Formal Methods for Quantum Programs: A Survey

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Abstract

While recent progress in quantum hardware open the door for significant speedup in certain key areas (cryptography, biology, chemistry, optimization, machine learning, etc), quantum algorithms are still hard to implement right, and the validation of such quantum programs is a challenge. Moreover, importing the testing and debugging practices at use in classical programming is extremely difficult in the quantum case, due to the destructive aspect of quantum measurement. As an alternative strategy, formal methods are prone to play a decisive role in the emerging field of quantum software. Recent works initiate solutions for problems occurring at every stage of the development process: high-level program design, implementation, compilation, etc. We review the induced challenges for an efficient use of formal methods in quantum computing and the current most promising research directions.
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1 Introduction

Cryptography and quantum information. Quantum computing birth act is usually dated back from 1982, when Richard Feynman raised the idea [58] of simulating quantum mechanics phenomena by storing information in particles and controlling them according to quantum mechanics laws. In the brief history of quantum computing, the description in 1994 by Peter Shor of an algorithm [149] performing the decomposition of prime integers in polynomial time on the size of the input, plays a major role. Indeed, it was the first ever described quantum algorithm with a practical utility – breaking the RSA public key cryptosystems in a tractable manner.

In an asymmetric cryptosystem such as RSA, information is encrypted via a key that is a solution for a given mathematical function – the decomposition of a given integer into prime factors for the case of RSA. The security of such a protocol is based on the fundamental assumption that no potential eavesdropper has means to compute this solution efficiently. Shor’s algorithm is based on (1) a reduction of the prime factor decomposition problem into the order-finding problem and (2) an adequate use of quantum parallelism to perform modular exponentiation of integers over many different inputs in a single row, enabling a polynomial resolution of the order-finding. Thus, the computation time for performing the prime decomposition is reduced from exponential to polynomial, and therefore breaks RSA’s fundamental assumption. Shor’s original article [149] also presents a variation of the order-finding resolution algorithm, solving the discrete logarithm problem with similar performances. Doing so, it brings a procedure for breaking elliptic curve cryptosystems.

Symmetric-key cryptosystems are also challenged by quantum computing [140]. As an example, Simon quantum algorithm [151] brings an exponential speedup for computing the period of a function (given the promise that this period indeed exists). Several applications in public-key cryptosystems were described, providing exponential gain in, e.g., distinguishing a three-round Feistel construction [104, 140], key recovering in the Evan Mansour encryption scheme [105] and attacking the CBC-MAC message authentication scheme [140].

Finally, Grover search quantum algorithm [72] brings a quadratic speedup in the search for a distinguished element in unstructured databases. Hence, while the complexity gain is less decisive here than for the procedures introduced above, its potential for cryptography is significant as it weakens any symmetric-key encryption system.

Thus, quantum computing challenges current cryptographic uses and practices. Shor’s algorithm opened a research program for cryptographic solutions resisting quantum computation power, called post-quantum cryptography [30].

Interestingly the post-quantum cryptography challenge also received answers from quantum information itself. Indeed, one of the major distinctive feature of quantum information is that, basically, it cannot be read without being affected. This entails that an eavesdropper trying to access a quantum information exchange cannot help betraying her attempt. Based on this feature, one can encode a cryptographic key in a quantum message and, in case of eavesdropping, detect it a posteriori, renounce to this particular key and try another sending. Quantum key distribution protocols is an active research area [141, 18, 113, 119].

Quantum computing and quantum software. These cryptographic aspects are one over many applications for the young research field of quantum computing. Others are, e.g., machine learning [19, 143, 118], optimization [54], solving linear systems [74], etc. In all these domains there are quantum algorithms beating the best known classical algorithms by quadratic or even exponential factors, complexity-wise.

These algorithms are based on laws and phenomena specific to quantum mechanics (such as quantum superposition, entanglement, unitary operations). Therefore, implementing them requires
both a dedicated hardware (quantum computers) and a dedicated software framework (quantum programming languages and compilation toolchains).

In the last 20 years, several such languages have been proposed, such as Qiskit [132], Liqui⟩ [165], Q# [155], Qupfer [71], ProjectQ [154], etc. Still, the field is in its infancy, and many questions need still to be answered before we can reach the level of maturity observed for classic programming languages. Still standing questions include for example foundational computing model and semantics for quantum programming languages, adequate programming abstractions and type systems, or the ability to interact with severely constrained hardware in an efficient way (optimizing compilers).

Verification of quantum programs. While testing and debugging are the common verification practice in classical programming, they become extremely complicated in the quantum case. Indeed, debugging and assertion checking are a priori very complicated due to the destructive aspect of quantum measurement (see Section 2.3.1 below). Moreover, the probabilistic nature of quantum algorithms seriously impedes system-level quantum testing. Finally, classical emulation of quantum algorithms is (strongly believed to be) intractable.

On the other hand, nothing prevents a priori the formal verification [34] of quantum programs, i.e. proving by (more or less) automated reasoning methods that a given quantum program behaves as expected for any input, or at least that it is free from certain classes of bugs.

Interestingly, while formal methods were first developed for the classic case where they are still used with parsimony – mainly for safety-critical domains – as testing remains the main validation methods, their application to quantum computing could become more mainstream, due to the inherent difficulties of testing quantum programs.

Goal of this chapter This chapter introduces both the requirements and challenges for formal methods in quantum computing, and the existing propositions to overcome these challenges.

The first sections give the general background. In Section 2 we introduce the main concepts at stake with quantum computing and quantum algorithms. We also need a state of the art introduction for formal methods, given in Section 3. The specific requirements for formal reasoning in the quantum case is then developed in Section 4. Then we come to concrete quantum programming and formal verification material. In Section 5 we introduce several existing solutions for the formal verification of quantum compilation and the equivalence of quantum program runs. Generating such runs requires specific programming languages. The formal interpretation of quantum languages is introduced in Section 6. Then in Section 7 we present the main existing solution for formally verified quantum programming languages. In Section 8 we introduce references for further usage of formal methods linked with quantum information, and we conclude this chapter with a discussion in Section 9.

2 General Background in Quantum Computing

By many aspects, quantum computing constitutes a new paradigm. Making great use of quantum superposition and quantum entanglement, it requires to define proper versions for such fundamental concepts as data structures at stake in computation, or the elementary logical operations at use. We introduce the well-known hybrid quantum computation model in Section 2.1.

Quantum computers are not intended to, and will not, replace classical ones. One should better see the opening of a new field, with possibilities to solve new problems. Section 2.2 presents these new problems and introduces quantum algorithms design.
As a new software technology, quantum computing comes with specific challenges and difficulties. These specificities are closely related to the particular needs for formal reasoning in quantum computing. They are introduced in Section 2.3.

2.1 Hybrid Computational Model

Let us first introduce the main concepts at stake in quantum programming. They concern the architecture of quantum computers, the structure of quantum information and quantum programs, and their formal interpretation.

2.1.1 Hybrid Circuit Model

The vast majority of quantum algorithms are described within the context of the quantum co-processor model [101], i.e., an hybrid model where a classical computer controls a quantum co-processor holding a quantum memory, as shown in Figure 1. The co-processor is able to apply a fixed set of elementary operations (buffered as quantum circuits) to update and query (measure) the quantum memory. Importantly, while measurement allows to retrieve classical (probabilistic) information from the quantum memory, it also modifies it (destructive effect).

![Figure 1: Scheme of the hybrid model](image)

Major quantum programming languages such as QUIPPER [71], LIQUI|⟩[165], Q# [155], PROJECTQ [154], SILQ [20], and the rich ecosystem of existing quantum programming frameworks [133] follow this hybrid model.

2.1.2 Quantum Data Registers

The following paragraphs introduce several definitions and notations for quantum data registers. In particular, we follow the standard Dirac notation. For more details about this content, we refer the reader to the standard literature [124].

Kets and basis-kets. While in classical computing the state of a bit is one between two possible states (0 or 1), in quantum computing the state of a quantum bit (or qubit) is described by amplitudes over the two elementary values 0 and 1 (denoted |0⟩ and |1⟩), i.e., linear combinations \( \alpha_0 |0⟩ + \alpha_1 |1⟩ \) where \( \alpha_0 \) and \( \alpha_1 \) are any complex values satisfying \( |\alpha_0|^2 + |\alpha_1|^2 = 1 \). In a sense, amplitudes are generalization of probabilities.

More generally, the state of a qubit register of \( n \) qubits (called a ket of length \( n \) — dimension \( 2^n \)) is a column vector with \( 2^n \) rows, formed as a superposition of the \( 2^n \) elementary basis vectors.
of length \( n \) (the “basis kets”), i.e. a ket is any linear combination of the form

\[
|u\rangle_n = \sum_{k=0}^{2^n-1} \alpha_k |k\rangle_n
\]

such that \( \sum_{k=0}^{2^n-1} |\alpha_k|^2 = 1 \).

**Bit-vectors and basis kets.** Depending on the context, it may be more convenient to index the terms in the sum above with bit vectors instead of integers. We call bit vector of length \( n \) any sequence \( x_0x_1 \ldots x_{n-1} \) of elements in \{0, 1\}. Along this chapter, we assume the implicit casting of these values to/from booleans (with the least significant bit on the right). For any positive \( n \), we denote the set of bit vectors of size \( n \) by \( BV_n \). We also surcharge notation \( |j\rangle_n \) shown above with bit vector inputs. Formally, for any bitvector \( \vec{x} \) of length \( n \), \( |\vec{x}\rangle_n = |\sum_{i=0}^{n-1} x_i \cdot 2^{n-1-i}\rangle_n \). Hence, one can write state \( |u\rangle_n \) from (1) as

\[
|u\rangle_n = \sum_{\vec{x} \in BV_n} \alpha_{\sum_{i=0}^{n-1} x_i \cdot 2^{n-1-i}} |\vec{x}\rangle_n
\]

It may also be convenient to represent basis kets through their index’s binary writing. For example, the two qubits basis is equivalently given as \{ |0\rangle_2, |1\rangle_2, |2\rangle_2, |3\rangle_2 \} or as \{ |00\rangle, |01\rangle, |10\rangle, |11\rangle \}.

We omit the length index \( n \) from notation \( |u\rangle_n \) when it is either obvious from the context or irrelevant. We also adopt the implicit convention of designing basis kets with either integer indexes \( k, i, j \) or bit-vector \( \vec{x} \) and general kets with indexes \( u, v, w \). Hence, in the following \( |u\rangle, |v\rangle, |i\rangle \) and \( |\vec{x}\rangle \) all designate kets, the last two having the additional characteristics of being basis kets.

When considering two registers of respective size \( m \) and \( n \), the state of the compound system lives in the Kronecker product\(^1\) —or tensor product— of the original state spaces: a general state is then of the form

\[
\sum_{\vec{x} \in BV_m, \vec{y} \in BV_n} \alpha_{\vec{x}, \vec{y}} |\vec{x}\rangle_m \otimes |\vec{y}\rangle_n.
\]

In particular, the state of a qubit register of \( n \) qubits lives in the tensor product of \( n \) state-space of one single qubit.

