A Lambda Calculus for Quantum Computation

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Abstract

The classical lambda calculus may be regarded both as a programming language and as a formal algebraic system for reasoning about computation. It provides a computational model equivalent to the Turing machine, and continues to be of enormous benefit in the classical theory of computation. We propose that quantum computation, like its classical counterpart, may benefit from a version of the lambda calculus suitable for expressing and reasoning about quantum algorithms. In this paper we develop a quantum lambda calculus as an alternative model of quantum computation, which combines some of the benefits of both the quantum Turing machine and the quantum circuit models. The calculus turns out to be closely related to the linear lambda calculi used in the study of Linear Logic. We set up a computational model and an equational proof system for this calculus, and we argue that it is equivalent to the quantum Turing machine.

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1 Introduction

Currently there exist two main approaches to the theory of quantum computation: The quantum Turing machine, introduced by Benioff and Deutsch [1, 2], and the quantum circuit model, introduced by Deutsch [3]. These two approaches were shown to be essentially equivalent by Yao [4].

The quantum Turing machine provides a fundamental model of quantum computation that may be regarded as a baseline for defining universality. However, reasoning about Turing machines can be a cumbersome process, requiring word-at-a-time thinking while keeping track of complicated machine and tape states. Turing machine programs do not satisfy a simple algebra.

For this reason, the quantum circuit model is more popular in the practical investigation of quantum algorithms. Quantum circuits are visual, compositional, and may be manipulated algebraically. However, no single finite quantum circuit is universal. Indeed, Yao’s proof of Turing equivalence relies on the concept of uniform circuit families generated by classical computation [4, 5]. To define what we mean by such a circuit family, we need to rely on a separate model of classical computation not described by any finite quantum circuit.

In classical computation, the lambda calculus provides an alternative computational model, equivalent to the Turing machine, which continues to be of enormous utility in the theory of computation, in mathematical logic, and in the study of computer languages and their semantics [6, 7, 8, 9, 10]. Due to its simplicity and expressive power, the lambda calculus has been used as the basis of several powerful computer languages, including Lisp, Scheme, ML and Haskell [11, 12, 13, 14].

In this article, we propose that quantum computing, like its classical counterpart, may benefit from an alternative computational model based on a version of the lambda calculus suitable for expressing and reasoning about quantum algorithms. We develop such a calculus, which turns out to be closely related to the linear lambda calculi used in the study of Linear Logic. We set up its computational model and equational proof system, and argue that the computational model is equivalent to the quantum Turing machine.

The quantum lambda calculus combines some of the benefits of both quantum circuits and the quantum Turing machine. The quantum lambda calculus describes functions that may be composed and manipulated algebraically, like quantum circuits. Programs can be algebraically transformed...
into equivalent programs, and one can solve equations whose unknowns are programs, in much the same way as one solves equations in high school algebra [15]. Unlike quantum circuits, the quantum lambda calculus provides a unified framework that is universal for quantum computation without the need to rely on a separate model of classical computation.

In a practical vein, we show how various known quantum algorithms may be expressed as simple programs in the lambda calculus. Indeed, the calculi described in this paper may be used as a programming language for prototyping quantum algorithms. In fact, the algorithms exhibited in this article were transcribed into Scheme for testing. The simulator, which was also written in Scheme, is available upon request from the author.

Since the first version of this paper was written, some progress has been made by the author in devising a typed version, with accompanying denotational semantics, of a fragment of the quantum calculus described here [16].

2 The classical lambda calculus

We begin by providing a reasonably self-contained introduction to concepts and constructions in the classical lambda calculus that will be used in the rest of the paper. The intended audience for this section includes physicists and general computer scientists. The expert may skip this section and refer back as needed.

The classical lambda calculus may be regarded both as a programming language and as a formal algebraic system for reasoning about computation. It was originally introduced by Church in the study of the foundations of mathematics [17, 18]. Church postulated that it provides a universal model of computation, which was later shown by Turing to be equivalent to the Turing machine [19].

As a formal system, the lambda calculus has axioms and rules of inference, and lends itself to analysis using the language and tools of mathematical logic. Computation may be regarded as guided deduction in this formal system. This provides a directed form of equational reasoning that corresponds to symbolic evaluation of programs via a sequence of algebraic simplifications called reductions [6, 7, 8, 9, 10].

The syntax of the classical untyped lambda calculus $\lambda$ is as follows: Expressions (also called terms) are constructed recursively from variables $x, y,$
z, \ldots, parentheses, spaces, the period, and the symbol \( \lambda \), according to the grammar of figure 1.

\[
t ::= \begin{array}{ll}
x & \text{variable} \\
(\lambda x. t) & \text{abstraction} \\
(t \ t) & \text{application}
\end{array}
\]

**Figure 1: Syntax of the lambda calculus \( \lambda \)**

A term of the form \( (\lambda x. t) \) is called a **functional abstraction**. It represents the function \( x \mapsto t \). For example, the identity function \( x \mapsto x \) is written as

\[
(\lambda x. x)
\]

The dummy variable \( x \) here is called a bound variable, and conforms to the usual rules governing bound variables in mathematical formulae. For example, we identify expressions that differ only in the renaming of bound variables.

A term of the form \( (t \ t) \) represents a **function application**. The sole means of computation in the lambda calculus is the operation of applying a function to its argument consistent with the following axiom:

\[
((\lambda x. t) \ v) = t[v/x] \quad (\beta)
\]

Here \( v \) denotes a **value**, to be defined shortly. Reading this axiom from left to right defines an algebraic rewrite rule for transforming terms, substituting the argument \( v \) in place of the variable \( x \) into the function body. This transformation is called **beta reduction**. We will use the arrow \( \rightarrow \) to indicate one (and sometimes more than one) beta reduction step. A reducible term is called a **redex**.

Unabridged lambda terms can be painful to read. For this reason, we will often introduce abbreviations using the symbol \( \equiv \). In addition, we will often omit parentheses according to the convention that nested lambda abstractions associate to the right and applications associate to the left.

Consider the simple program \((\lambda x. x) \text{apple}\) where \text{apple} stands for some term in our language. With the abbreviation \( \text{id} \equiv (\lambda x. x) \), this may be
written more legibly as \((\text{id \ apple})\), which should evaluate to \text{apple}. Indeed, beta reduction gives
\[
((\lambda x. \ x) \ \text{apple}) \longrightarrow \text{apple}
\]
in a single step.

In general, a computation consists of a sequence of beta reductions executed according to some deterministic strategy until the resulting term cannot be reduced any further, at which point the computation terminates.

A slightly more complicated example, which serves to show how multiple-argument functions can be represented in terms of nested single-argument functions (a technique known as \textit{currying}), is given by
\[
\text{apply} \equiv \lambda f. \lambda x. ( f \ x) \\
\equiv \lambda f. (\lambda x. (f \ x))
\]
which represents a function that applies its first argument \(f\), which should be a function, to its second argument \(x\). Applying the identity function to \text{banana} should give \text{banana}. To see this, the program \((\text{apply \ id \ banana})\), which is shorthand for \(((\text{apply \ id}) \ \text{banana})\), is now executed by the following sequence of beta reductions (underlining redexes)
\[
\begin{align*}
((\text{apply \ id}) \ \text{banana}) & \equiv (((\lambda f. (\lambda x. (f \ x))) \ \text{id}) \ \text{banana}) \\
& \longrightarrow ((\lambda x. (\text{id} \ x)) \ \text{banana}) \\
& \longrightarrow (\text{id \ banana}) \\
& \longrightarrow \text{banana}
\end{align*}
\]
Often there is more than one reducible subterm at any given step and a strategy is required to make the process unambiguous. For definiteness, we will use a \textit{call by value} strategy. This works as follows: Abstractions (terms of the form \((\lambda x. t)\)) are considered \textit{values} and may not be reduced any further. A function application \((t \ t)\) may only be reduced if both the operator and the operand are values. Otherwise the operator and operand must be reduced first. We will call the resulting calculus the call-by-value lambda calculus \(\lambda_v\). Formally, we state the syntax for values \[20, 21\] in figure \[2\]
The reduction rules are listed in figure \[3\].
v ::= values:
x variable
(λx. t) abstraction value

Figure 2: Values in the call-by-value calculus $\lambda_v$

\[
\begin{align*}
  t_1 & \rightarrow t'_1 \quad (app_1) \\
  (t_1 \ t_2) & \rightarrow (t'_1 \ t_2) \\
  t_2 & \rightarrow t'_2 \quad (app_2) \\
  (v_1 \ t_2) & \rightarrow (v'_1 \ t'_2) \\
  (\lambda x. t) \ v & \rightarrow t [v/x] \quad (\beta)
\end{align*}
\]

Figure 3: Reduction rules for the call-by-value calculus $\lambda_v$

We will denote by $\langle\langle t \rangle\rangle$ the term, when it exists, obtained by fully reducing $t$ to a value.

