```
Inductive quantum_data: qexp -> Prop :=
   vQVAR: forall i, quantum_data (CON (Qvar i))
```

```
| vSTAR: quantum_data (CON STAR)
| vTENSOr: forall a b, quantum_data a -> quantum_data b ->
quantum_data (Prod a b).
```

This subset of expressions are those whose types satisfy the valid predicate.

5.2 Encoding Proto-Quipper Semantics

The main purpose of this section is to discuss the implementation of the atomic predicates atm and the program context prog for Proto-Quipper. Here, atm contains three constructors, one that relates a Proto-Quipper type qtp to a Proto-Quipper expression qexp, one for representing reduction rules, and one that identifies valid (well-formed) expressions of Proto-Quipper.

```
Inductive atm : Set :=
| typeof : qexp -> qtp -> atm
| reduct : Econ -> qexp -> Econ -> qexp -> atm
| is_qexp : qexp -> atm.
```

It is important to clarify that the formalization presented in the previous section does not guarantee that all instances of the type qexp are valid in Proto-Quipper. (It just defines expressions that we are interested in.) This will be done as part of the program context prog with the help of the constructor is_qexp.

Now, we turn to the crucial step in our whole formalization, the implementation of prog. The formal definition of such a predicate is quite long. Accordingly, we choose to present it rule by rule, where we address only the major rules, and others can be found in [15]. We discuss clauses for <code>is_qexp</code> and <code>typeof</code> here, and leave the discussion of <code>reduct</code> to Section 6.

Now that we have instantiated the parameters con and atm, we can define the first two abbreviations below.

```
Definition oo_ := oo atm Econ.
Definition atom_: atm -> oo_ := atom Econ.
Definition seq_: nat -> list atm -> list atm -> oo_ -> Prop := seq prog.
Definition splitseq_:
  nat -> list atm -> list atm -> Prop := splitseq prog.
```

The third and fourth are useful once we have completed the definition of prog. Thus the general form of sequents of the SL will be written seq_ n IL LL G, where the arguments are the height of the proof, the intuitionistic and linear contexts of assumptions of type atm, and the conclusion (formula on the right of the turnstile), respectively. We will sometimes omit the height argument for readability when it is not important for the discussion, and in particular in the statements of theorems, seq_ IL LL G will mean that there exists an n such that seq_ n IL LL G.

The prog predicate has type <code>atm -> list oo_ -> list oo_ -> Prop</code>, whose arguments are: the atomic statement, the list of intuitionistic subgoals, and the list of linear subgoals. Recall that it appears in the definition of <code>seq</code> in the <code>s_bc</code> clause, which implements the bc rule in Figure 3. It is the implementation of the program clauses Π . In the upcoming rules, this predicate reads as follows: the atomic statement is valid in the context of Proto-Quipper program if the list of intuitionistic and linear subgoals can be proven using the linear specification logic presented in Figure 3 (as implemented by <code>seq</code>). We start by presenting examples of syntax rules that define valid expressions inside Proto-Quipper:

```
| starq: prog (is_qexp (CON STAR)) [] []
| trueq: prog (is_qexp (CON TRUE)) [] []
| boxq: prog (is_qexp (CON BOX)) [] []
```

Constants of Proto-Quipper are unconditionally valid; the list of linear and intuitionistic subgoals are empty. Similar clauses are included in prog for the constants FALSE, UNBOX, and REV.

Note that we have defined the syntax of terms in Section 2 as grammars. As argued in [6], grammars contain implicit information, and specifying well-formedness as inference rules makes some of this information explicit, which is useful for formally defining valid terms. For example, consider the sublanguage of Proto-Quipper terms containing term variables, application, and function abstraction. One possible set of rules expressing valid syntax is as follows:

$$\begin{array}{ll} \underline{is_qexp} \ x \in \underline{\Phi} \\ \overline{\Phi \vdash is_qexp} \ x \end{array} \qquad \underline{ \begin{array}{l} \underline{\Phi \vdash is_qexp} \ a \\ \overline{\Phi \vdash is_qexp} \ ab \end{array} } \\ \underline{ \begin{array}{l} \underline{\Phi, is_qexp} \ x \vdash is_qexp} \ a \\ \overline{\Phi \vdash is_qexp} \ \lambda x.a \end{array} }$$

Here, Φ is an explicit context of variables, and a term is only considered well-formed if all of its free variables come from this set. Stated formally in our setting, for a sequent seq_IL [] (atom_ (is_qexp a)) to be provable, for each free variable x of type qexp that appears in a, the atom is_qexp x must be in the intuitionistic context IL. Note that the list of linear subgoals is empty. This is the case for all well-formedness of syntax rules, as the context elements expressing validity of an expression can be used as many times as we want, i.e., they are infinitely consumable resources.

The following clause encodes the well-formedness of the application expression:

```
| apq: forall E1 E2:qexp,
prog (is_qexp (App E1 E2))
  [And (atom_ (is_qexp E1)) (atom_ (is_qexp E2))] []
```

As mentioned, the list of linear subgoals is empty. In the intuitionistic goals, notice is the use of additive conjunction. Actually, we cannot use multiplicative conjunction to express an intuitionistic subgoal according to the specification

logic defined in Section 4.2. The use of And for intuitionistic subgoals has the same power as the use of multiplicative conjunction because the use of the intuitionistic context involves infinitely consumable resources, and hence we can show the validity of E1 and E2 from the same context. Similar rules are defined for the Prod and Slet expressions, and also the If expression, where we have three sub-expressions instead of two.

The following clause corresponds to the function abstraction (Fun) case.

For a function expression containing E to be valid in Proto-Quipper, E should first satisfy the Hybrid abstr condition. This predicate guarantees that E encodes object-level syntax (discussed earlier and in more detail in Section 7). One of the big advantages of the Hybrid framework is that it hides such details when reasoning about OLs. The term (Fun E) is said to be valid if for all valid expressions \mathbf{x} , the expression E \mathbf{x} a is valid Proto-Quipper expression. Again, this subgoal needs to be proved intuitionistally. Proving this subgoal involves assuming that a new variable \mathbf{x} is a valid expression and showing that the term obtained by replacing the bound variable in E by \mathbf{x} is a valid expression. A similar clause can be developed for the Let expression, with the difference that E is a function of two parameters instead of one:

This case illustrates how abstr is used for functions of more than one argument. Another difference from the Fun case is that a second subgoal ensures the validity of the b argument representing the body of the let expression.