**Adjointness.** In the following we also use the adjoint transformation for matrices. The adjoint of matrix \( M \) with \( r \) rows and \( c \) columns is the matrix \( M^\dagger \), with \( c \) rows and \( r \) columns and such that for any indexes \( j,k \in \{0,c\} \times \{0,r\} \), cell \( M^\dagger(j,k) \) holds the conjugate value \( M(k,j)^* \) of \( M(k,j) \) (for any complex number \( c \), its conjugate \( c^* \) is the complex number with the same real part and the opposite imaginary part as \( c \)). The adjoint of a ket \( |u\rangle_n \) is called a bra. It is a row vector with \( 2^n \) columns denoted \( \langle u |_n \) — or simply \( \langle u \) — and with indices the conjugates of those of \( |u\rangle_n \). This bra-ket notation is particularly convenient for representing operations over vectors. Given a ket \( |u\rangle \) and a bra \( \langle v | \) \( |u\rangle \langle v | \) denotes their Kronecker product — or outer product —; furthermore, if \( |u\rangle \) and \( \langle v | \) have the same length, then \( \langle v | u \rangle \) denotes their scalar product — also called inner product—. In particular, in the case of basis states \( |i\rangle \) and \( \langle j \), \( \langle i | j \rangle = 1 \) if \( i = j \) and 0 otherwise and \( |i\rangle \langle j \) is the square matrix of width \( 2^n \) with null coefficient everywhere except for cell \( (i, j) \) with coefficient \( 1 \). If \( i = j \), then \( |i\rangle \langle j \) operates as the projector upon \( |i| \).

\(^1\)Given two matrices \( A \) (with \( r \) rows and \( c \) columns) and \( B \), their Kronecker product is the matrix \( A \otimes B = \begin{pmatrix} a_{11}B & \ldots & a_{1c}B \\ \vdots & \ddots & \vdots \\ a_{r1}B & \ldots & a_{rc}B \end{pmatrix} \). This operation is central in quantum information representation. It enjoys a number of useful algebraic properties such as associativity, bilinearity or the equality \( (A \otimes B) \cdot (C \otimes D) = (A \cdot C) \otimes (B \cdot D) \), where \( \cdot \) denotes matrix multiplication.
Quantum measurement and Born rule. The probabilistic law for measurement of kets is given by the so-called Born rule: for any \( k \in [0, 2^n] \), measuring state \( |u\rangle_n \) from Equation 1 results in \( k \) with probability \( |\alpha_k|^2 \). The measurement is destructive: if the result were \( k \), the state of the register is now \( |k\rangle_n \) (with amplitude 1).

2.1.3 Separable and Entangled States

From Section 2.1.2, a quantum state of length \( n \) is a superposition of basis element with coefficients whose squared moduli sum to one. Then, tensoring \( n \) quantum states \( |u_j\rangle_1 \) of length 1 results in a state \( |u\rangle_n = \bigotimes_{j=0}^{n-1} |u_j\rangle_1 \) of length \( n \). One can decompose back \( |u\rangle_n \) into the family \( \{ |u_j\rangle \}_{j=0}^{n-1} \); we say that \( |u\rangle_n \) is a separable state. Note that the structure of quantum information introduced above contains states missing the property of being separable. As an example, the state

\[
|\beta_{00}\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)
\]

cannot be written as a tensor product of two single qubit states. This phenomenon is called entanglement, and \( |\beta_{00}\rangle \) is an entangled state. It induces that one can store more quantum information in \( n \) qubits altogether than separately.

Example 2.1 (Bell states). State \( |\beta_{00}\rangle \) is a construction of particular interest in quantum mechanics and quantum computing. In their famous 1935 article [52], Einstein, Podolsky and Rosen argued for the incompleteness of quantum mechanics, based on considerations upon \( |\beta_{00}\rangle \). In 1964 [17], J.S. Bell proposed an experiment to test the argument. It was based on statistics over experiments on the four following states:

\[
|\beta_{00}\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \quad |\beta_{01}\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \\
|\beta_{10}\rangle = \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle) \quad |\beta_{11}\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)
\]

These four state are now known as the Bell states (notation \( \beta \) stands for the initial \( B \)) and are used in many quantum protocols, such as teleportation or superdense coding (see Section 5.1). We use them and their generation as a running example in the rest of this chapter.

2.1.4 Quantum Circuits

Three kinds of operations may be applied to quantum memory, exemplified in Figure 2 with the circuit generating and measuring Bell states:

- the initialization phase allocates and initializes quantum registers (arrays of qubits) from classical data. In Figure 2 it is represented on each qubit wire \( w \) as \( I_w \), indexed by value \( i_w \). It creates a quantum register in one of the basis states (that is, in the case of a two qubit registers as in Figure 2, in one of the four basis states \( |00\rangle, |01\rangle, |10\rangle, |11\rangle \)),

- the actual quantum computing part consists in transforming an initialized state. This is performed by applying a sequence of properly quantum operations, structured in a so-called quantum circuit. In Figure 2 this part is identified with a dashed box (itself sequenced with dotted box a. and b.),

- the extraction of useful information from a quantum computation is performed through the measurement operation, by which one probabilistically gets classical data from the quantum memory register. Measurement is represented, on each qubit it is applied to as \( \mathcal{M} \).
Note that we reserve the term circuit for the pure quantum part (the dashed box in Figure 2). We call generalized circuit a process made of a circuit together with, possibly, initialization and measurements.

Quantum circuits are built by combining, either in sequence or in parallel, a given set of elementary operations called quantum gates. In addition to sequence and parallelism, derived circuit combinators (controls, reversion, ancillas, etc) are often used in quantum circuit design (See Figure 8 in Section 6.1.1 for details). In any case, the circuit part of Figure 2 uses two different quantum gates, drawn in dotted box:

- the Hadamard gate \( H \) (a.), which operates a state superposition on a given qubit,
- the control not gate, often written \( CNOT \) (b.) and represented as \( \oplus \). It is a binary gate, flipping the target qubit (in wire 2 in our case) when the control qubit (wire 1) has value 1.

### 2.1.5 Quantum Matrix Semantics

The transformation operated by a quantum circuit on a quantum register is commonly interpreted as a matrix. In this setting, parallel combination of circuits is interpreted by Kronecker product and sequential combination by matrix multiplication.

**Quantum circuits.** Quantum circuits happen to operate as unitary operators (preserving the inner product between vectors). A set of elementary gates is (pseudo-) universal if, by combination of parallel and sequential composition, one can synthesize (or approximate) all unitary operations. Examples for elementary gates are given in Table 1, with their matrix semantics interpretation. Apart from the already encountered gates \( H \) and \( CNOT \), it figures two additional families of gates, \( PH(\theta) \) and \( R_Z(\theta) \), where \( \theta \) is an angle. \( PH(\theta) \) operates a simple scalar multiplication by a phase factor, while \( R_Z(\theta) \) operates as a rotation. Table 1 is given with indexes ranging over any angle \( \theta \), making the set of gates universal. Usually, we restrict it to angles of measure \( \pi n \), with \( n \) ranging over integers. This restriction makes the resulting set of gates pseudo-universal.

![Generalized circuit to create Bell states](image)

Table 1: Elementary gates and their matrix semantics

| \( H \) | \( CNOT \) | \( PH(\theta) \) | \( R_Z(\theta) \) |
| --- | --- | --- | --- |
| \( H \) | \( \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \) | \( e^{2\pi i \theta} \begin{pmatrix} 0 & 0 \\ 0 & e^{2\pi i \theta} \end{pmatrix} \) | \( e^{2\pi i \theta - \theta} \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \) |
Example 2.2 (Semantics for the Bell generating circuit). Let us look at Figure 2 again. First, an Hadamard gate is applied to the first wire and nothing happens to the second wire (it stays untouched, which is represented by the identity matrix). The matrix for the first column – the dotted box indexed with a.– of Figure 2 is
\[
\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}
\]
Then gate CNOT is applied, with matrix
\[
\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}
\]
and the sequential combination of the two sub-circuits translates, in the matrix semantics, as their usual product (mind the reverse ordering, wrt the figure):
\[
\text{Mat}(\text{Bell-circuit}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 \end{pmatrix}
\]

Application to input initialized kets. In the matrix formalism, we interpret \(|0\rangle\) as the column vector \(\begin{pmatrix} 1 \\ 0 \end{pmatrix}\), \(|1\rangle\) as \(\begin{pmatrix} 0 \\ 1 \end{pmatrix}\) and the concatenation \(|i\rangle\otimes|j\rangle\), where \(i\) and \(j\) both are sequences of 0 or 1, as the Kronecker product \(|i\rangle\otimes|j\rangle\). For example, the two qubits basis kets \(|00\rangle, |01\rangle, |10\rangle, |11\rangle\) are represented, respectively, as
\[
\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\]
The transformation performed by a quantum circuit \(C\) upon a quantum state \(|\psi\rangle\) is interpreted as the matrix product \(\text{Mat}(C) \cdot |\psi\rangle\) of the matrix for this circuit by the column vector for this quantum state. By notation abuse, we also simply write it \(C|\psi\rangle\).

Example 2.3. One can now directly verify that the Bell generating circuit from Figure 2 generates the Bell states from Example 2.1: for any \(a,b\in\{0,1\}\),
\[
\text{Bell-circuit} \cdot |ab\rangle = |\beta_{ab}\rangle
\]

Measurement. Last, measuring a quantum register results in a basis state, with probabilities following the Born rule introduced in Section 2.1.2: measuring any state \(|u\rangle_n\) results in basis state \(|k\rangle_n\) with probability \(\text{proba}_\text{measure}(|u\rangle_n, |k\rangle_n) = |\alpha_k|^2\), where \(\alpha_k\) is the amplitude of \(|k\rangle_n\) in \(|u\rangle_n\). Applying this rule to the Bell state, one easily state that for any \(a,b,i,j\in\{0,1\}\),
\[
\text{proba}_\text{measure}(|\beta_{ab}\rangle, |ij\rangle) = \frac{1}{2} (\text{if } b = 0 \text{ then } i \oplus j \text{ else } 1 - (i \oplus j))
\]
where \(\oplus\) denotes addition modulo 2.

Discussion. Matrix semantics is the usual standard formalism for quantum computing (see [124] for example). Still, the size of matrices grows exponentially with the width of circuits, so that it is often cumbersome when addressing circuits from non-trivial algorithm instances. Furthermore, algorithms usually manipulate parametrized families of circuits. The resulting parametrized families of matrices may not be conveniently writable.

Hence, more compact interpretation for quantum circuits may be helpful. In particular, path-sum semantics [5, 4] directly interprets quantum circuits by the input/output function they induce over kets – corresponding, in matrix terms, for any circuit \(C\) of width \(n\), to the function \(|u\rangle_n \mapsto \)
\( \textbf{Mat}(C) \cdot |\psi\rangle_n \). To do so, it exhibits a generic form for quantum registers description, which is generated by a restricted number of parameters and composes nicely with matrix and Kronecker products. Path-sum semantics plays a growing role in formal specification and verification. It is introduced with further details in Section 5.2.

### 2.1.6 Other Models for Quantum Computations

Many alternatives are currently explored for physical implementations of quantum computing machines, some of them (such as Measurement Based Quantum Calculus [136], topological quantum computations [64], linear optical networks [1], adiabatic quantum computing [55], etc.) differing on rather fundamental aspects (like, e.g., the elementary operations constituting computations). Nevertheless, they still use the fundamental data structures (ket, vectors, unitary transformation, Kronecker parallel composition, etc.) introduced above.

The ZX-calculus [37] also provides an alternative graphical formalism to reason about quantum processes. Basically, in this setting, quantum operations are represented by diagrams and their composition through sequence or parallelism corresponds to graphical compositions in the calculus. This language comes with a series of enabled transformations over graphs, preserving computational equivalence. ZX-calculus is presented in Section 5.1.