We will often use a less cumbersome informal notation when defining functions. For example, the apply function above satisfies the following property

\[
\text{apply} \ f \ x \rightarrow (f \ x)
\]

under beta reduction. Given this specification, the translation into a lambda term is straightforward.

How do we represent data in the lambda calculus? Since all we have at our disposal are lambda terms, we need a way of encoding data as lambda abstractions with specified properties. There is a technique which can be used for any kind of data structure, which we will illustrate with two examples: Natural numbers and lists.

Let us first consider how the natural numbers may be represented. As with any kind of data, we need a way to construct natural numbers and a way to deconstruct them, extracting their constituents.

One possible encoding is as the sequence

\[
0, \ 1 \equiv \langle\langle \text{succ} \ 0 \rangle\rangle, \ 2 \equiv \langle\langle \text{succ} \ 1 \rangle\rangle, \ \ldots,
\]
where

\[0 \equiv \lambda x. \lambda y. (x \text{id})\]
\[\text{succ} \equiv \lambda n. \lambda x. \lambda y. (y \, n)\]

are the constructors.\(^1\) The above definitions were motivated by the need to be able to define a case expression (deconstructor)

\[\text{case } t_1 \text{ of } (0 \rightarrow t_2, \text{succ } m \rightarrow t_3)\]

which may now be taken as an abbreviation for

\[t_1 \, (\lambda z. \, t_2) \, (\lambda m. \, t_3)\]

Here \(z\) denotes a variable that does not appear free in \(t_2\). This expression allows us to deconstruct a natural number, extracting the ingredients that went into its construction, i.e., either \(0\) or its predecessor \(m\). It is indeed not difficult to verify the following behavior under beta reduction:

\[\text{case } 0 \text{ of } (0 \rightarrow t_2, \text{succ } m \rightarrow t_3) \rightarrow t_2\]
\[\text{case } \langle \text{succ } t_0 \rangle \text{ of } (0 \rightarrow t_2, \text{succ } m \rightarrow t_3) \rightarrow t_3 [\langle t_0 \rangle / m]\]

As an example, it is now trivial to define the predecessor function (with the convention that \(\text{pred } 0 = 0\))

\[\text{pred} \equiv \lambda n. \text{case } n \text{ of } \begin{cases} 0 \rightarrow 0 \\ \text{succ } m \rightarrow m \end{cases}\]

In order to program arbitrary computations, we need to verify that the lambda calculus is sufficiently powerful to represent recursive functions. Indeed, recursion can be used to represent any kind of iterative or looping computation.

\(^1\)Explicitly

\[0 \equiv \lambda x. \lambda y. (x \, (\lambda w. \, w))\]
\[1 \equiv \lambda x. \lambda y. (y \, \lambda x. \lambda y. (x \, (\lambda w. \, w)))\]
\[2 \equiv \lambda x. \lambda y. (y \, \lambda x. \lambda y. (y \, \lambda x. \lambda y. (x \, (\lambda w. \, w))))\]

\vdots

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For example, in order to define addition, we need an expression \(\text{add}\) which behaves as follows under beta reduction:

\[
\text{add} \; m \; n \rightarrow \text{case} \; m \; \text{of} \; \begin{cases} 
0 \rightarrow n \\
\text{succ} \; k \rightarrow \text{add} \; k \; (\text{succ} \; n)
\end{cases}
\]

where the subterm denoted by \(\text{add}\) on the left has copied itself into the body of the term on the right hand side. One of the simplest ways of achieving this is to define

\[
\text{add} \equiv (t \; t) \tag{1}
\]

where

\[
t \equiv \lambda f. \left( \lambda m. \lambda n. \text{case} \; m \; \text{of} \; \begin{cases} 
0 \rightarrow n \\
\text{succ} \; k \rightarrow (f \; f) \; k \; (\text{succ} \; n)
\end{cases} \right) \tag{2}
\]

In other words, \(t\) is an abstraction consisting of the body of the addition function with the combination \((f \; f)\) in the position where \(\text{add}\) should insert itself after reduction. It is a simple exercise to show that \(\text{add}\) indeed has the specified behavior under beta reduction. This method can be applied to any recursive function.

The computation of the program \((\text{add} \; 2 \; 2)\) then proceeds via the following sequence of beta reductions:

\[
\begin{align*}
\text{add} \; 2 \; 2 & \equiv \text{add} \; \langle \text{succ} \; 1 \rangle \; 2 \\
& \rightarrow \text{case} \; \langle \text{succ} \; 1 \rangle \; \text{of} \; \langle 0 \rightarrow 2, \text{succ} \; k \rightarrow \text{add} \; k \; (\text{succ} \; 2) \rangle \\
& \rightarrow \text{add} \; 1 \; \langle \text{succ} \; 2 \rangle \equiv \text{add} \; \langle \text{succ} \; 0 \rangle \; 3 \\
& \rightarrow \text{case} \; \langle \text{succ} \; 0 \rangle \; \text{of} \; \langle 0 \rightarrow 3, \text{succ} \; k \rightarrow \text{add} \; k \; (\text{succ} \; 3) \rangle \\
& \rightarrow \text{add} \; 0 \; \langle \text{succ} \; 3 \rangle \equiv \text{add} \; 0 \; 4 \\
& \rightarrow \text{case} \; 0 \; \text{of} \; \langle 0 \rightarrow 4, \text{succ} \; k \rightarrow \text{add} \; k \; (\text{succ} \; 4) \rangle \\
& \rightarrow 4 
\end{align*}
\]

The above technique can be generalized to arbitrary data structures. For example, lists can be represented by the following constructors, which are entirely analogous to those of the natural numbers

\[
() \equiv \lambda x. \lambda y. (x \; \text{id}) \\
\text{cons} \equiv \lambda h. \lambda t. \lambda x. \lambda y. ((y \; h) \; t)
\]

8
where () denotes the empty list and \texttt{cons} constructs a list consisting of a first (head) element \( h \) followed by a list \( t \) (the tail) containing the rest of the elements. Again, the above definitions were motivated by the need to be able to define a deconstructor

\[
\text{case} \ t_1 \ \text{of} \ ((()) \rightarrow t_2, \ \text{cons} \ h \ t \rightarrow t_3)
\]

which may now be taken as an abbreviation for

\[
t_1 \ \lambda z. \ t_2 \ (\lambda h. \ \lambda t. \ t_3)
\]

We will often abbreviate \( h : t \equiv (\text{cons} \ h \ t) \). We can define tuples in terms of lists as \((x_1, \ldots, x_n) \equiv x_1 : x_2 : \cdots : x_n : ()\). Under beta reduction, we have the behavior

\[
\begin{align*}
\text{case} \ () \ \text{of} \ ((()) \rightarrow t_2, \ h : t \rightarrow t_3) & \rightarrow t_2 \\
\text{case} \ \langle \langle t_0 : t_1 \rangle \rangle \ \text{of} \ ((()) \rightarrow t_2, \ h : t \rightarrow t_3) & \rightarrow t_3 \ [\langle \langle t_0 \rangle \rangle / h, \ \langle \langle t_1 \rangle \rangle / t]
\end{align*}
\]

showing how the case expression may be used to deconstruct the list, extracting its head and tail. To see how these abstractions are used, consider the following recursive function

\[
\text{map} \ f \ \text{list} \rightarrow \text{case} \ \text{list} \ \text{of} \ \begin{cases} 
(()) \rightarrow () \\
(\lambda z. \ t_2) (\lambda h. \ \lambda t. \ t_3)
\end{cases}
\]

which takes as input a function and a list and applies the function to each element of the list. The reader may verify that, for example,

\[
\text{map} \ \text{double} \ (4, 7, 2) \rightarrow (8, 14, 4), \ \ \ \text{double} \equiv \lambda x. \ (\text{add} \ x \ x)
\]

Finally, we introduce some convenient notation. Since we can represent tuples as lists, we can define functions on tuples using notation such as

\[
\lambda (x, y). \ t \equiv \lambda u. \ \text{case} \ u \ \text{of} \ \begin{cases} 
(()) \rightarrow () \\
x : t' \rightarrow \text{case} \ t' \ \text{of} \ \begin{cases} 
(()) \rightarrow () \\
y : t'' \rightarrow t
\end{cases}
\end{cases}
\]

For example, \((\lambda (x, y). \ (\text{add} \ x \ y)) \ (7, 7)\) evaluates to 14. It is also useful to have a notation for representing intermediate results. The \texttt{let} notation

\[
\text{let} \ (x_1, \ldots, x_n) = (t_1, \ldots, t_n) \ \text{in} \ t \\
\equiv (\lambda (x_1, \ldots, x_n). \ t) (t_1, \ldots, t_n)
\]
allows us to write terms such as

\begin{verbatim}
let x = 1 in
let (y, z) = (2, 3) in
add x (add y z)
\end{verbatim}

which evaluates to 6.