The last syntactic rule to present is the quantum circuit rule circ. Note that in the sample rules for well-formedness of Proto-Quipper expressions given above, the context Φ should contain all the free term variables; we did not include a second context for quantum variables. Following the style of the typing rule circ, we use the In and Out functions to identify free quantum variables and then these variables occur in the corresponding premises, but not in the conclusion. In the rule below, if Q is a set of quantum variables q_1, \ldots, q_n for $n \geq 0$, we write Φ_Q to abbreviate the context is_qexp q_1, \ldots, is_qexp q_n .

This rule is encoded as the following clause of the prog definition.

```
| Circq: forall (C:nat) (t a:qexp), quantum_data t ->
prog (is_qexp (Circ t C a))
  [toimpexp (FQ a) (atom_ (is_qexp a))] []
```

Recall that quantum_data is a predicate that holds for expressions that only involve quantum variables, the star constant, and the product constructor Prod. This predicate is used to directly prove the first premise $\Phi, \Phi_{Q_1} \vdash is_qexp\ t$. The encoding of the second premise appears in the intuitionistic list of subgoals (the second argument to prog). The Coq function FQ returns a list of free quantum variables of an expression, and toimpexp is a function that takes a list quantum variables and using intuitionistic implication, adds them recursively as antecedents to a the predicate expressing well-formedness of the term. We illustrate by example:

In general, proving such an implication requires repeated applications of the \Rightarrow -R rule of the SL (Figure 3) in a backward direction, moving antecedents of the form $is_qexp\ q$ into the intuitionistic context, resulting in a context that encodes Φ_{Q_2} .

As stated above, we have defined FQ as a Coq function. In general, users of Hybrid need to take care when defining functions with arguments whose types instantiate expr (defined in Section 4), which in our specific case includes the type qexp (defined as expr Econ in Section 5.1). In particular, proving properties of such functions may require exposing the de Bruijn representation of these arguments. The FQ function is one such example. In particular, our proofs require the following three axioms:

```
Hypothesis FQ_FUN: forall i E,
  abstr E -> FQ (Fun E) = FQ (E (Var i)).
Hypothesis FQ_LET: forall i E b,
  abstr (fun x => lambda (E x)) ->
  (forall x, proper x -> abstr (E x)) ->
  FQ (Let E b) = (FQ (E (Var i) (Var i))) ++ (FQ b).
Hypothesis FQU_LET: forall i E b,
  abstr (fun x => lambda (E x)) ->
  (forall x, proper x -> abstr (E x)) ->
  FQU (Let E b) = (FQU (E (Var i) (Var i))) ++ (FQU b).
```

These axioms are admissible, but require complex proofs. Replacing the definition of the FQ function with an inductive predicate that relates the input and output would solve this problem.²

² This is straightforward change, but it affects a large portion of the proof development and is left for (very near) future work.

This concludes the presentation of the rules for well-formedness of Proto-Quipper terms. Such clauses actually play two roles in proofs of OL meta-theory. First, induction on well-formedness derivations is often useful, since induction directly on terms is not currently available in Hybrid. Second showing that rules are adequately represented requires these clauses. (See Section 7.)

In the following, we will present the formal typing rules that correspond to the sequent rules presented in Figure 2. Recall that the Proto-Quipper typing judgment has the form Φ ,! Ψ ; $Q \vdash a : A$. The latter context Q contains all free quantum variables that appear on the right of a sequent; they appear in such a context without specifying the type since it is implicitly known to be qubit. The other context contains term variables and their types and has two parts where the types in ! Ψ contain a leading! and the types in Φ do not. Recall also that the sequents of the SL, which we will now use to encode these rules, have the general form Γ ; $\Delta \vdash A$, where A is a formula of the SL, Γ is an intuitionistic context of atomic formulas, and Δ is a linear context, also of atomic formulas. In our formalization, elements of the contexts of the Proto-Quipper typing judgment will be encoded as atomic formulas of the form (typeof x A) in the SL; in particular, the encoding of elements of Ψ will appear in the intuitionistic context Γ of the SL, while elements of the typing context Φ will appear in the linear context Δ of the SL. Each quantum variable q in Q will be placed in Δ explicitly associated with the type qubit, i.e., typeof (CON (Qvar qi)) qubit, where qi is the natural number encoding variable q.

We start with the ax_c rule, which we specify as two clauses depending on whether or not the first argument to the subtype relation has a leading bang.

```
| axc1: forall (A B:qtp) (x:qexp), validT (bang A) ->
Subtyping A B ->
prog (typeof x B) [atom_ (is_qexp x)] [atom_ (typeof x A)]
| axc2: forall (A B:qtp) x, Subtyping (bang A) B ->
prog (typeof x B)
  [(And (atom_ (typeof x (bang A))) (atom_ (is_qexp x)))] []
```

In axc1, the validT (bang A) condition ensures that A has no leading bang, and as a consequence of theorem Subtyping_Prop6, B also has no leading bang. Thus it is required to linearly prove that atom_ (typeof x A), whereas in axc2, it is required to intuitionistically prove atom_ (typeof x (bang A)). Note that for reasons of adequacy, there is the additional proof obligation to show that x is a valid Proto-Quipper expression (in both cases).

Regarding the ax_q and ax_x rules, as mentioned they are not encoded as clauses of prog. In particular, they are already covered by the initial rule of the SL (l-init of Figure 3 encoded as part of the defintion of seq).

The following clauses implement the two versions of the \top rule, the first for n=0 and the second for n=1, and the *cst* rule for box^T . Similar to the well-formedness rules for constants, they are axioms and thus have no subgoals.

```
| truel: prog (typeof (CON TRUE) bool) [] []
```

The prog definition includes similar clauses for the other rules about constants and functions on circuits, i.e, the two versions of the $*_i$ and \bot rules, and the cst rules for unbox and rev.