### 2.2 Algorithms

As previously introduced, quantum computers are meant to perform calculus that classical computers are not able a priori to perform in a reasonable time. We give the formal complexity theory characterization for this point in Section 2.2.1, then Section 2.2.2 discusses the usual conventions for quantum algorithms descriptions.

#### 2.2.1 Quantum Algorithms and Complexity

It is commonly admitted that formal problems are tractable by a computer if there exists an algorithm to solve this problem in time (measured by the number of elementary operations it requires) that is bounded by a polynomial over the size of the input parameters. Formal problems satisfying this criterion for classical computers form a complexity class usually referred to as \( \text{P} \). It is schematically represented in Figure 3.

Since quantum computations are probabilistic, this tractability criterion needs to be slightly adapted for them. Instead of considering problems for which a polynomial algorithm brings a solution with certainty, we consider those for which a polynomial algorithm brings a solution with an error probability of at most \( \frac{1}{3} \). The corresponding class of problems for quantum computers is called bounded error quantum polynomial time (BQP).

In addition to \( \text{P} \) and \( \text{BQP} \), Figure 3 represents the non deterministic polynomial time class \( \text{NP} \). It gathers formal problems \( \mathcal{P} \) for which there is an algorithm that, given a candidate solution, checks whether this candidate is an actual solution for \( \mathcal{P} \) in polynomial time. It is trivial that \( \text{P} \) is included in \( \text{NP} \) and it is also proved that \( \text{P} \subseteq \text{BQP} \). There are good reasons to believe that these inclusions are strict. Nevertheless, strictness is not formally proved and there are a variety of problems that belong to \( \text{NP} \) without known tractable resolution algorithm.

Hence, quantum algorithm performance is not to be evaluated against the best possible performance of any classical computation (which depends on whether \( \text{BQP} = \text{P} \)) but, in a more pragmatic way, against the best classical known equivalent.

Then, the relevance field for quantum computing is easily schemed by Figure 3: it consists in problems that are polynomially solvable by a quantum computer (with a given probability of
success) but *intractable* by a classical one. It appears in gray. The question whether the dark gray part \( (\text{BQP} \setminus \text{NP}) \) is empty or not depends on whether \( \text{BQP} \subseteq \text{NP} \), which is unknown, but several BQP-complete problems have been described through the literature [170]. These are neither easily computable nor verifiable with known classical means, but may be computed with quantum means: since quantum computers output a right solution for them with probability \( > \frac{2}{3} \), after several runs one can select the best represented output as the seeked solution.

Let us stress that the correspondence between polynomial solvability and tractability is not strict. For a problem, not belonging to a polynomial class bounds the size of input parameters concretely tractable by a computer, but does not absolutely forbid computation for any instance of it. Hence, for some problems, the quantum advantage does not consist in providing a polynomial resolution, but in reducing computation time so as to extend the set of tractable inputs. A typical example is the Grover search algorithm [72], searching for a distinguished element in an unstructured data set, which provides a quadratic acceleration against classical procedures.

### 2.2.2 Quantum Algorithm Design

Before introducing the challenges at stake with implementations of quantum algorithms and their formal solutions, we make a few observations on the usual format used to describe quantum algorithms, based on an example: Figure 4 reproduces the core quantum part for the Shor’s algorithm [124, p. 232] — certainly the most emblematic of all quantum algorithms —.

The following observations generally hold for other quantum algorithms in the literature. We give them together with illustrations (within parenthesis) from the example of Figure 4.

1. An algorithm is structured in two main parts: a specification preamble and a Procedure description. The preamble indicates the minimal specification an implementation should satisfy. Note that it figures as a full-right part of the algorithm. It contains three types of entries:
   - a description of the Inputs, giving a signature for the parameters (a black-box circuit \( U \), integers \( x, N, L \) and two quantum registers of sizes \( t \) and \( L \)) and some preconditions for these elements (e.g. \( x \) co-prime to \( L \), \( L \) being \( N \) bits long, etc.)
   - a description of the Outputs of the algorithm. It contains, again, a signature (an integer) and a success condition for these Outputs (to be equal to the seeked modular order),
   - a Runtime specification, containing: (1) a probability of success for each run of the Procedure \( O(1) \), (2) resources requirements. In the example the latter consists in bounding the number of required elementary operations. Further metrics are also often used (the maximal width of required quantum circuits – the number of qubits a circuits...
2. The **Procedure** itself consists in a sequence of declared operations, interspersed with formal descriptions of the state of the system along the performance of these operations. (in Figure 4 these elements are given in parallel, declarations of operations constitute the right hand side column and intermediate formal assertions are on the left hand side column). These assertions serve as specifications for the declared operations. For instance, operation “create superposition” has precondition the formal expression of Line 1, left (framed in blue) and postcondition the one of Line 2, left (framed in red). They serve as arguments to convince the reader that the algorithm Outputs conditions are met at the end of the **Procedure** (notice that the ultimate such postcondition — the measured state being $r$ — corresponds to the success condition for the overall algorithm). But we can also interpret them as contracts for the programmer, committing her to implement each function in any way provided that whenever its inputs satisfy the preconditions, then its outputs satisfy the postconditions.

3. The algorithm description is parametric, and so should be any program implementing it. Hence, quantum programming paradigm is higher-order: a quantum program is a function from (classical data) input parameters to quantum circuits. Then, each instance of a quantum circuit behaves as a function from its (classical data) inputs to its (classical data) outputs.

| Inputs: | (1) A black-box $U_{x,N}$ which performs the transformation $|j\rangle|k\rangle \rightarrow |j\rangle| x^j \mod N\rangle$, for $x$ co-prime to the $L$–bit number $N$,  
(2) $t = 2L + 1 + \lceil \log(2 + \frac{1}{2}) \rceil$ qubits initialized to $|0\rangle$, and  
(3) $L$ qubits initialized to the state $|1\rangle$. |
| Outputs: | The least integer $r > 0$ such that $x^r = 1 \pmod N$. |
| Runtime: | $O(L^3)$ operations. Succeeds with probability $O(1)$. |
| Procedure: | |
| 1. $|0\rangle|u\rangle$ | initial state |
| 2. $\rightarrow \frac{1}{\sqrt{2^L}} \sum_{j=0}^{2^L-1} |j\rangle|1\rangle$ | create superposition |
| 3. $\rightarrow \frac{1}{\sqrt{2^L}} \sum_{j=0}^{2^L-1} |j\rangle|x^j \mod N\rangle$ | apply $U_{x,N}$ |
| $\approx \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} \sum_{j=0}^{2^L-1} e^{2\pi ij/r} |j\rangle|u_s\rangle$ |
| 4. $\rightarrow \frac{1}{\sqrt{r}} \sum_{s=0}^{r-1} |s/r\rangle|u_s\rangle$ | apply inverse Fourier transform to the first register |
| 5. $\rightarrow |s/r\rangle$ | measure first register |
| 6. $\rightarrow r$ | apply continued fraction algorithm |

Figure 4: Bird eye view of the circuit for [149]’s factoring algorithm (as presented in [124, p. 232])

Most of current quantum programs [132, 71, 165, 155, 154, 20, 107] proceed as implementation
for functions such as those declared in Figure 4 (right part of the Procedure part), providing no guarantee over the algorithm specifications, be it about their functional behavior of their resource requirements.

Based on the preceding comments, the purpose of formal verification can be summarized as completing algorithm implementations with their proved specifications. In other words:

*Formal verification in quantum programming aims at providing solutions to furnish, in addition to quantum programs, evidence that these programs meet their requirements, in terms both of success probability and of resource usage.*

### 2.3 Challenges for Quantum Computation

Let us now introduce some particularities of quantum programming with regards to classical computing. They raise design challenges that are proper to this programming paradigm.

#### 2.3.1 Destructive Measurement and Non-Determinism

One of the main particularity of quantum programming is that the output produced by the quantum memory device follows the probabilistic Born rule (see Section 2.1.2). So, in the general case, the result of a quantum computation is non deterministic.

Furthermore, a computation in the model of Figure 1 contains both probabilistic quantum computations and classical control structures, performed by the classical controller. Hence, control itself may depend on the probabilistic data received from the quantum device and the execution flow itself is probabilistic. This requires programming models: it is the subject of Section 6.1.

#### 2.3.2 Quantum Noise

Another particularity comes from the difficulty to maintain big quantum systems in a given state and to control the evolution of this state through time. Along a quantum computation, uncontrolled modifications (bit or phase flip, amplitude damping, etc.) of the quantum state may occur.

This phenomenon calls both for formal analysis of the risk of state deterioration and for an error correction mechanism, integrated in the compilation. The formal analysis of error propagation requires a typology of possible errors together with rules specifying how their probability of occurrences propagates along quantum circuits [84, 134]. Error correction design is an active research fields [31, 114, 69, 63]. Many propositions have been developed. They mainly consist in designing redundant quantum circuits (one logical qubit is implemented by many different physical qubit). Then the main challenge is to design solution for testing the redundancy along a computation without losing the state of the register due to destructive measurement.

#### 2.3.3 Efficient Compilation on Constrained Hardware

Languages such as LIQUID, Q#, QUIPPER, etc. enable the description and building of quantum circuits for so-called logical qubits. In practice, realizing a quantum circuit on an actual quantum machine (physical qubits) requires several compilation passes, in addition to the error correction mentioned in the preceding paragraph. Among others:

- the physical realization should respect the physical constraints of its target architecture, which concern, e.g. connectivity of qubits or register size limits. Considering this point requires
qubit reordering intermediary operations and an adequate mapping between theoretical and physical qubits,

• the set of possible quantum operations over physical qubits may not correspond to the set of elementary gates from the logical circuit description, which would require an adequate gate synthesis and circuit rewriting,

• last but not least, physical realization of algorithm should be as resource sober as possible, requiring the development of circuit optimization techniques.

Each of these steps consists in low-level operations over circuits. They must all preserve functional equivalence while reaching their proper purpose. For these low-level developing layers, one requires tools and languages formalizing functionally equivalent circuit transformation operations. ZX calculus [37] (Section 5.1) is particularly well-fitted for such design, other propositions include the proof of path-sum semantics equivalence [5, 4] (Section 5.2) and formally verified circuit optimization [78] (Section 5.3).

3 General Background on Formal Methods

We now present a brief overview of formal methods. While the domain is old and has led to a rich literature, we try to highlight the underlying main principles and to quickly describe the most popular classes of techniques so far.

3.1 Introduction

Formal methods and formal verification [34] denote a wide range of techniques aiming at proving the correctness of a system with mathematical guarantee — reasoning over all possible inputs and paths of the system, with methods drawn from logic, automated reasoning and program analysis. The last two decades have seen an extraordinary blooming of the field, with significant case-studies ranging from pure mathematics [68] to complete software architectures [100, 109] and industrial systems [16, 94]. In addition to offering an alternative to testing, formal verification has in principle the decisive additional advantages to both enable parametric proof certificates and offer once-for-all absolute guarantees for the correctness of programs.