3 A quantum computational model

In this section we will construct a computational model, based on the lambda calculus, suitable for describing quantum computations. The language used will be an adaptation of the classical lambda calculus, extended with a set of quantum primitives. We will denote it by \( \lambda_i \) where the subscript stands for \textit{intermediate}. For reasons to be discussed in the next section, this language is not suitable as a formal system. In particular, reduction in \( \lambda_i \) does not correspond to a simple system for equational reasoning. In section 5 we will correct these deficiencies to obtain the full quantum lambda calculus \( \lambda_q \).

In the classical lambda calculus, beta reduction consumes the program to give the result. At each step, information is discarded, which makes the process irreversible. For quantum computing, we need reduction rules that take computational states to superpositions of states in a way that is unitary and reversible.

Bennett [23] showed that any classical computation can be transformed into a reversible computation. The construction, adapted to our situation, is as follows: Let \( x \) denote the term being computed, and let \( \beta : x \mapsto \beta(x) \) denote a single beta reduction step. Instead of the non-invertible function \( \beta \), one considers the function \( x \mapsto (x, \beta(x)) \), which is invertible on its range. In its simplest version, the computation proceeds as

\begin{verbatim}
x \mapsto (x, \beta(x)) \mapsto (x, \beta(x), \beta^2(x)) \mapsto (x, \beta(x), \beta^2(x), \beta^3(x)) \mapsto \cdots
\end{verbatim}

More complicated schemes exist that reversibly erase the intermediate steps, saving space at the expense of running time. Although this process does not end by itself, we may observe it and regard the computation as having terminated when \( \beta^{n+1}(x) = \beta^n(x) \), at which time we may stop the machine by external intervention.

Although this scheme can be used to reversibly implement computations in the classical lambda calculus, we will soon see that it does not work unmodified in the quantum case.
In order to represent computations involving qubits, we will add a few constant symbols as additional primitives to our language as in figure 4.

\[
\begin{align*}
  t & ::= \text{terms:} \\
  & x \quad \text{variable} \\
  & (\lambda x. t) \quad \text{abstraction} \\
  & (t t) \quad \text{application} \\
  & c \quad \text{constant} \\
  c & ::= \text{constants:} \\
  & 0 \mid 1 \mid H \mid S \mid R_3 \mid \text{cnot} \mid X \mid Y \mid Z \mid \ldots
\end{align*}
\]

Figure 4: Syntax of the intermediate language $\lambda_i$

The symbols 0 and 1 here are primitives and should not be confused with the abbreviations $0$ and $1$ of the previous section. Additional constants $H$, $S$, . . . , will denote elementary gate operations on qubits. These should include symbols for a universal set of elementary quantum gates \[3, 24, 25\]. For example, the set consisting of the Hadamard gate $H$, the phase gate $S$, the $\pi/8$ gate $R_3$, and the controlled-not gate $\text{cnot}$ is universal \[25, 5\]. Additional primitives, such as the the Pauli gates $X$, $Y$ and $Z$, may be added for convenience.

We now allow the state of a computation to be a quantum superposition of terms in this language. As a model, one may imagine lambda terms encoded as strings of symbols on the tape of a quantum Turing machine.

As a first example, consider an initial state written in ket notation as

\[|H\ 0\rangle\.
\]

We would like to choose the transition rules of the quantum computer in such a way that this string will evaluate to the Hadamard operator applied to $|0\rangle$, which should give the superposition $\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$ of the states $|0\rangle$ and $|1\rangle$ containing unit-length strings. The candidate reduction rule

\[
\begin{align*}
  |H\ 0\rangle & \longrightarrow \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \\
  |H\ 1\rangle & \longrightarrow \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)
\end{align*}
\]
is not reversible. To make it reversible, we first try the same trick as in the classical case

\[ |(H \ 0)\rangle \rightarrow \frac{1}{\sqrt{2}} \left( |(H \ 0); 0\rangle + |(H \ 0); 1\rangle \right) \]

\[ = |(H \ 0)\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \]

where we have factored out the common substring. The semicolon denotes string concatenation. In this simple example, the answer indeed factors out on the right. However, notice what happens if we apply this method to the term

\[ |(H (H \ 0))\rangle \rightarrow \frac{1}{\sqrt{2}} \left( |(H (H \ 0)); (H \ 0)\rangle + |(H (H \ 0)); (H \ 1)\rangle \right) \]

\[ \rightarrow \frac{1}{2} |(H (H \ 0))\rangle \otimes \]

\[ \otimes \left( |(H \ 0); 0\rangle + |(H \ 0); 1\rangle + |(H \ 1); 0\rangle - |(H \ 1); 1\rangle \right) \]

Here the answer does not factor out. The fully reduced rightmost term is entangled with the intermediate term in the history.

Note, however, that this scheme keeps more information than necessary. For reversibility, it is sufficient to record at each step only which subterm has been reduced, and the operation that has been applied to it. We may encode this in our example as follows (to be formalized below):

\[ |(H (H \ 0))\rangle \rightarrow \frac{1}{\sqrt{2}} \left( |(\_ (H \_)); (H \ 0)\rangle + |(\_ (H \_)); (H \ 1)\rangle \right) \]

\[ \rightarrow \frac{1}{2} |(\_ (H \_))\rangle \otimes \]

\[ \otimes \left( |(H \_); 0\rangle + |(H \_); 1\rangle + |(H \_); 0\rangle - |(H \_); 1\rangle \right) \]

\[ = |(\_ (H \_)); (H \_) \otimes |0\rangle \]

Here we have at each step replaced subterms that do not need to be recorded by the constant placeholder symbol \_. Now the answer does indeed factor out on the right as required, consistent with \( H^2 |0\rangle = |0\rangle \). It is also clear that at each step we have kept enough information to reconstruct the previous step, thus ensuring reversibility.
The computational model may now be formalized with the following rules: First, we extend our definition of values to include constants as in figure 5. The computational state is taken to be a quantum superposition of sequences of the form

$$h_1; \ldots; h_n; t$$

where $$h_1; \ldots; h_n$$ will be called the **history track** and $$t$$ will be called the **computational register**. The classical subset of the transition rules is shown in figure 6.

$$\begin{align*}
    t_1 & \rightarrow h_1; t'_1 \\
    \mathcal{H}; (t_1 t_2) & \rightarrow \mathcal{H}; (h_1 \_); (t'_1 t_2) & \text{(app}_1) \\
    t_2 & \rightarrow h_2; t'_2 \\
    \mathcal{H}; (v_1 t_2) & \rightarrow \mathcal{H}; (\_ h_2); (v_1 t'_2) & \text{(app}_2) \\
    \mathcal{H}; ((\lambda x. t) v) & \rightarrow \mathcal{H}; ((\lambda x. \_ x) \_); t [v/x] & \text{($\beta_1$) if } x \text{ appears free in } t \\
    \mathcal{H}; ((\lambda x. t) v) & \rightarrow \mathcal{H}; ((\lambda x. \_ v) \_); t & \text{($\beta_2$) if } x \text{ not free in } t \\
    \mathcal{H}; t & \rightarrow \mathcal{H}; \_ ; t & \text{(Id) otherwise}
\end{align*}$$

**Figure 6: Operational model for the classical subset of } \lambda_i$$

In these rules $$\mathcal{H}$$ denotes the (possibly empty) history track, and $$\mathcal{T}_x$$ is obtained from $$t$$ by recursively replacing all subterms that do not contain $$x$$.
with the placeholder symbol and keeping $x$. More formally

\[
\begin{align*}
\bar{t}_x &\equiv x \quad \text{if } x \text{ not free in } t \\
(\lambda y. t)_x &\equiv (\_ \bar{t}_x) \\
(t \ t')_x &\equiv (\bar{t}_x \bar{t'}_x) \\
\overline{t}_x &\equiv x
\end{align*}
\]

These rules are sufficient to make classical computations reversible, provided that lambda terms which differ only by renaming of bound variables have been identified. In this regard, we note here that in a quantum Turing machine model, it is possible to represent terms on the tape of the quantum Turing machine in an unambiguous way (e.g., using De Bruijn indices instead of bound variables) \[7, 8\].