The next two clauses encode the λ_1 rules. Similar to the ax_c rule, we develop intuitionistic and linear versions of λ_1 , depending on the type of the bound variable (whether or not it has a leading!):

Note that in both cases, the subgoal is required to be proved linearly regardless of the type of the bound variable. This is because the type of the whole expression Fun (fun x => E x) is linear. The difference between the two rules is the use of lImp when the type of the bound variable is linear, and the use of Imp when the type of the bound variable. In contrast, the subgoal will be required to be proved intuitionistically for both cases of the λ_2 rule. We omit the clauses for these rules, as well as those for the \otimes_e rule, since they are similar to the encoding of λ_1 presented above.

The following clause implements the *app* rule. This case requires that both expressions be available at the same time. Accordingly, it uses multiplicative conjunction (Conj):

In other words, considering backward proof from the app rule of Figure 2, the linear context of the conclusion must be divided into two disjoint contexts. The use of Conj means that the \otimes -R rule of Figure 3 will be used to achieve this division. Note here that there is only one app rule, and thus only one corresponding clause in prog since, whether or not T has a leading bang, the typing judgments for E1 and E2 must be proved linearly.

The encoding of the two \otimes_i rules is similar to app:

We omit the clauses for $*_e$ and if, since their encoding is similar to rules already presented.

The last rule is *circ*. We encode this rule similarly to the encoding of the well-formedness rule for circuits: in this case the lists of free variables Q_1 and Q_2 have been moved in front of the turnstile symbol with the help of linear implication for typeof atoms, and intuitionistic implication for the <code>is_qexp</code> atoms:

```
| tCricl: forall (C:nat) (t a:qexp), forall T U,
    circIn (Crcons C) = FQ t ->
    circOut (Crcons C) = FQ a ->
    quantum_data t -> validT (circ T U) ->
        prog (typeof (Circ t C a) (circ T U))
        [And (toimp (FQ a) (atom_ (typeof a U)))
            (toimp (FQ t) (atom_ (typeof t T)))] []
| tCrici: forall (C:nat) (t a:qexp), forall T U,
        circIn (Crcons C) = FQ t ->
        circOut (Crcons C) = FQ a ->
        quantum_data t -> validT (circ T U) ->
        prog (typeof (Circ t C a) (bang (circ T U)))
        [And (toimp (FQ a) (atom_ (typeof a U)))
        (toimp (FQ t) (atom_ (typeof t T)))] []
```

Similar to the toimpexp presented earlier, we define toimp which iteratively adds well-formedness and typing assumptions for free quantum variables to a statement with the help of linear implication. Again, we illustrate by example:

```
toimp (FQ (Prod (CON (Qvar 0)) (CON (Qvar 1))))
          (atom_ (typeof (Prod (CON (Qvar 0)) (CON (Qvar 1))) A)) =
Imp (is_qexp (CON (Qvar 0)))
  (lImp (typeof (CON (Qvar 0)) qubit)
        (Imp (is_qexp (CON (Qvar 1)))
        (lImp (typeof (CON (Qvar 1)) qubit)
              (atom_ (typeof (Prod (CON (Qvar 0)) (CON (Qvar 1))) A)))))
```

It is important to note here that both the linear and duplicable versions of the circuit rule require the subgoal to be proved intuitionistically. Moreover, the subgoal is the same for both cases. Although this is in contrast with other rules, it reflects the real semantics of circuits, because if a circuit has been proven

to be of a certain type, then it should be possible to use as many instances of this circuit as needed; it is an autonomous component. If it happens that a free variable appears in a circuit construct, then this variable is of duplicable type. This semantics is imposed by the above rules since we keep the list of linear subgoals empty. According to [27], quantum variables appearing in the circuit constructs are called bounded quantum variables. That is why FQ of a circuit construct is supposed to return an empty list. Also, the free variables of t should match the input of the circuit C, and the free variables of a should match the output of C. The functions circIn and circOut are defined as abstract functions. In particular, [27] does not provide specific definitions for these functions. They are identified only by their domains and co-domains. In the Coq code, we define them as variables in a module. Before proving properties about a specific set of circuits, these variables must be instantiated with a particular definition. Since, like [27], we are proving only meta-level properties, we leave them abstract also.

6 Type Soundness

In this section, we formally verify the type soundness of Proto-Quipper by addressing three important properties: a type soundness under subtyping rule, inversion lemmas for Proto-Quipper *values*, and the subject reduction theorem.

6.1 Context Subtyping

In a type system with subtyping, an important soundness lemma is one that expresses that typing is preserved under the subtype relation extended to contexts. In our setting, the statement of this lemma is in a sense, a general form of the ax_c rule where the contexts in the premise and conclusion are not the same, but instead have a subtyping relation between them, in this case a kind of "contravariant" one. The lemma states, roughly, that if seq_i il 11 (atom_A) holds, A is a subtype of B, and the pair (i1',11') is a "subtype" of the pair (i1,11), then seq_i il' 11' (atom_B) holds. Context subtyping includes an extension of subtyping in the obvious way; an atom typeof a t1 occurs in il' or 11' if and only if an atom typeof b t2 occurs in the corresponding il or 11 and Subtyping t1 t2 holds.