3.2 Principles

Formal methods main principles were laid mostly in the 1970s. Pioneers include Floyd [61], Hoare [81], Dijkstra [49], Cousot [39] and Clark [32]. While there is a wide diversity of approaches in the field, any formal method builds upon the following three key ingredients:

• a formal semantic $M$ representing the possible behaviors of a system or program — $M$ is typically equipped with an operational semantic and behaviors are often represented as a set of traces $L(M)$;

• a formal specification $\varphi$ of the acceptable or correct behaviors — $\varphi$ is typically a logical formula or an automaton representing a set of traces $L_\varphi$;

• a (semi-)decision procedure verifying that possible behaviors are indeed correct, denoted $M \models \varphi$ — typically a semi-algorithm to check whether $L(M) \subseteq L_\varphi$ holds or not.
Regarding the complexity of realistic systems and programs, the verification problem is usually undecidable, hence the impossibility to have a fully automated and perfectly precise decision procedure for it. The different formal method communities bring different responses to get around this fundamental limitation, yielding different trade offs in the design space, favoring either restriction of the classes of systems under analysis, restrictions of the classes of properties, human guidance or one-sided answer (over-approximations or under-approximations).

Overall, after two decades of maturation, formal methods have made enough progress to be successfully applied to (mostly safety-critical) software [76, 163, 12, 24, 40, 102, 94].

3.3 The Formal Method Zoo

We present now in more details the main classes of formal methods. While recent techniques tend to blur the lines and combine aspects from several main approaches, this classification is still useful to understand the trade-off at stake in the field.

- Type checking and unification: at the crossroad of programming language design and formal methods, type systems [131] allow to forbid by design certain classes of errors or bad code patterns. Traditionally, type systems focus on simple "well-formedness" properties (good typing), but they scale very well (modular reasoning) and require only little manual annotation effort (type inference). While first type systems were based on basic unification [80, 121], advanced type systems with dependent types or flow-sensitivity come closer and closer to full-fledged verification techniques;

- Model checking and its many variants: while initially focused on finite-state systems [32] (typically, idealized protocols or hardware models) and complex temporal properties – with essentially graph-based and automata-based decision procedures, model checking [33] has notably evolved along the year to cope with infinite-state systems, either through specific decidable classes (e.g., Petri Nets or Timed Automata) or through abstractions. The current approaches to software model checking include notably symbolic bounded verification [102, 26] for bug finding and counter-example guided abstraction refinement [76] for bug finding and proof of invariants (but it may loop forever);

- Abstract Interpretation: Generally speaking, Abstract Interpretation (AI) [39] is a general theory of abstraction for fixpoint computations. AI-based static analysis [138] builds over Abstract Interpretation to effectively compute sound (i.e. overapproximated) abstractions of all reachable states of a program. Hence, these techniques are well suited for proving invariants. Historically speaking, the approach is rather geared at full automation and implicit properties (e.g., runtime error);

- Deductive verification and first-order reasoning: Deductive program verification [14, 60, 81] is probably the oldest formal method technique, dating back to 1969 [81]. In this approach, programs are annotated with logical assertions, such as pre- and post-conditions for operations or loop invariants, then so-called proof obligations are automatically generated (e.g., by the weakest precondition algorithm) in such a way that proving (a.k.a. discharging) them ensures that the logical assertions hold along any execution of the program. These proof obligations are commonly proven by help of proof assistants or automatic solvers.

- Interactive proof and second-order reasoning: some techniques completely drop the hope for automation in favor of expressivity, relying on 2nd order or even higher-order specification and proofs languages – typically in COQ [129] or ISABELLE/HOL [125]. Once programmed
and proved in the language, a certified functional program can then often be extracted. This family of approach is very versatile and almost any problem or specification can be encoded, yet it requires lots of manual effort, both for the specification and the proofs – higher-order proofs can be automatically checked but not found. Still, the technique has been for example used for certified compilers or operating systems [109, 100].

4 Overview of Formal Methods in Quantum Computing

As presented in Section 3, formal methods for proving properties of classical algorithms, programs and systems are well-developed and versatile. In this section, we present the needs for formal methods in the realm of quantum computation, while the later sections are devoted to answer them.

4.1 The Need for Formal Methods in Quantum Computing

As introduced in Section 2, the data structures at stake in quantum computing make the computations hard to represent for developers. Intermediary formal languages are of great help for understanding what quantum programs do and for describing their functional behavior.

Furthermore, as introduced in Section 1, directly importing the testing and debugging practices at use in classical programming is extremely difficult in the quantum case, due to the destructive aspect of quantum measurement. Moreover, the probabilistic nature of quantum algorithms seriously impedes system-level quantum testing. As a consequence, test-based programming strategies do not seem adequate in the quantum case and quantum computing needs alternative debugging strategies and methodologies.

So far, existing quantum processors were small enough that their behavior could be entirely simulated on classical device. Hence, a short-term solution for overcoming the debugging challenge lied on classical simulations of quantum programs. Since quantum computer prototypes are now reaching the size limit over which it will not be possible anymore (upon several, [9] is often referred to as the milestone for this context change, referred to as quantum supremacy), more robust solutions must be developed.

On the other hand, nothing prevents a priori the formal verification of quantum programs. In addition to constitute alternative debugging strategies, formal methods have several additional decisive advantages. In particular:

- They enable parametrized reasoning and certification in the higher-order quantum programming context introduced in Section 2.2.2: formal certification of a parametrized program holds for any circuit generated by this program, whatever the value of its parameters. In contrast, testing certification holds for the particular value of these parameters that is used in a test. Formal certification is not limited by the size of the parameters;

- It provides once for all an absolute, mathematically proven, certification of a program’s specifications, whereas testing furnishes at best only statistical arguments based on bounded-size input samples.

4.2 Typology of Properties to Verify

In this section we detail the different properties one has to mind for developing correct quantum programs. The goal of formal certification is to provide solutions for their verification.

\(^2\) It requires major adaptations and redefinitions, see Section 8.4 for details.
4.2.1 Functional Specifications

A major challenge is to give insurance on the input/output relationship computed by a given program, that is verifying whether a given program implements an intended function $f$. Functional specifications are two-layered:

**High-level specifications.** We give a circuit an overall specification independent from the concrete implementation. It is made of a success condition and a minimum probability, for any run of this circuit, to result in an output satisfying the success condition.

In the hybrid model, circuits are run on a quantum co-processor but controlled by a classical computer, performing control operations (such as if and while instructions, simple sequence, etc). As a simple example, an algorithm such as the one from Figure 4 outputs a success with probability $p$. It can be included in a control structure including $k$ iterations of it. This higher-level procedure has probability $(1 - p)^k$ to output a success at least once, which can be made arbitrarily close to 1.

More generally, a high-level quantum verification framework [116, 166] considers an algorithm as a controlled sequence of quantum functions. There, one considers quantum operations as primitives and composes them together via controlled sequence operations. These operations are interpreted as functions in the semantical formalism. As example, [116, 166] formalize quantum programs in the density operators formalism. This view is introduced in details in Section 7.1 together with the Quantum Hoare Logic (QHL) [116, 166].

**Mid-level specifications.** In the Procedure section from Figure 4, each mid-level step of the algorithm is given a formal specification, that is a description of the state of the system. These intermediate specifications are deterministic and concern quantum data.

In a lower-level verification approach view, instead of inputting quantum operations as primitive functions, one builds quantum circuit implementations of these operations, by adequately combining quantum gates. Such a framework [78, 135, 29] lies on a circuit description language such as QUIPPER or QWIRE. Then, an adequate semantics characterization for the built circuits enables to reason about the quantum data received as inputs and delivered as outputs. A certification solution for quantum circuits enables to reason compositionally about their semantics. This programming view is explored in Sections 7.2 and 7.3.

4.2.2 Complexity Requirements

The major reason for developing quantum computers and quantum algorithms is to lower computing complexity requirements, w.r.t. classical computing solutions (see Section 2.2.1 for precisions). Therefore, the relevance of a quantum implementation lies on its respect of some complexity requirements. As introduced in Section 2.2.2, they may be formulated through different metrics such as the width and/or depth of quantum circuits, their number of elementary gates or more complex metrics such as quantum volume [110].

The complexity requirement is also crucial for another reason: remind from Section 2.3.2 that quantum computation is subject to noise: the bigger a quantum circuit is, the most prone to error it is. Functional specifications introduced so far reason about the theoretical output of quantum computations, in the absence of errors. The risk of error in a circuit is closely related to structural characteristics of this circuit, among which are the different measures of complexity. Therefore, the information provided by these measures is also crucial to appreciate the functional trustfulness of an implementation.
4.2.3 Structural Constraints

Quantum circuit design must also consider various structural constraints that discriminate through several criteria:

1. They can be either relative to a target architecture or absolute (induced by quantum physics laws). The first category comprises, for example, the number of available qubits in a processor, the connectivity between physical qubits, the set of available elementary gates, etc. The second category mainly deals with aspects induced by quantum calculus unitarity (no cloning theorem, ancilla management, quantum control, etc.);

2. Now, depending on the programming language at stake, absolute structural constraints may either be taken into charge by the language design or left to the user’s responsibility. For example the no-cloning rule is derived from the unitarity of quantum processes. It forbids to use the same quantum data register twice:
   - in languages where quantum data registers are full right objects (e.g.: QUIPPER, QWIRE, etc), caring for the respect of no-cloning is left for the user. In this case, formal verification may help her to do so. Solutions like PROTOQUIPPER [139] or QWIRE [130, 135] tackle this problem through linear type systems (see Section 6.3);
   - another possibility is to reduce the expressivity of the language, so as to prevent any possible violation of no-cloning. In SQIR [78] or QBRICKS [29], quantum data registers are addressed to via integer indexes, but the data they hold only concern the semantics of the language and the specification language. Hence, the respecting conditions for the no cloning theorem are reduced to simple indexing rules for quantum circuits.

3. Last, structural program constraints can be either syntactic or semantic. The first category contains, for example, all constraints that are linked with qubit identification (e.g.: do not control an operation by the value of a qubit it is acting on). The most representative example for semantic constraints concerns a particular aspect of quantum computing that we do not detail in this chapter: the management of ancilla qubits. Basically, ancilla qubits provide additional memory for some sections of quantum circuits, the content of which is then discharged at some stage of the computation. Discharging a part of a register is possible (without affecting the rest of the memory) only if there is no intrication between the memory to discharge and the rest of the memory (See [124] for further details). Hence, ancilla management is possible modulo some non-intrication specifications, regarding the semantic of quantum circuits.

4.2.4 Circuit Equivalence

Compilation of quantum programs contains a number of circuit rewriting operations (see Section 2.3.3). They concern the implementation of logical qubits in a physical framework and require a certification for functional behavior preservation. Concretely, given a logical circuit $C$, compiling $C$ traces as a chain of circuits, starting from $C$ and each obtained from the precedent by applying a circuit rewriting operation. Each such rewriting must preserve the input/output relation, so as to ensure that, provided $C$ fits its functional requirements, then so does the final physical qubits circuit. In Section 5 we present two tools enabling the verification of circuit equivalence: the ZX-calculus (Section 5.1) and the path-sum equivalence verification (Section 5.2).
Further formal comparisons between quantum processes. Different notions of equivalence between quantum processes are also at stake with further uses of quantum information, such as communication protocols. Recent developments [158, 15, 157] generalize the equivalence specification to further comparison predicates between quantum processes. Since they are not designed for the formalization of algorithm, which is the scope of the present chapter, we do not detail these propositions in the present chapter.