Here is an example computation:

\[
\begin{align*}
|(\text{apply id } \text{ banana}) &\equiv (\text{apply id } (\lambda f. (\lambda x. (f x)) (\lambda z. z) \text{ banana}) \\
\rightarrow |((\lambda f. (\_ (f \_))) \_ \_); (\lambda x. ((\lambda z. z) x) \_ \_)); (\_ \_)); (\_ \_)); (\text{banana}) \\
\rightarrow |((\lambda f. (\_ (f \_))) \_ \_); (\lambda x. ((\lambda z. z) x) \_ \_)); (\_ \_)); (\text{banana}) \\
\rightarrow |((\lambda f. (\_ (f \_))) \_ \_); (\lambda x. ((\lambda z. z) x) \_ \_)); (\_ \_)); (\_ \_)); (\_ \_)); (\text{banana}) \\
\rightarrow |((\lambda f. (\_ (f \_))) \_ \_); (\lambda x. ((\lambda z. z) x) \_ \_)); (\_ \_)); (\_ \_)); (\_ \_)); (\_ \_)); (\_ \_)); (\_ \_)); (\text{banana}) \\
\rightarrow \ldots
\end{align*}
\]

At each step just enough information is kept to reconstruct the previous step. Although in this particular example, termination can be tested by observing and comparing the last expression in the history with \_, in general we do not have a well-defined criterion for termination in the calculus $\lambda_i$, due to the fact that the state may involve a superposition of several computational histories, some of which have terminated and others not. Thus, to observe termination would potentially disturb the state. This problem will be solved in the quantum calculus $\lambda_q$ of section 5.

In addition, we have some extra reduction rules involving the quantum gate symbols such as:

The rules for quantum primitives are summarized in figure 8.

Here $c_U$ denotes any one of the quantum primitive symbols and $U$ the corresponding unitary transformation, while $\phi$ stands for 0 or 1 in the case
\[
|\mathcal{H}; (H \ 0)\rangle \longrightarrow |\mathcal{H}; (H \ 0)\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)
\]

\[
|\mathcal{H}; (H \ 1)\rangle \longrightarrow |\mathcal{H}; (H \ 0)\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)
\]

Figure 7: Operational model for $H$

\[
|\mathcal{H}; (cU \ \phi)\rangle \longrightarrow |\mathcal{H}; (cU\ \phi)\rangle \otimes U |\phi\rangle
\]

Figure 8: Operational model for the quantum primitives of $\lambda_i$

Towards an equational theory

While the language $\lambda_i$ constructed in the previous section can be used to describe quantum computations, reduction in $\lambda_i$ does not correspond to a simple system for equational reasoning. This makes $\lambda_i$ unsuitable as a formal proof system for quantum computation. We will discuss the problem in this section and resolve it in the next with the introduction of the quantum lambda calculus $\lambda_q$.

In the classical lambda calculus, program evaluation through beta reduction can be regarded as a directed form of equational reasoning consistent with the axiom

\[
(\lambda x. t) \ v = t [v/x] \quad (\beta)
\]

Indeed, the classical lambda calculus provides both a model of computation and a formal system for reasoning about functions, a property we would like to keep in the quantum case.

To understand the difficulty, notice what happens when a function application discards its argument (in other words, the argument does not appear...
in the function body). For example
\[ |((\lambda x. \text{apple}) \text{banana}) \rangle \longrightarrow |((\lambda x. \_ \text{banana}); \text{apple}) \rangle \]

We see that in order to maintain reversibility, a record of the argument \text{banana} is kept in the history. Restricting our attention to the computational register, we see that its evolution is consistent with replacing the original expression with an equal expression according to the axiom \((\beta)\). In other words, in this example reduction is consistent with equational reasoning.

However, we run into problems when the discarded subterm is in a quantum superposition with respect to the computational basis. For example, consider the reduction of
\[ |(\lambda x. 0) (H \: 0) \rangle \longrightarrow |(\_ (H \_)) \rangle \otimes \frac{1}{\sqrt{2}} \left( |(\lambda x. 0) \: 0 \rangle + |(\lambda x. 0) \: 1 \rangle \right) \]
\[ \longrightarrow |(\_ (H \_)) \rangle \otimes \frac{1}{\sqrt{2}} \left( |(\lambda x. \_) \: 0 \rangle + |(\lambda x. \_) \: 1 \rangle \right) \otimes |0 \rangle \]

In the second step, a discarded subterm in a superposition is saved in the history and the computational register becomes |0\rangle. However, if we were to apply the axiom \((\beta)\) to the contents of the computational register, we would get the equation
\[ \frac{1}{\sqrt{2}} \left( |(\lambda x. 0) \: 0 \rangle + |(\lambda x. 0) \: 1 \rangle \right) = \sqrt{2} |0 \rangle \]
which is invalid since the right hand side is not a legal normalized state.

As a second example, consider the following computation, where the inner function discards its argument \(x\):
\[ |((\lambda y. ((\lambda x. y) \: y)) (H \: 0))) \rangle \]
\[ \longrightarrow \frac{1}{\sqrt{2}} |(\_ (H \_)) \rangle \otimes \left( |((\lambda y. ((\lambda x. y) \: y)) \: 0) \rangle + |((\lambda y. ((\lambda x. y) \: y)) \: 1) \rangle \right) \]
\[ \longrightarrow \frac{1}{\sqrt{2}} |(\_ (H \_)); ((\lambda y. ((\_ y) \: y)) \_)) \rangle \otimes \]
\[ \otimes \left( |((\lambda x. 0) \: 0) \rangle + |((\lambda x. 1) \: 1) \rangle \right) \]
\[ \longrightarrow \frac{1}{\sqrt{2}} |(\_ (H \_)); ((\lambda y. ((\_ y) \: y)) \_)) \rangle \otimes \]
\[ \otimes \left( |((\lambda x. \_) \: 0) \rangle + |((\lambda x. \_) \: 1) \rangle \right) \]
Now the computational register is entangled with the last expression in the history. Ignoring the history, the computational register would be in a mixed state with density matrix
\[
\begin{pmatrix}
\frac{1}{2} & 0 \\
0 & \frac{1}{2}
\end{pmatrix}
\]
However, an attempt to apply the equational axiom \((\beta)\) to the contents of the computational register would give
\[
\frac{1}{\sqrt{2}} \left( |(\lambda x. 0) 0)\rangle + |(\lambda x. 1) 1)\rangle \right) = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)
\]
which is clearly inconsistent.

5 A quantum lambda calculus

We will resolve the shortcomings of the language \(\lambda_i\) by developing a quantum lambda calculus \(\lambda_q\) which has a consistent equational theory. This section will be somewhat heavier on the formalities, and the reader who wishes to see some concrete examples may wish to skip ahead to section 7 after reading the introductory paragraphs.

The previous discussion suggests that the problems with equational reasoning in the presence of quantum operations can be avoided by preventing functions from discarding arguments which may be in a superposition with respect to the computational basis.

Let us call a subexpression definite with respect to the computational basis if it is textually the same in all branches of the superposition. For example, in the state
\[
\frac{1}{\sqrt{2}} \left( |(\lambda x. 0) 0)\rangle + |(\lambda x. 0) 1)\rangle \right)
\]
the subexpression \((\lambda x. 0)\) is definite, whereas the argument \(\frac{1}{2} (|0\rangle + |1\rangle)\) is non-definite. Definite subexpressions may be thought of as a classical resource. They can be observed without affecting the state of the computation. On the other hand, non-definite subexpressions represent purely quantum resources.