Before we can make the above statement formal, we must consider additional constraints on the contexts in the sequents. As discussed in [6], in general when formalizing meta-theory, statements of theorems often relate two or more judgments and if the contexts in these judgments are non-empty, a context relation is often needed to specify the constraints in the form of a relation between them. The above lemma is an example that relates exactly two statements about the seq_predicate with their corresponding contexts. A variety of examples in a simpler setting with an intuitionistic SL are discussed in detail in [8]. We adopt this notion of context relation here, extending it to

express our requirements, which are significantly more complex. We capture both the subtyping constraints as well as the necessary additional constraints in the following inductive definition.

```
Inductive Subtypecontext :=
| subcnxt_i: Subtypecontext [] [] []
| subcnxt_q: forall a il il' ll ll',
 Subtypecontext il' 11' il 11 ->
 Subtypecontext (is_qexp a::il') 11' (is_qexp a::il) 11
| subcnxt_iig: forall a t1 t2 il il' ll ll',
 Subtyping t1 t2 -> (exists c, t2 = bang c) ->
 Subtypecontext il' 11' il 11 ->
 Subtypecontext (is_qexp a::typeof a t1::il') ll'
                 (is_qexp a::typeof a t2::il) 11
| subcnxt_llg: forall a t1 t2 il il', ll ll',
 validT (bang t1) -> validT (bang t2) ->
 Subtyping t1 t2 -> Subtypecontext il' 11' il 11 ->
 Subtypecontext (is_qexp a::il') (typeof a t1::ll')
                 (is_qexp a::il) (typeof a t2::ll)
| subcnxt_lig: forall a t1 t2 il il' ll ll',
  validT (bang t2) -> (exists c, t1 = bang c) ->
 Subtyping t1 t2 -> Subtypecontext il' il' il ll ->
 Subtypecontext (is_qexp a::typeof a t1::il') ll'
                 (is_qexp a::il) (typeof a t2::11).
```

The additional constraints include, for example, that every time there is a typing assumption (typeof a t) in either a linear or intuitionistic context, there must be an assumption of the form (is_qexp a) in the intuitionistic context. Note that we can write Subtypecontext il 11 il 11, where the first and third arguments are the same, and similarly for the second and fourth, when we want to ignore subtyping and care only that these additional constraints are met. We will use Subtypecontext for this secondary purpose rather than define a new context relation.

Before expressing and proving the central lemma mentioned above, we have to tackle a crucial theorem that is very helpful for splitting a linear context:

```
Theorem subcnxt_split: forall il il' 11 11' 111 112,

Subtypecontext il' 11' il 11 -> split 11 111 112 ->
exists il1 il2 111' 112',
split 11' 111' 112' /\
(forall a, In a il -> In a il1) /\
(forall a, In a il -> In a il2) /\
Subtypecontext il' 111' il1 111 /\
Subtypecontext il' 112' il2 112.
```

This theorem explains the effect of splitting a linear context in the Subtype-context relation. Recall that list splitting means dividing a list into two lists with elements in any order. This theorem helps when we are dealing with

several subgoals in **splitseq** or multiplicative conjunction goals, and we want to split the linear context without losing the benefit of the **Subtypecontext** relation. This situation is pretty common in our proofs.

We are now ready to state the central lemma.

```
Theorem subtypecontext_subtyping: forall a IL IL' LL LL' B A, Subtypecontext IL' LL' IL LL -> seq_ IL LL (atom_ (typeof a A)) -> Subtyping A B -> seq_ IL' LL' (atom_ (typeof a B)).
```

With the help of the above lemma and others, we successfully prove this theorem. The proof amounts to 800 lines of Coq script. The proof is by induction on the height of the sequent derivations, with cases for every possible typing rule defined in the program context prog.

6.2 Inversion Rules for Values

A Proto-Quipper expression is considered a *value*, or non-reducible expression, if it matches one of the following cases:

The major role of these special expressions is in defining the language reduction rules (i.e., operational semantics), as detailed in the next section, where the main objective is to reduce a Proto-Quipper expression to one of these forms. The cases mentioned above in the definition are obvious, except for Unboxappv. The reason behind considering (App (CON UNBOX) v) a value is because the resulting expression is of function type; as stated in [27], the unbox operator turns a circuit into a circuit-generating function, and thus this case is similar to Funvv.

Now that we have the language values, we can prove a number of inversion lemmas (corresponding to lemmas in [27]). In each, we prove that a well typed value v should follow certain Proto-Quipper format(s). Here is the first example:

```
Theorem sub_one_inv: forall IL a,
    ~(In (is_qexp (CON UNBOX)) IL) -> is_value a ->
    Subtypecontext IL [] IL [] -> ~(In (is_qexp a) IL) ->
    seq_ IL [] (atom_ (typeof a one)) -> a = CON STAR.
```

In this particular inversion theorem, a value of type one should be the STAR constant. To make sure that the context is not misused, we must prevent assumptions about well-formedness of value terms from occurring in the context. To do so, we use the Subtypecontext relation to ensure that every (is_qexp a) that appears in IL is associated with a typing atom (typeof a A) in IL This way, if ~(In (is_qexp a) IL) is assumed in the inversion theorem then no typing hypothesis for the value "a" appears in IL. We add a similar condition for the UNBOX due to the fact that (App (CON UNBOX) v) is a value: if UNBOX is assumed in IL to be of type (arrow A one) (which is a false assumption according to Proto-Quipper typing rules), then by assuming the existence of a value v of type A, one can prove that "a" has the form (App (CON UNBOX) v), which is wrong. The conclusion of the above theorem is also valid for the type (bang one), which is also formally proved. Similar results have been proved for all other values. To avoid repetition, we pick one more interesting example to illustrate, however, the reader still can find a full list of the inversion rules online at [15].

The following theorem is concerned with the values of the arrow type constructor. In contrast to the previous theorem (and all other cases), we have several possibilities that satisfy this typing format:

According to above theorem, the value "a" would be a function, a quantum circuit conversion function, or a function application over the UNBOX constant.

The proofs of the above inversion rules are done by case analysis of the possible values. For each case, it is proved that seq_ IL LL (atom_ (typeof a A)) requires that (In (typeof a A) IL) or (In (typeof a A) LL), which leads to a contradiction except for the particular value we are interested in. For instance, in the theorem sub_one_inv, assuming that seq_ IL LL (atom_ (typeof a one)) leads to a contradiction in all cases except for the STAR constant.