5 Low-Level Verification: Compilation and Equivalence

Realizing logical circuits into physical devices (circuit compilation) requires to deal with severe constraints: the number of available qubits, their connectivity, the set of elementary operations, the instability of quantum information—requiring the insertion of error correction mechanisms, etc. As mentioned in Section 4.2.4, the underlying circuit transformations must preserve functional equivalence with the initial circuit representation, all along the compilation process. In the present section we introduce formal tools for checking such equivalences and certifying compilation correctness.

5.1 ZX Calculus and Quantomatic/pyZX

ZX-Calculus [36] is a powerful graphical language for representing and manipulating quantum information. This language historically stems from category theory applied to quantum mechanics, through the program Categorical Quantum Mechanics initiated by Samson Abramsky and Bob Coecke [2].

For our purposes, it is interesting to see ZX-diagrams as a lax version of quantum circuits. This laxness on the one hand implies that not all ZX-diagrams are implementable with physical qubits, but on the other hand, it allows the formalism to get powerful results on the underlying equational theory (rewriting rules, pseudo-normal forms).

The level of abstraction provided by the language allows the user to reason about quantum programs or protocols while significantly alleviating the “bureaucracy checks” typically coming with circuit-level reasoning, in particular checking sub-circuit equivalence in the presence of ancillas. It also allows to unify different models of quantum computation (circuits, measurement-based quantum computing, lattice surgery, etc.), as well as to provide optimization strategies for these models. Last but not least, it can be used to formally (yet, graphically) verify properties on protocols or programs—all that based on simple graph-based manipulations.

5.1.1 Semantical Model

The ZX-diagrams are generated from a set of primitives:

\[
\left\{ \otimes, \bigcirc, \bigotimes, \bigoplus, \left\lfloor \begin{array}{c} n \cdot m \cdot \alpha \end{array} \right\rfloor \right\}_{n, m \in \mathbb{N}, \alpha \in \mathbb{R}}
\]

which can be composed either:

- sequentially:

\[
\begin{align*}
\ldots & \\
D_1 & \\
\ldots & \\
D_2 & \\
\ldots & 
\end{align*}
\]
• or in parallel: \[
\begin{bmatrix}
\cdots & D_1 & \cdots \\
D_2 & \cdots & \cdots \\
\cdots & D_2 & \cdots
\end{bmatrix}
\]

We denote by \(ZX\) the set of ZX-diagrams. These diagrams are used to represent linear maps, thanks to the so-called \textit{standard interpretation} of ZX-diagrams as complex number matrices \([\cdot] : ZX \to \mathcal{M}(\mathbb{C})\). It is inductively defined as:

\[
\begin{bmatrix}
\cdots & D_1 & \cdots \\
D_2 & \cdots & \cdots \\
\cdots & D_2 & \cdots
\end{bmatrix}
= id_{C^2} = |0\rangle\langle 0| + |1\rangle\langle 1|
\]

\[
\begin{bmatrix}
\cdots & D_1 & \cdots \\
\bigotimes & \cdots & \cdots \\
\cdots & D_1 & \cdots
\end{bmatrix}
= \sum_{i,j \in \{0,1\}} |ij\rangle\langle ij|
\]

where \(|+\rangle := \frac{|0\rangle + |1\rangle}{\sqrt{2}}\) and \(|-\rangle := \frac{|0\rangle - |1\rangle}{\sqrt{2}}\) and \(\langle u| \langle v|\) is the ket bra outer product from Section 2.1.2.

For example, \(id_{C^2} = |0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\).

In ZX-diagrams, information flows from top to bottom, which is in contrast with quantum circuits where it flows from left to right. This is only a matter of convention, as string diagrams, on which the ZX-Calculus formalism relies upon, are oriented vertically.

Notice that the green (light) and red (dark) nodes only differ from the basis in which they are defined (as \((|+\rangle, |-\rangle)\) defines an orthonormal basis of \(\mathbb{C}^2\)), and that they can have an arbitrary number of inputs and outputs. It often happens that a green or red node has a parameter of value 0. In this case, by convention, this angle 0 is omitted. Finally, notice that \(\bigotimes\) represents exactly the Hadamard gate of quantum circuits. This is not a coincidence, as ZX-diagrams can be seen as a generalization of quantum circuits. In particular, we can map any quantum circuit to a ZX-diagram that represents exactly the same quantum operator:

\[
PH(\theta) \mapsto \begin{array}{c}
\includegraphics[width=0.2\textwidth]{phasor_diagram.png}
\end{array}
RZ(\theta) \mapsto \begin{array}{c}
\includegraphics[width=0.2\textwidth]{rotation_diagram.png}
\end{array}
H \mapsto \begin{array}{c}
\includegraphics[width=0.2\textwidth]{hadamard_diagram.png}
\end{array}
CNOT \mapsto \begin{array}{c}
\includegraphics[width=0.2\textwidth]{cnot_diagram.png}
\end{array}
\]

and that preserves sequential and parallel compositions. The elementary gates given above are the ones detailed in Table 1.

We can actually map any \textit{generalized} quantum circuit (i.e. circuit including measure) into a ZX-diagram. Indeed, initializations of qubits are easy to represent: \(|0\rangle \mapsto \begin{array}{c}
\includegraphics[width=0.1\textwidth]{initialization_diagram.png}
\end{array}\), and there exists an extension of the ZX-Calculus [38, 27] that allows the language to represent measurements. In this extension, we represent the environment as \(\bigotimes\), which becomes an additional generator of the diagrams (we denote by \(ZX^+\) this updated set of ZX-diagrams). This generator can also be understood as discarding a qubit. However, contrary to classical data, this action affects the rest of the system. Introducing \(\bigotimes\) forces us to change the codomain of the standard interpretation, but we will not give the details here. Simply keep in mind that the measurement in the computational basis \((|0\rangle, |1\rangle)\) is represented by \(\begin{array}{c}
\includegraphics[width=0.1\textwidth]{measurement_diagram.png}
\end{array}\).
In this way, we can (fairly) easily represent any generalized quantum circuit as a ZX-diagram. But we can actually represent more, and this is an active field of research to try and characterize diagrams that can be put in circuit form (we talk about “extracting a circuit”). First was introduced the notion of causal flow [42] which was then extended to that of “gflow” (for generalized flow) [25]. Some other variations exist [11].

Quantum circuits, however, are not the only computational model one might want ZX-diagrams to compile to. Indeed, it so happens that the primitives of the ZX-Calculus quite naturally match those of lattice surgery [45], a scheme for error correction [63, 82]. In particular, ZX-diagrams implementing a (physical) lattice surgery procedure features a special notion of flow, the PF flow (for Pauli fusion flow) [44].

5.1.2 Verified Properties

The strength of ZX-Calculus comes from its powerful equational theory. This equational theory, allowing to define equivalence classes of ZX-diagrams and to conveniently decide whether two different diagrams represent the same quantum operator.

This question can be asked for quantum circuits as well, as two different circuits may represent the same operator (e.g. $H^2 = I$). Some such equational theories exist for quantum circuits [145, 6], but none, as of today, for a universal fragment of quantum mechanics.

The main difference between the two formalisms is that the equational theory of the ZX-Calculus allows for a powerful result in this language, aggregated under the paradigm “only connectivity matters”. This result states that we can treat any ZX-diagram as an undirected open graph, where the Hadamard box and the green and red nodes are considered as vertices. In particular, any (open) graph isomorphism is an allowed transformation.

**Example 5.1.**

\[
\begin{array}{c}
\text{\includegraphics[width=0.5\textwidth]{example51.png}}
\end{array}
\]

because the two diagrams can be obtained from one another by simply “moving their nodes around” (while keeping inputs and outputs fixed).

This result also allows us to unambiguously represent a horizontal wire. For instance:

\[
\begin{array}{c}
\text{\includegraphics[width=0.5\textwidth]{example52.png}}
\end{array}
\]

This “meta”-rule, that all isomorphisms of open graphs are allowed, constitutes the backbone of the ZX-Calculus. In what follows, different sets of axioms, that satisfy different needs, will be presented, but this meta-rule will always be there implicitly.

When two diagrams $D_1$ and $D_2$ are proven to be equal using the equational theory $\mathcal{T}$, we write $\mathcal{T} \vdash D_1 = D_2$. The axiomatization $zx$ for the ZX-calculus can be found in Figure 5, and it was recently proven to be complete [161]:

**Theorem 5.2.** **ZX/zx is complete:**

\[
\forall D_1, D_2 \in \mathbf{ZX}, \quad \llbracket D_1 \rrbracket = \llbracket D_2 \rrbracket \iff \mathcal{Zx} \vdash D_1 = D_2
\]

Here $\mathbf{ZX}/\mathbf{zx}$ represents the quotient of $\mathbf{ZX}$ by the equational theory $\mathbf{zx}$. The completeness property is fundamental. It allows us to reason on quantum processes through diagrammatic transformations rather than by matrix computations. In particular, it tells us that whenever two diagrams represent the same quantum operator, they can be turned into one another using only the rules of $\mathbf{zx}$. 
It is customary in quantum computing to work with particular (restricted) sets of gates. For a lot of such restrictions, there exist complete axiomatizations [73, 88, 89, 87, 90, 91]. The ZX-Calculus with measurements has a similar completeness result for $\text{ZX}^\|_x$ [27] with an updated set of rules $\text{zx}^\|_x$ which we will not give here for conciseness purposes.

Some properties of quantum protocols or algorithms can then be verified by diagram transformations. To give the reader the flavor of such verifications, we detail the example of superdense coding.

**Example 5.3 (Superdense Coding).** The idea of the superdense coding protocol is to transmit two classical bits using a single qubit. This is not possible in general, but it is when the two parties initially share an entangled pair of qubits. The protocol goes as follows:

- Alice and Bob initially share the (previously defined) EPR pair $\beta_{00} = \frac{\lvert 00 \rangle + \lvert 11 \rangle}{\sqrt{2}}$, and Alice moreover has two bits she wants to send to Bob
- Alice applies $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ to her qubit if her first bit is 1, then $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ if her second bit is 1
- Alice sends her qubit to Bob
- Bob applies a $\text{cnot}$ between his qubit and the one he received from Alice, then a had gate on his qubit, and finally measures his two qubits
This protocol can be represented with a ZX-diagram as follows.

It is then possible to verify that Bob eventually does get (copies of) Alice’s bits, using the equational theory (although the whole derivation is not given here):

We can hence see that data is transmitted from Alice to Bob, without any loss. Interestingly, this protocol can be extended for secure communication between the two parties [164]. The larger protocol uses instances of the smaller one to also check whether an eavesdropper has tried intercepting or copying data.

If Bob is aware that the data he received was compromised, he can abort everything by simply discarding his qubits, so that the eavesdropper (Eve) gets absolutely no information:

where $U$ denotes an unknown operator applied by Eve to the qubit she intercepted. Notice here how no information can pass from Alice to Eve. No information is retrieved by the latter.

A plethora of quantum protocols have been verified with ZX-Calculus in a similar manner [79]. Note however that the theory is ever evolving, and in particular, $\frac{1}{\phi}$ was not introduced in the language at that time, so the author had to use a trick to make up for the absence of measurement (namely case-based reasoning).
5.1.3 Algorithms and Tools

It is possible to manipulate ZX-diagrams in a computer-verified way. For instance, Quantomatic [99, 95] allows the users to define at the same time diagrams in graphical form and equational theories. It is also possible to work with user-defined nodes in the diagram, so that even though $\perp$ is not part of the “vanilla” ZX-Calculus, it can be defined as a new node. It is then possible in the tool to manipulate diagrams in a way that satisfies the equational theory, and even to define rewriting strategies that can be then applied in an automated way.