To avoid the problems pointed out in the previous section, we seek a calculus that will keep track of whether an argument is definite or non-definite, and which will make it impossible to write a function that discards
a non-definite resource. Calculi that are resource sensitive, known as linear
lambda calculi, have been studied intensively in recent years [26, 27, 28, 29]. So-called typed linear lambda calculi are very closely related to the
field of linear logic [30, 31]. Linear logic is a resource sensitive logic where,
for example, certain assumptions may only be used once in the course of a
derivation.

For our purposes it will be sufficient to study a simple untyped linear
calculus. The syntax is a fragment of the one introduced in [27], extended
with quantum operations as in figure 9.

\[
\begin{align*}
t ::= & \quad \text{terms:} \\
x & \quad \text{variable} \\
(\lambda x. t) & \quad \text{abstraction} \\
(t t) & \quad \text{application} \\
c & \quad \text{constant} \\
!t & \quad \text{nonlinear term} \\
(\lambda !x. t) & \quad \text{nonlinear abstraction} \\
c ::= & \quad \text{constants:} \\
0 & | 1 | H | S | R_3 | \text{cnot} | X | Y | Z | \ldots
\end{align*}
\]

**Figure 9:** Syntax of the quantum calculus $\lambda q$

Here terms of the form $!t$ are called nonlinear. Nonlinear terms will be
guaranteed to be definite with respect to the computational basis, and may
be thought of physically as classical strings of symbols that may be discarded
and duplicated at will. On the other hand, linear terms may be non-definite,
possibly containing embedded qubits in superpositions with respect to the
computational basis. Abstractions of the form $(\lambda !x. t)$ denote functions of
nonlinear arguments. In an abstraction of the form $(\lambda x. t)$, the argument is
called linear.

A functional abstraction may use a nonlinear argument any number of
times in its body, or not at all. On the other hand, a linear argument must
appear exactly once in the function body (hence the name linear).

To enforce these rules, we require terms to be well-formed. This corre-
sponds to the constraint that linear arguments appear linearly in a function
body, and that all free variables appearing in a term \( !t \) refer to nonlinear variables \([28]\). In the following examples, the terms in the left column are well-formed, while those in the right column are ill-formed \(^2\):

\[
\begin{align*}
(\lambda x. 0) & \quad (\lambda x. 0) \\
(\lambda x. x) & \quad (\lambda x. !x) \\
(\lambda x. (x x)) & \quad (\lambda x. (x x)) \\
(\lambda y. (\lambda x. y)) & \quad (\lambda y. (\lambda x. y)) \\
(\lambda y. !(\lambda x. y)) & \quad (\lambda y. !(\lambda x. y))
\end{align*}
\]

Well-formedness is a property that can be checked syntactically. For completeness, we formally state the rules for well-formedness \([28]\), which the reader satisfied with the above informal characterization may skip, in figure 10.

These rules may be related to the typed linear calculi described in \([28, 27]\) by erasing the type annotations from the typing rules of the latter. Here \( \Gamma \) and \( \Delta \) denote contexts, which are sets containing linearity assumptions of the form \( x \) and \( !x \), where each variable \( x \) is distinct. If \( \Gamma \) and \( \Delta \) are contexts with no variables in common, then \( \Gamma, \Delta \) denotes their union. For example, the rule \( \rightarrow_E \) implicitly assumes that \( \Gamma \cap \Delta = \emptyset \). Rules may be read as follows: For example, the promotion rule says that if \( t \) is a well-formed term under the assumption that \( x_1 \) to \( x_n \) are nonlinear, then \( !t \) is a well-formed term under the same assumption. The condition \( \Gamma \cap \Delta = \emptyset \) in \( \rightarrow_E \) ensures that a linear variable can only appear once in the body of a formula. The weakening and \( \rightarrow_I \) rules allow a function to discard a nonlinear argument, whereas the contraction and \( \rightarrow_E \) rules allow us to duplicate a nonlinear argument any number of times in the body of a function.

The well-formedness constraint prevents us from writing a function which discards a linear argument. However, this is not sufficient to prevent unsafe computations without further specification of the substitution order. To see this, consider the expression \( ((\lambda x. 0) !(H 0)) \), which is well-formed. The problem is that we are allowed to use \( ! \) to promote the expression \( (H 0) \) to a nonlinear value, which can then be discarded. If we were allowed to reduce

\(^2\)Notice that while well-formedness guarantees that linear resources will be used appropriately, it does not guarantee that terms are meaningful. For example the term \( (\lambda y. (\lambda z. 0) y) \) is well-formed, but may or may not get stuck at run-time, according to the operational model of figure 12 when applied to a linear or nonlinear argument respectively. A typed calculus would be needed to specify which terms can be legally substituted for \( y \). For recent progress in this direction, see \([16]\).
\[ \frac{\vdash c}{\Gamma, x \vdash t} \quad \frac{\vdash x}{\vdash x} \quad \frac{\vdash !x_1, \ldots, !x_n \vdash t}{\vdash !x_1, \ldots, !x_n \vdash !t} \quad \frac{\Gamma, x \vdash t}{\Gamma, !x \vdash t} \quad \frac{\Gamma, !x, !y \vdash t}{\Gamma, !z \vdash t \ [z/x, z/y]} \quad \frac{\Gamma \vdash t}{\Gamma, !x \vdash t} \quad \frac{\Gamma, !x \vdash t}{\Gamma \vdash \lambda x. t} \quad \frac{\Gamma \vdash t}{\Gamma \vdash \lambda !x. t} \quad \frac{\Gamma \vdash t_1 \quad \Delta \vdash t_2}{\Gamma, \Delta \vdash (t_1 \ t_2)} \]

\[ \text{Const} \quad \text{Id} \quad \text{Pomotion} \quad \text{Dereliction} \quad \text{Contraction} \quad \text{Weakening} \quad \text{\textit{\small -I}} \quad \text{\textit{\small \rightarrow-I}} \quad \text{\textit{\small -E}} \]

Figure 10: Rules for well-formed terms in the quantum calculus $\lambda_q$

the subterm $(H \ 0)$ first, equational reasoning would give

\[
|((\lambda !x. \ 0) \ !(H \ 0))) = \frac{1}{\sqrt{2}} \left(||((\lambda !x. \ 0) \ !0)|| + ||((\lambda !x. \ 0) \ !1)||\right) \\
= \sqrt{2} |0\rangle
\]

which is an invalid equation since the last line is not a valid normalized state. On the other hand, if we consider $!(H \ 0)$ as an irreducible value, we may use beta reduction immediately to obtain

\[
|((\lambda !x. \ 0) \ !(H \ 0))) = |0\rangle
\]

which is a valid result, since we are discarding the unevaluated expression $!(H \ 0)$, which is definite.

20
To prevent terms of the form !t from being evaluated, we follow Abramsky \cite{abramsky1994} and extend our definition of values as in figure 11.

\[
v ::= \text{values: } \\
x \quad \text{variable} \\
c \quad \text{constant} \\
(\lambda x. t) \quad \text{linear abstraction} \\
(\lambda! x. t) \quad \text{nonlinear abstraction} \\
!t \quad \text{!-suspension}
\]

Figure 11: Values in the quantum calculus \(\lambda_q\)

The computational model is described in figure 12, where \(\bar{t}\) is defined as in \(\bar{t}\).

\[
\begin{align*}
t_1 \rightarrow h_1; t'_1 & \quad (\text{app}_1) \\
\mathcal{H}; (t_1 t_2) \rightarrow \mathcal{H}; (h_1 \_); (t'_1 t_2) \\
t_2 \rightarrow h_2; t'_2 & \quad (\text{app}_2) \\
\mathcal{H}; (v_1 t_2) \rightarrow \mathcal{H}; (\_ h_2); (v_1 t'_2) \\
\mathcal{H}; ((\lambda x. t) v) \rightarrow \mathcal{H}; ((\lambda x. \bar{t}_x) \_); t [v/x] & \quad (\beta) \\
\mathcal{H}; ((\lambda! x. t) !t') \rightarrow \mathcal{H}; ((\lambda! x. \bar{t}_x) \_); t [t'/x] & \quad (!\beta_1) \text{ if } x \text{ appears free in } t \\
\mathcal{H}; ((\lambda! x. t) !t') \rightarrow \mathcal{H}; ((\lambda! x. \_ !t')}; t & \quad (!\beta_2) \text{ if } x \text{ not free in } t \\
|\mathcal{H}; (c_U \phi) \rangle \rightarrow |\mathcal{H}; (c_U \_\_ \_)); \otimes U |\phi\rangle & \quad (U) \\
\mathcal{H}; t \rightarrow \mathcal{H}; \_ \_; t & \quad (\text{Id}) \text{ otherwise}
\end{align*}
\]