We also prove inversion rules that serve the opposite purpose from the above ones, where the expression format is provided and the theorems conclude the right corresponding type and/or typing rules. Those rules are more general, i.e., they are not restricted to values. For instance, the following theorem characterizes the typing rules for the Slet statement:

```
Theorem sub_slet_inv: forall IL LL a b A,

Subtypecontext IL LL IL LL ->

seq_ IL LL (atom_ (typeof (Slet a b) A)) ->

~(In (is_qexp (Slet a b)) IL) ->

(exists B, Subtyping B A /\

(splitseq_ IL LL

[Conj (atom_ (typeof a B)) (atom_ (typeof b (bang one)))] \/

splitseq_ IL LL

[Conj (atom_ (typeof a B)) (atom_ (typeof b one))])) \/

(validT A /\

(splitseq_ IL LL

[Conj (atom_ (typeof a A)) (atom_ (typeof b (bang one)))] \/

splitseq_ IL LL

[Conj (atom_ (typeof a A)) (atom_ (typeof b one))])).
```

The Subtypecontext is used here again to ensure that we are dealing with a valid typing context as explained earlier; it has nothing to do with the subtyping between contexts since the super-context and subcontext are the same. The above theorem concludes two possible cases for a well-typed Slet expression. First, the right side of the main disjunction corresponds to the case when the type A is deduced directly from the SLet typing rules (see the tsletl and tsleti of the Prog definition in [15]). Second, the left disjunct corresponds to the case when the typing deduction has gone through one or more subtyping rules (see rules axc1 and axc2 of the prog definition discussed above and in [15]) followed by the regular SLet typing rules).

Here is another example for the circuit construct:

```
Theorem sub_Circ_inv: forall IL LL t a c A,
  Subtypecontext IL LL IL LL ->
  seq_ IL LL (atom_ (typeof (Circ t c a) A)) ->
  ~(In (is_qexp (Circ t c a)) IL) ->
  (exists T T' B,
    Subtyping B A / validT (circ T T') / LL = [] /
    splitseq_IL []
     [And (toimp (FQ a) (atom_(typeof a T')))
           (toimp (FQ t) (atom_(typeof t T)))] /\
    (B = circ T T' \setminus B = bang (circ T T'))) \setminus /
  (exists T T',
    validT (circ T T') /\ LL = [] /\
    splitseq_ IL []
     [And (toimp (FQ a) (atom_(typeof a T')))
           (toimp (FQ t) (atom_(typeof t T)))] /\
    (A = circ T T' \setminus A = bang (circ T T'))).
```

An interesting fact about a well-typed circuit construct is that its linear context should be empty, and this is expected as the circuit is supposed to be used several times, and hence it does not depend on linear typing atoms. Re-

Fig. 4 If statement reduction rules

call that the quantum variables that appear in "t" and "a" are considered bound variables.

Similar results have been proved for other Proto-Quipper expressions, e.g., functions, function application, circuit conversion constants, etc.

6.3 Subject Reduction

Reduction rules, i.e., operational semantics, are crucial for any programming language, defining how valid expressions in a language are simplified until a non-reducible expression is reached, i.e. a value. In the context of a language's reduction rules, it is very important to ensure the integrity of typing rules by ensuring that a reduction of a well-typed expression should not affect the expression's type (i.e., type soundess). In Proto-Quipper, there are seventeen reduction rules, which handle all possible cases while ensuring that only one reduction rule can be applied at a time. To keep the description concise, we choose five reduction rules to explain in this paper, which are good representative samples. Similar to typing rules, we encode Proto-Quipper reduction rules as part of the inductive definition of prog. For the complete set of rules, we refer the reader to [27], and for their complete encoding in Coq, see [15].

Given a closure pair [C, a], where C is a circuit constant and a is a Proto-Quipper expression such that $FQ(a) \in Out(C)$, an if statement is reduced according to the rules listed in Figure 4. The formal Coq presentation of the rules in Figure 4 as part of the prog definition is as follows:

```
| ifr: forall C C' b b' a1 a2, valid_c C (If b a1 a2) ->
valid_c C' (If b' a1 a2) -> ~(is_value b) ->
prog (reduct C (If b a1 a2) C' (If b' a1 a2))
    [atom_ (reduct C b C' b');
    atom_ (is_qexp a1); atom_ (is_qexp a2)] []
| truer: forall C a1 a2, valid_c C (If (CON TRUE) a1 a2) ->
prog (reduct C (If (CON TRUE) a1 a2) C a1)
    [atom_ (is_qexp a1); atom_(is_qexp a2)] []
| falser: forall C a1 a2, valid_c C (If (CON FALSE) a1 a2) ->
prog (reduct C (If (CON FALSE) a1 a2) C a1)
    [atom_ (is_qexp a1); atom_(is_qexp a2)] []
```

where valid_c ensures that [C',(If b' a1 a2)] forms a valid closure. Note that the rule ifr is only applicable if "b" is not a value, otherwise this rule

$$\frac{[D,a] \rightarrow [D',a']}{[C,(t,D,a)] \rightarrow [C,(t,D',a')]} circ$$

$$\frac{Spec_{FQ(v)}(T) = t \qquad New(FQ(t)) = D}{[C,box(v)] \rightarrow [C,(t,D,v\ t)]} box$$

$$\frac{bind(u,v) = b \qquad Append(C,D,b) = (C',b')}{[C,(unbox\ (u,D,u'))\ v] \rightarrow [C',b'(u')]} unbox$$

Fig. 5 Circuit reduction rules

would be applied an infinite number of times without achieving any progress. When "b" is a value, i.e., True or False one of the other two rules can be applied.

The remaining examples of Proto-Quipper reduction rules that we consider here are the circuit construct and its conversion function boxing and unboxing rules, which appear in Figure 5. $Spec_Q$ is a function that given a quantum data type T, returns a $specimen\ t$ of that type, i.e., a quantum data term having type T that has the further property that all quantum variables in t are "fresh" with respect to the quantum variables occurring in Q. New is a function that creates a new identity circuit, i.e., given a set of quantum variables, these variables serve as the inputs and outputs, and the new circuit contains only wires where inputs are mapped directly to the same outputs.