The verification of protocols and programs using the ZX-Calculus relies on diagrammatic equivalence. This problem in general is at least QMA-complete, [22, 85] (the quantum counterpart of NP-completeness). This problem is linked to the one of simplification/optimization, which asks how a quantum operator can be simplified, given a particular metric (e.g. the number of non-Clifford gates). Indeed, for instance if $D_1$ and $D_2$ are two diagrams representing the same unitary (i.e. $[D_1] = [D_2]$), then simplifying $D_2^\dagger \circ D_1$ should ideally get us to the identity.

In the case of the Clifford fragment (obtained when the angles in $\alpha_n^{n\pi}$ and $\alpha_m^{m\pi}$ are restricted to multiples of $\frac{\pi}{2}$), there exists a strategy that reduces the diagram in (pseudo-)normal form [10]. When this algorithm terminates, the resulting diagram is of size $O(n^2)$ where $n$ is the number of inputs and outputs in the diagram. The algorithm is polynomial in the overall size of the diagram it is applied on.

Turning an arbitrary diagram into a normal form can be done in principle [90], however the complexity of this algorithm is EXPSPACE for universal fragments. So this approach is obviously not preferred in general. However, one can use the ideas of the algorithm for the Clifford fragment as a starting point to get a rewriting strategy for the general case. Applications to quantum circuits and improvements on this strategy can be found in the literature [98, 43, 50, 11], and implementations in the PyZX tool [96]. Finally, we can mention that the path-sum formalism described in Section 5.2 below can be used in this context. Indeed, it was shown [108, 162] that one can pass from one formalism to the other “freely”, allowing us to apply strategies for path-sums to the ZX-Calculus.

5.2 Path-Sum circuit Equivalence Verification

A recent direction for verifying the equivalence between quantum circuits is provided by the path-sum semantics formalism [5, 4]. In this section we briefly introduce it, together with the main verification achievements so far.

Note that a generalization of path-sum semantics is introduced in Section 7.2, for parametrized families of circuits. For sake of readability, conciseness and coherence with this further content, in the coming paragraphs we slightly simplify path-sums related notations with regard to their original definitions [5, 4]. We refer the reader to the original definitions for the full formalism and underlying mathematical structures.

5.2.1 Semantical Model

The standard semantics for quantum circuits is the matrix formalism, introduced in Section 2.1.5. It associates to each quantum circuit $C$ a matrix $\text{Mat}(C)$ and it interprets the behavior of this circuit as a function $|x\rangle \rightarrow \text{Mat}(C) \cdot |x\rangle$ from kets to kets, where $\cdot$ stands for the usual matrix product.

Notice that this standard semantics builds on intermediary object – the matrix– to derive and interprets the functional behavior of circuits. And it does so by use of an higher-order function –
the matrix product. Contrarily, path-sums are a straight construction of the input/output function performed by circuits, enabling compositional reasoning.

Concretely, a path-sum $PS(x)$ is a quantum register state (a ket), parametrized by an input basis ket $|x\rangle$ and defined as the sum of kets

$$PS(x) := \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{\frac{2\pi i}{2^n} P_k(x)} |\phi_k(x)\rangle$$

(2)

where the $P_k(x)$ are called phase polynomials while the $|\phi_k(x)\rangle$ are basis-kets. This representation is closed under functional composition and Kronecker product. For instance, if

$$C : |x\rangle \mapsto PS(x) = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} \exp\left(\frac{2\pi i P_k(y)}{2^n}\right) |\phi_k(y)\rangle,$$

$$C' : |y\rangle \mapsto PS'(y) = \frac{1}{\sqrt{2^{n'}}} \sum_{k=0}^{2^{n'}-1} \exp\left(\frac{2\pi i P_k'(y)}{2^{n'}}\right) |\phi_k'(y)\rangle,$$

then their parallel combination parallel$(C, C')$ sends $|x\rangle \otimes |y\rangle$ to:

$$\frac{1}{\sqrt{2^{n+n'}}} \sum_{j=0}^{2^{n+n'}-1} e^{\frac{2\pi i}{2^{n+n'} (2^{n} P_j(x) + 2^{n'} P_j'(y))}} |\phi_{j/2^n}(x)\rangle \otimes |\phi_{j/2^{n'}}(y)\rangle$$

The sequential combination of quantum circuits $C$ and $C'$ receives a similar compositional definition, parametrized by path-sums components for circuits $C$ and $C'$.

### 5.2.2 Path-Sums Reduction

While path-sums compose nicely, a given linear map (e.g. the input/output function for a quantum circuit) does not have a unique representative path-sum. To solve this problem, an equivalence relation is defined with a few, simple rules that can be oriented. All these rules transform a path-sum into an equivalent one, with a lower number of path variables (parameter $n$ in the notation of Equation 2).

The corresponding proof system was proved strongly normalizing, meaning that every sequence of reduction rules application terminates with an irreducible path-sum. Furthermore, finding and applying such a normalizing sequence is feasible in time polynomial in the width of the circuit at stake, which makes the overall reduction procedure tractable.

### 5.2.3 Verified Properties

Hence, path-sums provides a human readable formalism for the interpretation of quantum circuits as ket data functions. Furthermore it is given a polynomial normalization procedure, based on a restricted set of rewriting rules. The methods was probed against both circuit equivalence and functional specifications verification. More precisely:

**Translation validation** consists, for a given quantum algorithm, in (1) computing the path-sums for both a non optimized and an optimized circuit realization and (2) using the normalization procedure for the automatic checking of their equivalence. It was performed on various quantum routines instances (Grover, modular adder, Galois field multiplication, etc) of various size (up to several dozens of qubits). Interestingly, the methods proved as efficient for identifying non-equivalence (over erroneous instances) as for checking equivalence.
**Quantum algorithms verification** consists in verifying whether a given circuit instance respects its functional description. It was performed for instances of similar case studies as for the translation validation (QFT, Hidden Shift [159]), with up to an hundred qubits.

As a conclusion, the path-sum formalism provides a fully automatized procedure for verifying the equivalence between two circuits. Hence, given two quantum circuits, the latter being a supposed optimized version of the former, path-sums treatment enables to verify that they implement the same quantum function. Since path-sums perform internal complexity reduction, an open direction is to efficiently extract an optimized quantum circuit from a reduced path-sums. This kind of procedure would indeed provide a verified optimization process.

In its present state of development, using path-sums for quantum algorithm verification is restricted to compilation time, when program parameters are instantiated. Furthermore, a new run of the path-sum reduction is required at each new call of a given quantum function. In Section 7.2 we introduce the QBRICKS language, whose semantics is based on a parametrized extension of path-sums. It enables the verification, once for all, of parametrized programs, holding for any possible future parameter instances – yet at the price of full automation as the manipulation of parametrized path-sums requires first-order logic reasoning.

### 5.3 Toward Integrated Verified Optimization: VOQC

A noticeable effort for an integrated verified quantum optimization was recently led through the development of a **Verified Optimizer for Quantum Circuits** (VOQC) [78]. As main aspects, in comparison to ZX- and path-sum calculus, VOQC:

- is integrated in a core programming environment, and applies on circuit issued from parametrized programs;
- not only validates the equivalence between an input quantum circuit and a candidate optimized version of it, but also provides the formally verified optimization procedure, directly generating this optimized version.

![Figure 6: A simplified view of VOQC architecture](image)

**5.3.1 Architecture**

In Figure 6 we give a simplified view of VOQC architecture: it lies on an Intermediate Representation Language named SQIR. Since it may also be used as a verified programming environment,
SQIR is introduced and developed per se in a dedicated section below (Section 7.3). In the present context we can think of it as a core language generating parametrized quantum circuits. Then, for any instance of the parameters, VOQC extracts the corresponding sequence of operations, applies an optimization procedure upon this sequence of operations and extracts back an optimized proved equivalent SQIR quantum circuit. Furthermore,

- in addition to optimization, VOQC also contains some circuit mapping functionalities, performing further circuit transformation fitting to specific quantum architecture qubit connectivity constraints, addressing the problem raised as first bullet in Section 2.3.3,
- VOQC environment also provides both ways compilations between SQIR and the standard assembly language OPENQASM [41]. Hence, it opens way for a modular easy integration in any standard programming environment, in particular QISKIT [132], which uses OPENQASM as assembly language.

5.3.2 Optimization Procedure

VOQC optimization process provides two functionalities, one is deterministic (optimization by propagation and cancellation) and the other one requires a replacing circuit input.

**Optimization by propagation and cancellation** is based on local circuit rewriting schemes and self composition properties of elementary gates, borrowed from [123] (eg., even sequences of either Hadamard, Control Not or X gate annihilate as the identity, successive occurrences of R\_\_ gates melt by summing their angle parameters, etc). Hence, the procedure consists in two successive steps:

- propagate: for any elementary gate, it considers a number of identified patterns, enabling gate commutations, it finds all occurrences of these patterns and it performs them so as to push any occurrence of this elementary gate to the end of the computation,
- cancellation then consists in deleting the resulting repetitive occurrences of the elementary gate at stake.

**Optimization by circuit replacement**, by contrast, is non-deterministic and requires an oracle. Basically it consists in substituting a part of a quantum circuit (a subcircuit) by another one which is proven to be functionally equivalent. In this case the equivalence proof is led by help of the path-sums semantics (see Section 5.2).

**Performance and Achievements.** VOQC performance has been evaluated against a number of standard quantum computation routines, and compared with several existing optimizers [7, 132, 123, 153, 97]. Note that in VOQC, since optimization is performed as a succession of rewriting operations, the formal verification consists in assessing the equivalence between the input and the output of the optimization, it does not address the optimization performance. Still, on reported experiments, VOQC performance competes with other existing non verified optimizers, both regarding computation time and circuit complexity reduction — precise performance comparison tables appear in [78]. Thus, in the current state of the art, the benefits of formally verified circuit optimization comes for free.
6  Formal Quantum Programming Languages

The notion of quantum circuit is the natural paradigm to reason on concrete run of quantum algorithms for solving specific problem instance. Yet, a quantum algorithm is not reducible to a quantum circuit: the latter is only a by-product of a run of the former. To run and reason on quantum algorithms, one needs quantum programming languages (QPL): this is the topic of the current section.

6.1  Quantum Programming Language Design

In Section 5, circuits were merely seen as sequences of elementary gates. However, in most quantum algorithms circuits follow a more complex structure: they are built compositionally from smaller sub-circuits and circuits combinators. If they are usually static objects, buffered until completion before being flushed to the quantum co-processor, in some algorithms circuits are dynamically generated: the tail of the circuit depends on the result of former measurements.

In this section, we discuss the high-level structure of quantum algorithms, the requirements for a quantum programming language, and review some of the existing proposals.

6.1.1  Structure of Quantum Algorithms

![Figure 7: Workflows for quantum algorithm](image)

The usual model for quantum computation was depicted in Figure 1: a classical computer controls a quantum co-processor, whose role is to hold a quantum memory. A programmatic interface for interacting with the co-processor is provided to the programmer sitting in front of the classical computer. The interface gives methods to send instructions to the quantum memory to allocate and initialize new quantum registers, apply unitary gates on qubits, and eventually perform measurements. If the set of instructions is commonly represented as a circuit, it is merely the result of a trace of classical execution of a classical program on the classical computer.