Figure 12: Operational model for the quantum lambda calculus \(\lambda_q\)

According to these rules, quantum superpositions can only be created by evaluating terms containing quantum primitives. The result of applying a

\footnote{See \cite{abramsky1994, olejnik1997, olejnik2000} for related operational interpretations of linear lambda calculi. Our evaluation model recomputes !-closures (see \cite{olejnik2000}).}
quantum gate is a linear value, not preceded by a !. As we prove below, there is no way of including such a linear value in a nonlinear subterm. It follows that subterms that may be quantum non-definite will never be discarded since, by (!\(\beta_1\)) and (!\(\beta_2\)), nonlinear functions can only be applied to nonlinear terms.

Note that when a nonlinear function encounters a linear argument, it simply gets stuck. More precisely, the rule (Id) applies.

The above reduction rules may create superpositions. However, such superpositions are not arbitrary. Indeed, terms in a superposition will only differ in positions containing the constants 0 and 1. Otherwise they will have the same shape. We may formalize this by defining two terms to be congruent if they coincide symbol by symbol except possibly in positions containing 0 or 1. It then follows that

**Lemma 5.1.** All terms in a superposition obtained via a reduction sequence from a definite initial term are congruent.

**Proof.** The proof is by a simple induction on the length of the reduction sequence, analyzing the reduction rules case by case. \(\square\)

Another case by case induction argument may be used to prove that reduction preserves well-formedness. More precisely

**Lemma 5.2.** If \(t\) is well-formed and \(|H; t\rangle \rightarrow \sum_i c_i |H'_i; t'_i\rangle\), then all terms \(t'_i\) appearing in the resulting superposition are well-formed.\(^4\)

Because terms appearing in a superposition have the same shape, it makes sense to talk about specific subterms of the expression in the computational register. We can therefore formulate the following lemma:

**Lemma 5.3.** Starting from a definite initial term, any !-suspension subterm occurring during reduction is definite with respect to the computational basis.

**Proof.** This follows by induction on the length of the reduction sequence. The initial term is definite by assumption. Assume that the lemma holds after \(n\) steps. We have argued that all terms in a superposition obtained from a definite initial term are congruent. They therefore have the same

---

\(^4\)Thanks to one of the referees for suggesting improvements in the exposition of this section.
structure of subterms and the same reduction rule applies to them all. Since we have argued that these terms are well-formed, there are then three ways in which we may obtain a !-suspension subterm after \( n + 1 \) steps. First, the suspension may not be part of the redex, in which case it is included unmodified in the resulting expression. Second, it may be the result of beta reduction of an application of the form

\[
(\lambda x. (\cdots x \cdots)) \ (\cdots t \cdots)
\]

where \( t \) is definite by the induction assumption. The result is \((\cdots (\cdots t \cdots) \cdots)\), where \( t \) has been copied without modification. Third, it may be the result of beta reduction of an application of the form

\[
(\lambda !x. \cdots !(\cdots x \cdots) \cdots) \ t
\]

where \( t \) and \( !(\cdots x \cdots) \) are definite by the induction assumption. This creates a suspension \( !(\cdots t \cdots) \), which is definite because all its subterms are definite. This completes the proof.

It is worth pointing out that we cannot create possibly non-definite suspensions by reducing terms like

\[
(\lambda x. \cdots !(\cdots x \cdots) \cdots) \ (H \ 0)
\]

because \( x \) is linear, which implies that \( !(\cdots x \cdots) \) is not a well-formed subterm.

**Lemma 5.4.** Given a definite initial term, the contents of the history track remains definite throughout reduction.

**Proof.** We have argued that all terms in a superposition obtained from a definite initial term are congruent. They therefore have the same structure of subterms and the same reduction rule applies to them all. Since our reduction rules allow only !-suspensions to be discarded (which saves a copy in the history), and since !-suspensions are always definite by the previous lemma, the result follows by induction on the length of the reduction sequence.

Since both the history and the shape of the term in the computational register remain definite throughout reduction, we can state the following conclusion.

Corollary 5.5. Termination can be tested without disturbing the computation by observing the last term in the history. When this term becomes equal to the placeholder $\_\_$, the result can be read off from the computational register.

Not only is termination a “classical” property, but so is the entire shape of the term itself, i.e., term shapes can be implemented in classical memory, and only their data slots need to point to qubits on a quantum device.\(^5\)

The fact that the history remains definite in $\lambda_q$ eliminates the specific impediments to setting up an equational theory that were pointed out in the previous section. Indeed, since the state of the computation is now always guaranteed to be a direct product $|H\rangle \otimes |c\rangle$ of the history $|H\rangle$ and the computational register $|c\rangle$, reduction can never lead to a computational register $|c\rangle$ that is in a mixed state. In addition, since $|H\rangle$ remains definite, the restriction of the reduction rules to the computational register will preserve the normalization. We are therefore led to the following theorem:

\[
\begin{align*}
& t_1 \rightarrow t'_1 \\
& (t_1 t_2) \rightarrow (t'_1 t'_2) \quad (app_1) \\
& t_2 \rightarrow t'_2 \\
& (v_1 t_2) \rightarrow (v'_1 t'_2) \quad (app_2) \\
& (\lambda x. t) v \rightarrow t [v/x] \quad (\beta) \\
& (\lambda !x. t) !t' \rightarrow t [t'/x] \quad (!\beta) \\
& |cU \phi\rangle \rightarrow U |\phi\rangle \quad (U)
\end{align*}
\]

Figure 13: Reduction rules for the quantum calculus $\lambda_q$

Theorem 5.6. In the quantum calculus $\lambda_q$, the evolution of the computational register is governed by the reduction rules of figure 13.

Proof. This easily follows from a case-by-case analysis of the computational rules of figure 12.

\(^5\)I would like to thank one of the referees for suggesting this improved formulation.
For example, consider the rule (!β2) applied to a state of the form |H⟩⊗|c⟩ where |c⟩ is a normalized superposition of the form

\[ \sum_i c_i |(\cdots i ((λ!x. t_i) !t') \cdots i)⟩ \]

in which, by lemma 5.1, all terms have the same structure and by lemma 5.3 the subterm !t' does not depend on i. This then reduces to

\[ |H⟩ ⊗ \sum_i c_i |(\cdots i (λ!x. t_i) !t') \cdots i)⟩ \]

= \[ |H; (\cdots i (λ!x. t_i) !t') \cdots i)⟩ ⊗ \sum_i c_i |(\cdots i t_i [t'/x] \cdots i)⟩ \]

with the computational register in the normalized state \[ \sum_i c_i |(\cdots i t_i [t'/x] \cdots i)⟩ \], consistent with applying the reduction rule (λ!x. t_i) !t' → t_i [t'/x] to its contents.

The big win is that we now have a simple set of reduction rules that can be used to reason about the computation without having to keep track of the history.

In order to define an equational theory for this calculus, we will simply define a notion of equality that is compatible with the the reduction rules of figure 13. Intuitively, reduction should be understood as a simple algebraic operation of replacing subterms with equal subterms. However, we need to take into account that reduction may not take place inside !-suspending.