The notion of a binding expresses the way in which wires should be connected. The bind function is a bijection on quantum variables, where it wires each quantum variable in u with the corresponding one in v. For example, $bind(\langle q_1,q_2\rangle,\langle q_3,q_4\rangle)=\{(q_1,q_3);(q_2,q_4)\}$. The Append function is responsible for appending two circuits. It returns the new circuit and a binder to rename the outputs of the newly created circuit. This rename step is not really required since the newly created circuit can use the same names of the output of the circuit D as its output; however, it is considered an added feature in the Proto-Quipper language. The following are the corresponding formal reduction rules of the box and unbox rules listed in Figure 5:

In the boxr clause, the function newqvar returns a variable that is fresh with respect to its argument, which is a quantum term. In our implementation of the Spec function, the first argument is a natural number and all quantum variables in the result are represented by numbers greater than this input number. Together Spec and newqvar implement the Spec function in the box rule.

In our formalization, we implement a relation (bind u v), which holds if u and v are related by some binding, i.e., they are the same quantum data terms up to the renaming of quantum variables. This relation is used twice in the unboxr clause to implement the binding relations in the unbox rule. We note that the Append function is formalized as an abstract function without concrete implementation, where Proto-Quipper does not provide one; rather it provides its properties which we axiomatize in the above rule.

Similar rules have been formalized for the rest of Proto-Quipper expressions and can be found in [15].

Now, we can present the most important property of the Proto-Quipper language, namely subject reduction, which completes the type soundness result of the Proto-Quipper type system and its operational semantics:

The three underlined predicates represent the core of the the subject reduction theorem. The three predicates translate the typical meaning of the subject reduction: an expression a, that is the reduction of a well-typed expression a, is also well-typed and hold the same type as the original expression a.

The remaining hypotheses belong to two categories and require explanation. The three lines following the theorem name are additional well-formedness constraints. As we will describe below, the one involving <code>get_boxed</code> was unexpected and illustrates the merits of formal proofs to check paper-and-pencil ones, which often overlook the kind of detail captured by this definition. The remaining lines are conditions on contexts. We are able to reuse our <code>Subtypecontext</code> definition to capture some of the requirements, but in addition, we define an additional context relation <code>common_ll</code> as well as add some additional requirements on the form of assumptions appearing in contexts.

In general, type soundness results are often stated and proved for typing of closed terms and empty contexts. Here, we could restrict terms so that they contain no free term variables (in particular, require that a and a' contain no free term variables), but we cannot do the same for quantum variables since there is no lambda binder for quantum variables in the language. Most of our additional hypotheses provide the required structure for the appearance of assumptions about quantum variables in contexts, but we go beyond that and also allow free term variables in a and a'. Doing so requires some additional hypotheses in the statement of the theorem, but allows us to prove a more general form. The version requiring a and a' to be closed follows as a corollary. In summary, the basic requirements for free quantum variables are that for every variable q (of the form (CON (Qvar n))), q is free in a or a' if and only if there is an assumption (is_qexp q) in IL, q is free in a if and only if there is an assumption of the form (typeof q qubit) in LL1, and q is free in a' if and only if there is an assumption of the form (typeof q qubit) in LL2.

We explain the hypotheses in more detail one by one in the following.

This hypothesis restricts the intuitionistic context so that it includes only typing and well-formedness assumptions about term variables and quantum variables. Note that the inversion rules sub_one_inv, sub_bangarrow_inv, sub_slet_inv, and sub_Circ_inv in Section 6.2 all restrict the form of the argument to is_qexp, which is the expression subject to inversion, when it appears in the intuitionistic context. In these theorems, the restrictions are carried over to the linear contexts because of the way the contexts are related according to the Subtypecontext predicate. The same applies here.

- Subtypecontext IL LL1 IL LL1 and Subtypecontext IL LL2 IL LL2: These predicates ensures that the constraints discussed in Section 6.1 about the relationship between the intuitionistic and linear contexts are met. For example, each typing assumption of the form (typeof a t) in any context must be associated with a well-formedness assumption (is_qexp a) in the intuitionistic context. In addition, it restricts the linear context to contain typeof assumptions only.
- common_ll a a' LL1 LL2:

One might wonder why the theorem requires two different linear contexts (LL1 and LL2); in particular, the common subject reduction for classical OLs maintains the same context in all judgments. The answer is quantum variables. Proto-Quipper reduction rules allow for quantum variable renaming (i.e., in the case of circuit appending), and allow introduction of new quantum variables (e.g., a circuit with zero inputs that produces quantum variables at the output, which typically represents an initialization circuit). As a result, the linear context of the original expression is

usually a bit different from the context for the reduced one; they are similar modulo quantum variables. That is why we have defined the predicate <code>common_ll</code>, which ensures that all typing assumptions in LL1 and LL2 are the same except for quantum variables, where quantum variables in LL1 belong to the set of free quantum variables of a, and quantum variables in LL2 belong to the set of free quantum variables of a'.

- (forall q, In q (FQ a') -> In (typeof q qubit) LL2):

The previous predicate does not assure that LL2 contains assumptions about all free quantum variables of a'; it only ensures if a quantum variables exists in LL2 then it belongs to (FQ a'). That is why we added this assumption. One might ask why not to do the same for LL1; the answer that we do not need that assumption since a is well-typed under LL1 and hence it must contain all quantum variable of (FQ a). This fact is proved as per the following theorem (note the equivalence in the last two lines):

- NoDup (FQUC a') and NoDup (FQU a'):

FQU is similar to FQ in that it returns the free quantum variables occurring in a term. The difference is that FQ returns a set, while FQU returns a list so that if there is more than one occurrence of a free variable in a term, it occurs more than once in the output list. FQUC is similar, but also includes bounded quantum variables of quantum circuits. (In FQ and FQU, those variables are excluded.) The predicate NoDup comes from Coq's list library and is true of lists that contain no duplicates. In quantum calculus, quantum variables are processed once. We use FQU to rule out expressions that involve quantum replicas. FQUC ensures no quantum variable replicas inside circuit bodies.

The function $\mathtt{get_boxed}$ returns a list of all expression that are arguments to the box^T operator, i.e., for the expression (APP (CON (BOX T)) a), it returns a. We want to make sure that those expressions are neither free variables nor quantum variables. Unlike the other hypotheses in the theorem, which are mostly due to our method of formalization, this condition

should be respected in the language implementation itself; otherwise the language allows for expressions that are not *values* and there is no reduction rule that applies. Without this, neither subject reduction nor progress properties hold for Proto-Quipper.