Figure 7 presents two standard workflows with a quantum co-processor. In Figure 7a, the classical execution inputs some (classical) parameters, performs some pre-processing, generates a circuit, sends the circuit to the coprocessor, collects the result of the measurement, and finally performs some post-processing to decide whether an output can be produced or if one needs to start over. Shor’s factoring algorithm [150] or Grover’s algorithm [72] fall into this scheme: the circuit is used
as a fancy probabilistic oracle. Most of the recent variational algorithms \[120\] also fall into this scheme, with the subtlety that the circuit might be updated at each step. The other, less standard workflow is presented in Figure 7b. In this scheme, the circuit is built “on the fly”, and measurements might be performed on a sub-part of the memory along the course of execution of the circuit. The latter part of the circuit might then depend on the result of classical processing in the middle of the computation.

Understanding a quantum circuit as a by-product of the execution of classical program shines a fresh view on quantum algorithms: it cannot be identified with a quantum circuit. Instead, in general, at the very least a quantum algorithm describes a family of quantum circuits. Indeed, consider the setting of Figure 7a. The algorithm is fed with some parameters and then build a circuit: the circuit will depend on the shape of the parameters. If for instance we were using Shor’s factoring algorithm, we would not build the same circuit for factoring 15 or 114,908,028,227. The bottom line is that a quantum programming language should be able to describe parametrized families of circuits.

The circuits described by quantum algorithms are potentially very large — a concrete instance of the HHL algorithm \[74\] for solving linear systems of equations has been shown \[142\] to count as much as $\sim 10^{40}$ elementary gates, if not optimized. Unlike the circuit-construction schemes hinted at in Section 5, this circuit is not uniquely given as a list of elementary gates: it is built from sub-circuits — possibly described as list of elementary gates but not only — and from high-level circuit combinators. These combinators build a circuit by (classically) processing a possibly large sub-circuit. Some standard such combinators are shown in Figure 8 (where we represent inverse with reflected letters). There is a distinction to be made between the combinator, applied on a sub-circuit, and its semantics, which is an action on each elementary gate. Combinators are abstractions that can be composed to build larger combinators, such as the one presented in Figure 9, built from inversion, controlling and sequential composition.

![Figure 8: Standard Circuits Combinators](image)

![Figure 9: Example of derived circuit combinator](image)
6.1.2 Requirements for Quantum Programming Languages

Any scalable quantum programming language should therefore allow the following operations within a common framework.

- Manipulation of quantum registers and quantum circuits as first-class objects. The programmer should both be able to refer to “wires” in a natural manner and handle circuits as independent objects.

- Description of parametric families of quantum circuits, both in a procedural manner as sequence of operations —gates or subcircuits— and in an applicative manner, using circuit combinators;

- Classical processing. In our experience [71], quantum algorithms mostly consist of classical processing —processing the parameters, building the circuits, processing the result of the measurement.

This broad description of course calls for refinements. For instance some of the classical processing might be performed on the quantum co-processor —typically the simple classical controls involved in quantum error correction—. The level of classical processing performed on the classical computer and performed on the quantum co-processor is dependent on the physical implementation. If some recent proposals such as Quingo [156] discuss the design of quantum programming languages aware of the two levels of classical processing—in and out of the co-processor—, this is still work in progress.

6.1.3 Review of the Existing Approaches

Most of the current existing quantum programming languages follow the requirements discussed in Section 6.1.2. In this section, we review some typical approaches followed both in academic and in industrial settings. This review is by no mean meant to be exhaustive: its only purpose is to discuss the possible strategies for the design of QPLs.

When designing a realistic programming language from scratch, the main problem is the access to existing libraries and tools. In the context of quantum computation, one would need for instance to access the file system, make use of specific libraries such as Lapack or BLAS, etc. One can also rely on the well-maintained and optimized compiler or interpreter of the host language. In order to quickly come up with a scalable language, the easiest strategy consists in embedding the target language in a host language. Indeed, a quantum programming language can be seen as a domain-specific language (DSL), and it can be built over a regular language.

If the advantages of working inside a host language are clear, there are two main drawbacks, the first one is the potential rigidity of the host language: there might be constructs natural to the DSL that are hardly realizable inside the host language. The second drawback has to do with the compilation toolchain: the shallow embedding of the DSL makes it impossible to access its abstract syntax tree, rendering specific manipulation thereof impossible.

Embedded QPLs. The first scalable embedded proposal is QUIPPER [71, 70]. Embedded in Haskell, it capitalizes on monads to model the interaction with the quantum co-processor. QUIPPER’s monadic semantics is meant to be easily abstracted and reasoned over: it is the subject of Section 6.2.2. Since QUIPPER, there has been a steady stream of embedded quantum programming languages, often dedicated to a specific quantum co-processor or attached to a specific vendor, and mostly in Python: QISKIT [152] and PROJECTQ [154] for IBMQ, CirQ [107] for Google, Strawberry Fields [93] for Xanadu, AQASM for Atos, etc. From a language-design point of view, most of
these approaches heavily rely on Python objects to represent circuits and operations: the focus is on usability and versatility rather than safety and well-foundness.

**Standalone QPLs.** On the other side of the spectrum, some quantum programming languages have been designed as standalone languages, with their own parser and abstract syntax tree. Maybe the first proposed scalable language was Ömer’s QCL [126]. Ömer experimented several features such as circuit-as-function, automatic inversion and oracle generation. However, due to its non-modular approach the language did not have successors.

LIQU|⟩ [165] and its sequel Q# [155] developed by Microsoft are good examples of an attempt at building a standalone language while keeping a tight link with an existing programming environment, as Q# is tightly linked with the F# framework, making it possible to easily “reuse” library functions from within a Q# piece of code. On the other hand, Q# has its own syntax and type system, to capture run-time errors specific to quantum computation.

ScaffCC [86] is another example of a standalone QPL. If the language is rather low-level its compiler has been heavily optimized and experimented over, and it serves as support for a long stream of research on quantum compiler optimizations.

The last noteworthy language to cite in series is SILQ [20], as it serves as a good interface with the next paragraph: aimed at capturing most of the best practice in term of soundness and safety, it is nonetheless targeted toward usability.

**Formal QPLs.** The last line of works on QPLs we would like to mention here are formal languages aimed at exploring and understanding the design principles and the semantics of quantum algorithms. We shall be brief as this is the topic of the remainder of this chapter. The initial line of work was initiated by Selinger [144] with the study of a small flow-chart language with primitive constructs to interact with the quantum co-processor: qubit initialization, elementary gate application and measurement. This language was later extended to a simple lambda-calculus with similar primitive quantum features [147]. If the language is not aimed at full-scale quantum algorithms, it is nonetheless enough to serve as a testbed for experimenting type systems and many operational [146, 47, 106] and denotational [127, 148, 48, 75] semantics.

The study of formal QPLs took a turn toward circuit-description languages à la QUIPPER with the development of scalable quantum languages. One of the first proposal of formalization is QWIRE [130], embedded in the proof assistant COQ. QWIRE uses Coq expressive system to encode the sophisticated typing rules of QWIRE. In a sense, CoQ type system is expressive enough to use CoQ as a host language and still be able to manipulate the abstract syntax tree of a program. The main design choice for QWIRE is to separate pure quantum computation with its constraints such as no-cloning, from classical computation.

Albeit disconnected from CoQ, the formalization of QUIPPER has followed a similar root. This development is based on the formal language PROTOQUIPPER [139], which extracts the critical features out of QUIPPER: the creation and manipulation of circuits using a minimal lambda-calculus. The language is equipped with a linear type system and a simple operational semantics based on circuit-construction. The simple core proposed by PROTOQUIPPER has stirred a line of research on the topic, including the formalization of inductive datatypes and recursion in this context [137, 115].

The last class of formal programming language we want to mention focuses on the specification and verification of high-level properties of programs, and are solely based on circuit manipulation: unlike QWIRE or QUIPPER, qubits are not first-class objects, and circuits are simple “bricks” to be horizontally or vertically stacked. In this class of languages, one can mention qPCF [128], mainly a theoretical exploration of dependent type systems in this setting, and QBRICKS, presented in Section 7.2.
6.2 Formalizing the Operational Semantics

In order to reason on quantum programming languages, one needs to have a formal understanding of their operational semantics.

6.2.1 Quantum Lambda-Calculi

The lambda-calculus [13] is a formal language encapsulating the main property of higher-order functional languages: functions are first-class citizens that can be passed as arguments to other functions. Lambda-calculus features many extensions to model and reason about side-effects such as probabilistic or non-deterministic behaviors, shared memory, read/write, etc.

One of the first formal proposal of a quantum, functional language has precisely been a quantum extension of lambda-calculus [147]. On top of the regular lambda-calculus constructs, the quantum lambda-calculus features constants to name the operations of qubit initialization, unitary maps and measurements. A minimal system consists of the following terms:

\[ M, N ::= x \mid \lambda x. M \mid MN \]
\[ \text{tt } \mid \text{ff } \mid \text{if } M \text{ then } N_1 \text{ else } N_2 \]
\[ \text{qinit } \mid U \mid \text{meas}. \]

Terms are represented with \( M \) and \( N \), while variables \( x \) range over an enumerable set of identifiers. The term \( \lambda x. M \) is an abstraction: it stands for a function of argument \( x \) and of body \( M \). The application of a function \( M \) to an argument \( N \) is represented with \( M N \). To this core lambda-calculus, we can add constructs to deal with booleans: \( \text{tt } \) and \( \text{ff } \) are the boolean constant values, while \( \text{if } M \text{ then } N_1 \text{ else } N_2 \) is the usual test. Finally, \( \text{qinit } \) stands for qubit initialization, \( \text{meas } \) for measurement and \( U \) ranges over a set of (unary) unitary operations. These three constants are functions: for instance, \( \text{qinit } \text{tt} \) corresponds to \( |1\rangle \) and \( \text{qinit } \text{ff} \) to \( |0\rangle \), while \( \text{meas } \) applied to a qubit stands for the measurement of this qubit. A fair coin can then be represented by the term

\[ \text{meas}(\text{Had(\text{qinit } \text{tt})}), \quad (3) \]

where \( \text{Had} \) stands for the Hadamard gate.

The question is now: how do we formalize the evaluation of a piece of code? In the regular lambda-calculus, evaluation is performed with substitution as follows:

\[ (\lambda x. M) N \rightarrow M[x := N] \]

where \( M[x := N] \) stands for \( M \) where all free occurrences of \( x \) —i.e., those corresponding to the argument of the function— have been replaced by \( N \). If we can still require such a rule in the context of the quantum lambda-calculus, this does not say how to deal with the term \( \text{qinit } \text{tt} \).