We therefore need to introduce algebraic rules governing just when we can replace subterms in an expression with equal subterms [20, 21]. One way to do that is to introduce the notion of a term context, which are expressions with a hole [ ] in place of a subexpression:

\[ C, C_i ::= [ ] | (t C) | (C t) | (λx. C) | (λ!x. C) | \sum_i c_i C_i, \]

where the last term denotes a superposition of shape-congruent contexts. It is important to note that there are no contexts of the form !([\cdots [ ] \cdots]). As a result, subterms preceded by ! will be opaque in the sense that we will not be able to perform substitutions under the ! sign.
**Definition 5.7.** The equational theory of $\lambda_q$ is the least equivalence relation $\equiv$ containing the reduction relation ($\rightarrow$) of figure 13 and which is closed under substitution in term contexts [20, 21]. In other words

$$\frac{t_1 = t_2}{C[t_1] = C[t_2]} \quad (\text{subst})$$

where $C$ is an arbitrary term context and $C[t]$ denotes the textual replacement of the hole in $C$ by the term $t$, extended by linearity to superpositions of congruent terms and congruent contexts, i.e., for $t = \sum_i c_i t_i$, we define $C[t] = \sum_i c_i C[t_i]$ and for $C = \sum_i c_i C_i$, we define $C[t] = \sum_i c_i C_i[t]$.

An alternative way of presenting the equational theory is by listing a set of axioms and rules of inference as in figure 14. These rules should again be understood as extending via linearity to congruent superpositions of terms. In this formulation, the rules ($\text{app}$), ($\lambda_1$) and ($\lambda_2$) are together equivalent to

\begin{align*}
& t = t \quad (\text{refl}) \\
& \frac{t_1 = t_2}{t_2 = t_1} \quad (\text{sym}) \\
& \frac{t_1 = t_2 \quad t_2 = t_3}{t_1 = t_3} \quad (\text{trans}) \\
& \frac{t_1 = t_2 \quad t_3 = t_4}{(t_1 \ t_3) = (t_2 \ t_4)} \quad (\text{app}) \\
& \frac{t_1 = t_2}{\lambda x. t_1 = \lambda x. t_2} \quad (\lambda_1) \\
& \frac{t_1 = t_2}{\lambda! x. t_1 = \lambda! x. t_2} \quad (\lambda_2) \\
& (\lambda x. t) \ v = t \ [v / x] \quad (\beta) \\
& (\lambda! x. t) \ !t' = t \ [t' / x] \quad (!\beta) \\
& |(cU \ \phi)) = U \ |\phi \rangle \quad (U)
\end{align*}

**Figure 14:** Equational proof system for the quantum calculus $\lambda_q$
the term context substitution rule \((\text{subst})\) above. Again, there is no rule that permits substitutions inside \(!\)-suspensions.

**Theorem 5.8.** In the quantum lambda calculus, the evolution of the computational register proceeds by replacing terms by equal terms according to the equational theory of definition 5.7.

**Proof.** True by construction. \(\square\)

### 6 Recursion and a fixed point operator

Recursive functions may be defined in the calculus \(\lambda_q\) in a way analogous to that described in section 2. We simply replace \((t \ t)\) in equation (1) with \((t \ !t)\), where now \(t \equiv \lambda f. (\cdots (f \ !f) \cdots)\).

Here we describe a related approach based on so-called fixed point combinators. A fixed point operator suitable for the linear lambda calculus is given by the following adaptation of the classical Turing combinator

\[
\text{fix} \equiv ( (\lambda u. \lambda f. ((u \ !u) \ !f)) \\
\quad \quad \quad \quad \quad \quad (\lambda u. \lambda f. ((u \ !u) \ !f)))
\]

It is easy to check that under reduction

\[
\text{fix} \ !t \rightarrow u [\text{fix} \ !t]/f
\]

where the \(!\)-suspension prevents further reduction of the term in brackets. Recursive functions can be defined as follows: If

\[
t \equiv \lambda f. u
\]

then it easily follows that

\[
\text{fix} \ !t \rightarrow u [(\text{fix} \ !t)/f]
\]

In other words, \(\text{fix} \ !t\) copies itself into the body \(u\) of \(t\) under reduction, as required for recursion.
7 Examples of algorithms

We are now ready to formulate some algorithms in the quantum lambda calculus. First, we reproduce some classical constructions, now decorated with the proper nonlinearity annotations.

First, we introduce list constructors that will enable us to build lists of linear values (qubits or structures containing qubits)

\[
\begin{align*}
() & \equiv \lambda x. \lambda y. (x \text{id}) \\
\text{cons} & \equiv \lambda h. \lambda t. \lambda x. \lambda y. ((y h) t)
\end{align*}
\]

with abbreviations \( h : t \equiv (\text{cons} h t) \) and \( (x_1, \ldots, x_n) \equiv x_1 : x_2 : \cdots : x_n : () \) as before. Since the arguments \(!x\) and \(!y\) above are nonlinear, we need to redefine our \text{case} abbreviation as follows:

\[
\text{case } t_1 \text{ of } (() \to t_2, h : t \to t_3)
\]

now stands for

\[
t_1 !((\lambda z. t_2) !((\lambda h. \lambda t. t_3))
\]

Deutsch’s algorithm \cite{1,5} can be very simply expressed as follows:

\[
\text{deutsch } U_f \rightarrow \text{let } (x, y) = U_f ((H 0), (H 1)) \text{ in } ((H x), y)
\]

Here the argument \(U_f\) is assumed to be a function that takes \((x, y)\) to

\[
(x, y \oplus f(x)), \text{ where } f \text{ is some (unknown) function of one bit. For example, if } f \text{ is the identity function, then we should take } U_f \text{ to be cnot. Indeed, the reader may check that}
\]

\[
|\text{deutsch cnot}\rangle \rightarrow |1\rangle \otimes \frac{1}{2} \left(|0\rangle - |1\rangle \right).
\]
where the first bit $1 = f(0) \oplus f(1)$ indicates that the function is balanced, as required.

Let us write a simple expression that creates an EPR pair

$$\text{epr} \equiv \text{cnot } ((H \ 0), 0)$$

The quantum teleportation gate array with deferred measurement [34, 5] can easily be translated into the following code: We create an EPR pair and pass the first EPR qubit, along with the unknown qubit $x$ to be teleported, to Alice. The outcome $(x', y')$ of Alice’s computation then gets sent to Bob, who has access to the second EPR qubit $e_2$

$$\text{teleport } x \rightarrow \text{let } (e_1, e_2) = \text{epr} \text{ in}$$
$$\text{let } (x', y') = \text{alice } (x, e_1) \text{ in}$$
$$\text{bob } (x', y', e_2)$$

Here

$$\text{alice } (x, e_1) \rightarrow \text{let } (x', y') = \text{cnot } (x, e_1) \text{ in } ((H \ x'), y')$$

and

$$\text{bob } (x', y', e_2) \rightarrow \text{let } (y'', e'_2) = \text{cX } (y', e_2) \text{ in}$$
$$\text{let } (x'', e''_2) = \text{cZ } (x', e'_2) \text{ in}$$

$$(x'', y'', e''_2)$$

The outcome of the computation consists of the list of three qubits $(x'', y'', e''_2)$. The teleported qubit is $e''_2$, but notice how linearity requires us to keep the other two qubits in the answer. The reader may check that throughout the computation, linear arguments are used exactly once. Implementing the
conditional operations \( cX \) and \( cZ \) in terms of the primitive constants is left as an easy exercise.

Given recursion and lists, the map function, which applies a given function \( f \) to each element of a list, may be defined as

\[
\text{map } ! f \text{ list } \rightarrow \text{case list of } \begin{cases} \() \rightarrow () \\ h : t \rightarrow (f \ h) : (\text{map } ! f \ t) \end{cases}
\]

The arguments \( \text{list, } h \text{ and } t \) may refer to qubits or data structures containing qubits and are therefore chosen linear. The expression is well-formed because \( \text{list, } h \text{ and } t \) are each used exactly once.