The proof of the above theorem involves several lemmas and theorems and makes significant use of a number of the inversion rules discussed in the previous section. It is proved by induction on i, the height of the proof of the sequent containing the typing judgment, followed by a case analysis of 17 reduction rules, each of which require at least 10 major subgoals due to case analysis and inversions.

This concludes our formalization of Proto-Quipper in Hybrid, along with our development of a generic linear specification logic used as a platform to reason about quantum programming languages. In the following section, we will discuss a very critical aspect of our development where we ensure that the developed formalization models the intended behavior of Proto-Quipper as presented in [27].

7 Adequacy

It is important to show that both syntax and inference rules are adequately represented in Hybrid. Adequacy of syntax encoding, also called *representational adequacy*, is discussed for the lambda calculus as an OL in Hybrid in [2] and proved in detail in [4], while adequacy for a fragment of a functional programming language known as Mini-ML is proved in [7]. Proto-Quipper contains the lambda calculus as a sublanguage, and representational adequacy for the full language is a straightforward extension of these other results. We give a brief overview here.

First, the proper and abstr predicates, defined in the Hybrid library, provide important tools for proving representational adequacy of any OL. As mentioned, the proper predicate rules out terms with dangling indices, which clearly cannot occur in well-formed terms of any OL. The abstr predicate, as mentioned, applies to arguments of the lambda operator. Recall that this operator has one argument of functional type (expr \rightarrow expr). To adequately represent OL syntax, we must rule out *exotic* functions, i.e., functions that do not encode OL lambda terms. To illustrate, we consider the example from [7]. Suppose we have (lambda e), where $e = (\lambda x.\text{count } x)$ where (count x) counts the total number of variables and constants occurring in x. This function clearly does not represent syntax. Only functions that behave uniformly or parametrically on their arguments, such as the one discussed in the introduction, represent OL terms. The abstr predicate identifies exactly this set of functions. See [5] and the related work section of [7] for a careful analysis of this phenomenon. The former applies specifically in the context of Coq. Also, see [15] for the precise definitions of these two predicates.

Second, proving representational adequacy requires defining an encoding function between OL terms and their representation in Hybrid, and showing

that this function is a bijection. In particular, we write $\varepsilon_{\varGamma}(\cdot)$ for the encoding function from Proto-Quipper terms with free term variables in \varGamma to terms of type qexp. We omit its definition, but note that it maps each term variable x in \varGamma to a distinct Coq variable x: qexp, and each quantum variable q in \varGamma to an expression of the form (CON (Qvar q_i)), where q_i is a distinct natural number for each quantum variable. Consider the judgment $\varGamma \vdash is_qexp$ a and a full set of inference rules for this judgment in the style of those presented in Section 5.2. Let $\{x_1,\ldots,x_n\}$ be the set of term variables in \varGamma and let x_1,\ldots,x_n be the encodings of these variables. We must prove that for any Proto-Quipper term a, if $\varGamma \vdash is_qexp$ a, then the following is provable in Coq:

```
\begin{array}{l} \texttt{proper} \ \mathtt{x_1} \to \cdots \texttt{proper} \ \mathtt{x_n} \to \\ \texttt{exists} \ (\texttt{i} : \texttt{nat}), \\ \texttt{seq} \ \texttt{i} \ [(\texttt{is\_qexp} \ \mathtt{x_1}); \ldots; (\texttt{is\_qexp} \ \mathtt{x_n})] \ [] \\ \texttt{(atom\_} \ (\texttt{is\_qexp} \ \varepsilon_{\varGamma}(a))) \end{array}
```

Furthermore, we write $\delta_{\Gamma}(\cdot)$ for the decoding function. Let Γ be Coq variables and terms $\{x_1, \ldots, x_n, (CON (Qvar q_{i_1})), \ldots, (CON (Qvar q_{i_m}))\}$ of type qexp, let E be a term of type qexp, and let Γ be:

```
\{\delta_{\Gamma}(\mathbf{x_1}), \ldots, \delta_{\Gamma}(\mathbf{x_n}), \delta_{\Gamma}(\mathtt{CON} (\mathtt{Qvar} \ q_{i_1})), \ldots, \delta_{\Gamma}(\mathtt{CON} (\mathtt{Qvar} \ q_{i_m}))\}.
```

We must prove that if the following is provable in Coq:

```
\begin{array}{l} \texttt{proper} \ x_1 \to \cdots \texttt{proper} \ x_n \to \\ \texttt{exists} \ (\texttt{i} : \texttt{nat}), \\ \texttt{seq} \ \texttt{i} \ [(\texttt{is\_qexp} \ x_1); \ldots; (\texttt{is\_qexp} \ x_n)] \ [] \ (\texttt{atom\_} \ (\texttt{is\_qexp} \ E)) \end{array}
```

then $\delta_{\Gamma}(E)$ is defined and yields a Proto-Quipper term a such that $\Gamma \vdash is_qexp\ a$. Additionally, $\varepsilon_{\Gamma}(\delta_{\Gamma}(E)) = E$ and $\delta_{\Gamma}(\varepsilon_{\Gamma}(a)) = a$. The above results correspond to Lemma 21 (called *Validity of Representation*) and Lemma 22 (*Completeness of Representation*), respectively, in [7].³

Proving the adequacy of the encoding of inference rules is similar. Note that in the above statements, well-formedness was expressed as a set of inference rules of a judgment of the form $\Gamma \vdash is_qexp\ a$, and the proofs of these statements require showing a bijection between proofs (on paper) using the inference rules of this judgment, and proofs using our encodings of prog and seq. The same approach is used to prove the adequacy of the other two judgments $\Gamma; Q \vdash a : A$ and $[C, a] \to [C', a']$. Additionally, for all judgments except well-formedness, internal adequacy lemmas must be proven. Such lemmas correspond to Lemma 20, clauses 2 and 4 for the reduction and typing judgments, respectively, of MiniML in [7]. They are called internal adequacy lemmas because they can be formalized in Hybrid and they are an important part of the general adequacy proofs for these judgments. In general, such properties state that whenever an OL judgment that is defined as part of the definition

 $^{^3}$ We also impose the restriction that the Coq derivation must be minimal in the same sense as described there. See [7] for details.