It is now trivial to define a program that computes a uniform superposition of a list of qubits by applying the Hadamard gate to each qubit in the list:

\[
H^{\otimes n} \text{ list } \rightarrow \text{map } ! H \text{ list}
\]

For example, we may evaluate

\[
\left| H^{\otimes n} (0,0) \right> \rightarrow \frac{1}{2} \left( |(0,0)> + |(0,1)\rangle + |(1,0)> + |(1,1)> \right)
\]

Note that the well-formedness conditions may be somewhat subtle, as the following example illustrates. A naive attempt at defining an append function that concatenates two linear lists

\[
\text{append } x \ y \rightarrow \text{case } x \text{ of } \begin{cases} \() \rightarrow y \\ h : t \rightarrow h : (\text{append } t \ y) \end{cases}
\]

fails to be well-formed. The problem can be seen by expanding the case abbreviation

\[x \ !(\lambda z. \ y) \ !(\lambda h. \ \lambda t. \ (h : (\text{append } t \ y)))\]

Since \( y \) is a linear variable, we may not promote the \( \lambda \) subterms to nonlinear values with the prepended \(!\). An alternative definition that does work is

\[
\text{append } x \ y \rightarrow \left( \text{case } x \text{ of } \begin{cases} \() \rightarrow (\lambda u. \ u) \\ h : t \rightarrow \lambda u. \ (h : (\text{append } t \ u)) \end{cases} \right) y
\]

Next we define a reverse function

\[
\text{reverse } \text{list } \rightarrow \text{case } \text{list of } \begin{cases} \() \rightarrow () \\ h : t \rightarrow \text{append } (\text{reverse } t) \ (h) \end{cases}
\]
The quantum Fourier transform \cite{35, 36, 37} can now be defined as a direct translation of the corresponding quantum circuit \cite{34} as follows:

$$\text{fourier list} \rightarrow \text{reverse fourier'} list$$

where

$$\text{fourier'} list \rightarrow \text{case list of} \begin{cases} () \rightarrow () \hfill \\
 h : t \rightarrow \text{let } h' : t' = \text{phases } (H \ h) \ t \ 1/2 \text{ in } \\
 h': (\text{fourier'} t') \hfill 
\end{cases}$$

recursively applies the appropriate conditional phase operations to the first qubit in the list, using the helper function

$$\text{phases target controls } \downarrow n$$

$$\rightarrow \text{case controls of} \begin{cases} () \rightarrow (\text{target}) \\
 \text{control} : t \rightarrow \text{let } (\text{control}', \text{target}') \\
 = (cR \ n) \ (\text{control}, \text{target}) \text{ in} \\
 \text{let } \text{target}'' : t' \\
 = \text{phases target'} t' \ (\text{succ } n) \text{ in} \\
 \text{target}'' : \text{control}' : t' \hfill 
\end{cases}$$

Here \((cR \ n)\) composes an appropriate combination of elementary gates to implement a conditional phase operation with phase \(2\pi i/2^n\). Since this is
essentially a classical computation and depends on the particular set of primitive constants chosen, we will not write it out here.

Note that we have assumed that the classical construction of the natural numbers may be adapted to the quantum lambda calculus. That this is possible for all classical constructions follows from the fact that there is an embedding of the classical lambda calculus into the linear lambda calculus, as shown in formula (4) of section 8.

8 Relating $\lambda_q$ to quantum Turing machines

In this section we will sketch a proof of the following theorem, leaving a more rigorous analysis to future work:

\textbf{Theorem 8.1.} The computational model provided by the quantum lambda calculus $\lambda_q$ is equivalent to the quantum Turing machine.

\textit{Proof.} First, we argue that the quantum lambda calculus $\lambda_q$ may be efficiently simulated on a quantum Turing machine.

In $\lambda_q$ the current state of the computation consists of a superposition of term sequences of the form $\mathcal{H}; t$, which may be encoded as strings of symbols on the tape of the quantum Turing machine. By lemma 5.1 term sequences in different branches of the superposition are congruent, and the same reduction rule will apply for all branches at each time step. The subset of $\lambda_q$ not involving quantum operations consists of a set of reversible classical rewritings, which can be unitarily and efficiently implemented on a quantum Turing machine by [2, 38, 39]. The fragment involving quantum operators again involves simple classical rewritings followed by a unitary transformation involving one or two symbols on the tape. Once again, the methods of [2, 38, 39] may be used to construct a quantum Turing machine that can execute these transformations. This completes the proof of the first half of the equivalence.

Next we argue that a quantum Turing machine can be efficiently simulated by the calculus $\lambda_q$.

Yao shows in [4] that for any quantum Turing machine $T$, there is quantum circuit $C_{n,t}$ that efficiently simulates $T$ on inputs of size $n$ after $t$ steps. The circuit family $C_{n,t}$ may be efficiently constructed via a classical computation. But $\lambda_q$ is universal for classical computation. This follows from the
fact that the classical call-by-value lambda calculus may be embedded in $\lambda_q$ via the following translation, adapted from \cite{28}:

\[
(t_1 \ t_2)^* = ((\lambda z. z) \ t_1^*) \ t_2^* \\
x^* = !x \\
(\lambda x. t)^* = !(\lambda x. t^*)
\]

So, given the specification of a quantum Turing machine and an input of length $n$, a classical computation in $\lambda_q$ first constructs a representation of the appropriate quantum circuit family $C_{n,t}$. It then follows the circuit diagram and applies the appropriate quantum operations one by one to the input. Since $\lambda_q$ has primitive quantum operations available corresponding to a universal set of quantum gates, this proves the second half of the equivalence. \hfill $\square$

9 Related work

In a series of papers, Henry Baker \cite{40, 41, 42} develops an untyped linear language based on Lisp. His language is similar to the classical fragment of the lambda calculus developed in the current article. It served as the initial inspiration for the linear approach followed here.

Ideas stemming from linear logic have been used previously by Abramsky in the study of classical reversible computation \cite{43}.

One of the earlier attempts at formulating a language for quantum computation was Greg Baker’s Qgol \cite{44}. Its implementation (which remained incomplete) used so-called uniqueness types (similar but not identical to our linear variables) for quantum objects \cite{45}. The language is not universal for quantum computation.

The language QCL, developed by Ömer, is described in \cite{46, 47}. QCL is an imperative language with classical control structures combined with special operations on quantum registers. It provides facilities for inverting quantum functions and for scratch space management. No formal program calculus is provided. A simulator is publicly available.

Another imperative language, based on C++, is the Q language developed by Bettelli, Calarco and Serafini \cite{48}. As in the case of QCL, no formal calculus is provided. A simulator is also available.
A more theoretical approach is taken by Selinger in his description of the functional language QPL [49]. This language has both a graphical and a textual representation. A formal semantics is provided.

The imperative language qGCL, developed by Sanders and Zuliani [50], is based on Dijkstra’s guarded command language. It has a formal semantics and proof system.

A previous attempt to construct a lambda calculus for quantum computation is described by Maymin in [51]. However, his calculus appears to be strictly stronger than the quantum Turing machine [52]. It seems to go beyond quantum mechanics in that it does not appear to have a unitary and reversible operational model, instead relying on a more general class of transformations. It is an open question whether the calculus is physically realizable.

A seminar by Wehr [53] suggests that linear logic may be useful in constructing a calculus for quantum computation within the mathematical framework of Chu spaces. However, the author stops short of developing such a calculus.

Abramsky and Coecke describe a realization of a model of multiplicative linear logic via the quantum processes of entangling and de-entangling by means of typed projectors. They briefly discuss how these processes can be represented as terms of an affine lambda calculus [54].

10 Conclusion

In this article we developed a lambda calculus $\lambda_q$ suitable for expressing and reasoning about quantum algorithms. We discussed both its computational model and its equational proof system. We argued that the resulting calculus provides a computational model equivalent to the quantum Turing machine and is therefore universal for quantum computation.

There are many possible directions for future work. The proof of Turing equivalence should be fleshed out. Formal issues relating to consistency and semantics need to be addressed further. While our computational model provides an operational semantics, the problem of providing a denotational semantics is open. The formalism of [55] may be useful in this regard.

In this article, the introduction of a linear calculus was motivated by requiring consistency of its operational model with equational reasoning. The fact that linear arguments, denoting quantum resources, may not be dupli-
cated suggests a separate motivation for linearity, not addressed here, based on the no-cloning theorem [56, 57].

While our calculus is untyped, it would be interesting to investigate typed linear calculi with quantum primitives and, via the Curry-Howard correspondence, the corresponding generalizations of linear logic [58, 59]. We might mention that there have been prior attempts to relate linear logic to quantum mechanics, starting with a suggestion by Girard [30, 60, 61].

On the practical side, the calculi described in this paper may be used as a programming language for prototyping quantum algorithms. Indeed, the algorithms exhibited in this article were transcribed into Scheme for testing. The simulator, which was also written in Scheme, is available upon request from the author.

It is our hope that the field of quantum computation, like its classical counterpart, may benefit from the insights provided by the alternative computational model provided by the quantum lambda calculus.

Note added

Since the first version of this paper was written, some progress has been made by the author in devising a typed version, with accompanying denotational semantics, of a fragment of the quantum calculus described here [16].

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