⁴ A variety of other internal adequacy lemmas are shown in [8].

of prog can be proved, then the OL terms in this judgment are well-formed. The abstr conditions are important for proving these lemmas. The following theorem expresses internal adequacy for the Proto-Quipper typing judgment.

```
Lemma hastype_isterm_ctx :
  forall (M:qexp) (T:qtp) (iq it lt:list atm),
  ctxR iq it lt ->
  seq_ it lt (atom_ (typeof M T)) ->
  seq_ iq [] (atom_ (is_qexp M)).
```

Note that it uses a context relation ctxR relating the intuitionistic and linear contexts of the typeof predicate to the intuitionistic context of the is_qexp predicate. (The linear context is always empty when proving well-formedness of terms.) The definition of this relation is as follows:

```
Inductive ctxR: list atm -> list atm -> list atm -> Prop :=
| nil_cr: ctxR nil nil nil
| cons_q_cr: forall (iq it lt:list atm) (x:qexp),
    proper x -> ctxR iq it lt ->
        ctxR (is_qexp x::iq) (is_qexp x::it) (lt)
| cons_l_cr: forall (iq it lt:list atm) (x:qexp)
        (T:qtp),    proper x -> ctxR iq it lt ->
        ctxR (is_qexp x::iq) (is_qexp x::it) (typeof x T::lt)
| cons_i_cr: forall (iq it lt:list atm) (x:qexp)
        (T:qtp),    proper x -> ctxR iq it lt ->
        ctxR (is_qexp x::iq) (typeof x T::is_qexp x::it) lt.
```

In addition the following two lemmas are needed. The first is a standard lemma about intuitionistic contexts as found in the examples in [8]. The second is unique to linear contexts, and thus is new.

```
forall (M:qexp) (Phi1 Phi2:list atm),
  (forall (M:qexp),
    In (is_qexp M) Phi1 -> In (is_qexp M) Phi2) ->
  seq_ Phi1 [] (atom_ (is_qexp M)) ->
  seq_ Phi2 [] (atom_ (is_qexp M)).
```

Lemma qexp_strengthen_weaken:

```
Theorem ctxRconcat: forall iq it lt lt1 lt2, ctxR iq it lt -> lt = lt1++lt2 -> exists it1 it2, (forall a, In a it -> In a it1) /\ (forall a, In a it -> In a it2) /\ ctxR iq it1 lt1 /\ ctxR iq it2 lt2.
```

Note that the conclusion of the hastype_isterm_ctx lemma only involves the term M. No similar conclusion is required for T because Proto-Quipper types are defined directly as an inductive type in Coq. There are no binders in types, and thus the correspondence between terms of type T and types of Proto-Quipper is direct.

We have proved a similar result for the reduction rules, showing that the language's operational semantics does not lead to invalid expressions (see [15]).

8 Conclusion

We have presented our formalization of Proto-Quipper in Hybrid. This work involved encoding a linear specification logic and carrying out a large case study in Hybrid, in the sense that we encode and reason about the complete Proto-Quipper specification, the most complex OL considered so far, and we prove type soundness, one of the central results in [27].

In order for Hybrid with a linear SL to become a fully operational logical framework, we will need to provide suitable automation of proofs, based on lessons learned from this case study. Adding such automation is an important direction for future work.

Another important direction is extending the formalization to other more complex properties and to other quantum programming languages. For example, the other main result [27] is a progress theorem for Proto-Quipper, which is an obvious next step for us. We do not foresee any difficulty, though its proof will likely be as long and detailed as the proof of type soundness. Also, it should be straightforward to adapt the existing formal proofs to new versions of Proto-Quipper. For example, a new version called Proto-Quipper-M is introduced in [26]. This version does not have subtyping, which should mean that certain aspects of formal proofs of its metatheory will be easier. In the future, we hope to use our system as an environment in which new Proto-Quipper metatheory can be simultaneously developed and formalized as versions of the language evolve.

It should also be possible to directly extend our work from Proto-Quipper, which is fairly expressive though not Turing complete, to the full Turing-complete Quipper language. Similarly, we expect to be able to extend this work directly in order to apply it to other Turing-complete quantum lambda calculi such as those introduced by Zorski et. al. [13,14,31] and Grattage et. al. [1, 9]. As another example, the QWIRE language in [25] is implemented in Coq and is expressive enough to include languages like Proto-Quipper. The work in that paper focuses on proving properties of quantum programs and program transformations, such as proving that a program meets its formal specification. In our framework, it would be interesting to also study the meta-theory of this language.

A variety of other logical frameworks implementing linear logic have been developed. The ordered linear logic (OLF) mentioned earlier [24] is one such example, where type soundness for a *continuation*-based abstract machine for the functional programming language Mini-ML (an OL that is simpler than Proto-Quipper) is proven [7] following the statement in [3]. Another example of OLs that benefit from a framework based on linear logic are those with

imperative features. A common thread of such examples is that they contain the notion of updatable state, which can be handled fairly directly by the linear features of the framework. The case study we present in this paper is the first one in Hybrid where the OL itself is linear, in the sense that the linear lambda calculus forms the core of Proto-Quipper.

Examples involving mutable state have motivated a variety of proposals for frameworks based on linear logics that support HOAS. For other examples that benefit from linear features, see the overview in [20]. Examples of frameworks proposed include Lolli [12], Forum [19], and LLF [3]. The logical framework LF [11] and its implementation in Twelf represents one of the earliest logical frameworks supporting HOAS and based on minimal intuitionistic logic. LLF is a conservative extension of LF with multiplicative implication, additive conjunction, and unit.

Type soundness proofs for various OLs has been a common benchmark for logical frameworks supporting HOAS and implementing an intuitionistic logic, starting with some of the earliest logical frameworks like LF [30]. In [17], Mini-ML with mutable references, an imperative version of the Mini-ML language mentioned above, is studied in Hybrid. Five versions of type soundness are proved using three different SLs, intuitionistic, linear, and OLF as implemented in [7], and their formalizations compared.

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