In order to give an operational semantics to the lambda-calculus, a naive idea could be to add yet another construction: a set of constants \( c_{\phi} \), once for every possible qubit state \( |\phi\rangle \). If —as shown by van Tonder [160]— this can somehow be made to work, a more natural presentation consists in mimicking the behavior of a quantum co-processor, in the style of Knill’s QRAM model [101]: we define an abstract machine \( (|\phi\rangle_n, L, M) \) consisting of a finite memory state \( |\phi\rangle_n \) of \( n \) qubits, a term \( M \) with \( n \) free variables \( x_1, \ldots, x_n \), and a linking function \( L \), bijection between \( \{x_1, \ldots, x_n\} \) and the qubit indices \( \{1, \ldots, n\} \). Variables of \( M \) captured by \( L \) are essentially pointers to qubits standing in
the quantum memory. The fair coin of Eq. (3) then evaluates as follows.

$$
(\langle 0 \vert_0, \{} \rangle, \text{meas}(\text{Had}(q_{\text{init t}})))
\rightarrow (\langle 1 \vert_1, \{x \mapsto 1\} \rangle, \text{meas}(\text{Had} x))
\rightarrow \left(\frac{1}{\sqrt{2}}(\langle 0 \vert_1 - |1 \rangle_1), \{x \mapsto 1\} \text{meas}(x)\right)
\rightarrow \begin{cases} 
(\langle 0 \vert_1, \}, \text{ff} \rangle & \text{with prob. 0.5} \\
(\langle 1 \vert_1, \}, \text{tt} \rangle & \text{with prob. 0.5.}
\end{cases}
$$

In this evaluation, most of quantum computation has been exemplified: initialization of qubits, unitary operations and measurements. Handling the latter in particular requires a probabilistic evaluation, and this requires some care — we invite the interested reader to consult for example Selinger & Valiron [146] for details.

6.2.2 Monadic Semantics

The operational semantics of the quantum lambda-calculus is very limited. Indeed, as discussed in Section 6.1, quantum algorithms do not in general send operations one by one to the quantum coprocessor: instead, a quantum program must build circuits (or pieces thereof) before sending them to the co-processor as batch jobs. The quantum lambda-calculus does not allow to build circuits: operations can only be sent one at a time. In particular, there is no possibility to create, manipulate and process circuits: circuit generation in the quantum lambda-calculus is a side-effect that is external to the language. One cannot interfere with it, and embedding the quantum lambda-calculus as it stands inside a host language as suggested in Section 6.1.3 would not help.

The solution devised by QUIPPER consists in relying on a special language feature from Haskell called monad. A monad is a type operator encapsulating a side effect. Consider for instance a probabilistic side effect. There are therefore two classes of terms: terms without side-effect, with types e.g. $\text{Bool}$, or $\text{Int}$, and terms with side-effect, with types e.g. $\text{P(Bool)}$ or $\text{P(Int)}$ standing for “term evaluating to a boolean/integer, possibly with a probabilistic effect”. The operator $\text{P(-)}$ captures the probabilistic side effect.

A monad comes with two standard maps. In the case of $\text{P}$ we would have:

$$
\text{return} :: \text{A} \rightarrow \text{P(A)}
\text{eval} :: (\text{A} \rightarrow \text{P(B)}) \rightarrow \text{P(A)} \rightarrow \text{P(B)}
$$

The return operation says that an effect-free term can be considered as having an effect — in the case of the probabilistic effect, it just means “with probability 1” —. The eval operation\(^3\) says how to compose effectful operations: given a function inputting A and returning an object of type B with a probabilistic side-effect, how to apply this function to a term of type A also having a probabilistic effect? We surely get something of type $\text{P(B)}$, but the way to construct it is described by eval. A few equations have to be satisfied by return and eval for them to describe a monad. For instance, eval return is the identity on $\text{P(A)}$. There can of course be more operations: for instance, we can add to the signature of $\text{P}$ an operator coin of type $() \rightarrow \text{P(Bool)}$\(^4\).

A nice property of monads is that effectful operations can be written with syntactic sugar in an imperative style:

```
    do
        x <- coin ()
        if x then return 0 else return 1
```

\(^3\)In Haskell this map is denoted with >>=. For the sake of legibility, here we denote it with eval.

\(^4\)In Haskell, the unit type is denoted with ().
is a term of type $P(\text{Int})$ equals to

$$\text{eval} \left( \lambda x. \text{if } x \text{ then return } 0 \text{ else return } 1 \right) (\text{coin}())$$

once the syntactic sugar has been removed.

Following this approach, quantum computation can be understood as side-effect: it combines both (1) Read/Write effect, since gates are sent to the coprocessor, and results of measurements are received; (2) Probabilistic effects, since measurement is a probabilistic operation. The first attempt at formalizing this monad is Green’s quantum IO monad [3]: it has then been further developed in QUIPPER [71], subject of Section 6.2.3.

### 6.2.3 The QUIPPER Language

QUIPPER [71] is a programming language for quantum circuit description and manipulation based on the hybrid circuit model of quantum computation. In particular, in QUIPPER there are two stages of evaluation: the first evaluation generates a quantum circuit and the second runs the quantum circuit on the quantum co-processor. This is different from the quantum $\lambda$-calculus discussed in Section 6.2.1, where the program has only one phase of evaluation which includes quantum gate operations. Although both the quantum $\lambda$-calculus and QUIPPER represent quantum computations mathematically, QUIPPER efficiently builds quantum circuits using the circuit-related operations which allows to consider quantum circuit as classical object, whereas quantum $\lambda$-calculus basically applies quantum gates one after another.

QUIPPER’s programming features can be summarized as follows.

- All of Haskell computations;
- Parametrized families of circuits;
- Circuit construction and manipulation both in an imperative and in a functional, applicative approach;
- Wires can be of type Qubit or Bit: this can place some simple classical operation inside the co-processor;
- Sound methods for circuit manipulation and modification;
- Dynamic lifting —that is, retrieval of classical booleans in the control flow of the program—and circuit execution.

Circuits in QUIPPER are constructed and sent to the quantum computer using a specific monad Circ. The signature of the monad in particular includes

- $\text{qinit} :: \text{Bool} \rightarrow \text{Circ}(\text{Qubit})$
- $\text{measure} :: \text{Qubit} \rightarrow \text{Circ}(\text{Bit})$
- $\text{dynamic\_lift} :: \text{Bit} \rightarrow \text{Circ}(\text{Bool})$
- $\text{had} :: \text{Qubit} \rightarrow \text{Circ}(\text{Qubit})$

The toss-coin of Section 6.2.2 can then be written as the code

```haskell
coin () = do
  q <- qinit True
  q' <- had q
  r <- measure q'
  dynamic_lift r
```
The function `coin` is of type `() -> Circ(Bool)`: running `coin` will merely generate a computation—producing a circuit—waiting to be executed.

Thanks to the monadic encapsulation, circuits can be manipulated within Haskell. For instance, inversion and control can be coded in Haskell as circuit combinators with the following types.

```haskell
inverse :: (a -> Circ b) -> (b -> Circ a)
control :: (a -> Circ b) -> ((a, Qubit) -> Circ (b, Qubit))
```

### 6.3 Type Systems

In Section 6.2, we discussed how to model the operational behavior of a quantum program. We have however not mentioned yet the run-time errors inherent to quantum computation. In the classical world, type systems are a standard strategy to catch run-time errors at compile-time. Several run-time errors specific to quantum computation can also be caught with a type system, with a few specificities that we discuss in this section.

#### 6.3.1 Quantum Data and Type Linearity

The main problem with quantum information is that it is non-duplicable (a.k.a. non clonable, see Section 4.2.3). In term of quantum programming language, this means that a program cannot duplicate a quantum bit: if \( U \) is a unitary map acting on two qubits, the function \( \lambda x. U(x \otimes x) \) trying to feed \( U \) with two copies of its argument make no sense. Similarly, it is not possible to control a gate acting on a qubit with the same qubit. The QUPPER code of Figure 10 is therefore buggy—and the generated circuit shown on the right is meaningless compared to the code.

```haskell
exp :: Circ Qubit
exp = do
  q1 <- qinit True
  q2 <- qinit True
  r <- qnot q1 'controlled' q1
  return r
```

![Figure 10: An example of erroneous circuit generated by a QUPPER program](image)

Type systems, in a broad sense, provide a predicate which says that a well-typed program does not have certain class of bugs: in the case of quantum programming languages, a large class of bugs comes from duplicating non-duplicable objects. This calls for a linear type system, enforcing the non-duplication at least of qubits. This has been taken into account in recent scalable implementations such as Silq [20].

On the theoretical side, type systems for quantum lambda-calculi and PROTOQUIPPER [139]—the formalization of QUPPER—are typically based on linear logic. Originally designed by Girard [67], linear logic assumes that formulas are linear—i.e. non-duplicable and non erasable—by default, and the logic comes equipped with a logic constructor “!” to annotate duplicable and erasable formulas. Linear logic also proposes a special pairing constructor \( \otimes \) replacing the usual product and compatible with both the linearity constructs and the (linear) implication.

A core type system for a quantum lambda-calculus with pairing therefore consists of the following grammar:

\[
A, B ::= qubit | bool | A \rightarrow B | A \otimes B | !A.
\]
Type $A \rightarrow B$ represents the type of (linear) functions, using their argument only once. Type $A \otimes B$ represents the pair of a term of type $A$ and a term of type $B$. Type $!A$ stands for a duplicable term of type $A$. We give a few examples as follows.

- The identity function $\lambda x.x$ is of type $A \rightarrow A$, but also of type $!(A \rightarrow A)$ as it is duplicable (since it does not contain any non-duplicable object);
- If the pairing construct is represented with $\langle -,- \rangle$, the function $\lambda x.\langle x,x \rangle$ is of type $!A \rightarrow (!A \otimes !A)$: it asks for a duplicable argument.
- The operator qinit is of type $\text{bool} \rightarrow \text{qubit}$: it does not generate a duplicable qubit;
- The operator meas can however be typed with $\text{qubit} \rightarrow !\text{bool}$ as a boolean should be duplicable;
- Provided that $U$ is a unitary acting on two qubits, one can type it in a functional manner with $\text{qubit} \otimes \text{qubit} \rightarrow \text{qubit} \otimes \text{qubit}$: it inputs two (non-duplicable) qubits and outputs the (still non-duplicable) modified qubits;
- In particular, provided that we assume implicit dereliction casting duplicable elements of type $!A$ to $A$, the term $\lambda x. U(x,x)$ can only be typed with $\text{qubit} \rightarrow \text{qubit} \otimes \text{qubit}$: its argument has to be duplicable. The fact that this program can never be actually used on a concrete qubit is a property of the type system (intuitively, qinit only generates non-duplicable qubits).

### 6.3.2 Example: Quantum Teleportation

Mixing quantum computation and higher-order can yield non-trivial objects. For instance, quantum teleportation can be understood as two non-duplicable functions. The scheme of teleportation is given in Figure 11. It consists of three steps: (A) creation of an Bell state, (B) measure in the Bell basis to retrieve two booleans and (C) application of a gate $U_{b_1 b_2}$ dependent on the result of the measure. The state of the top wire is then “teleported” to the bottom wire. It is possible to understand the pieces of the quantum teleportation protocol as three functions:

- (A) $() \rightarrow \text{qubit} \otimes \text{qubit}$
- (B) $\text{qubit} \rightarrow (\text{qubit} \rightarrow \text{bool} \otimes \text{bool})$
- (C) $\text{qubit} \rightarrow (\text{bool} \otimes \text{bool} \rightarrow \text{qubit})$
The teleportation algorithm then feed the two qubits of (A) to (B) and (C), and this gives a general type
\[(\cdot) \to (\text{qubit} \to \text{bool}) \otimes (\text{bool} \otimes \text{bool} \to \text{qubit})\]
for the protocol: it morally generates two functions, and the specification of the protocol states that these two functions are inverse one of the other.

One can also note that these two functions are non-duplicable. Indeed, each of them holds a (non-duplicable) qubit. Moreover, in a sense these functions are entangled, since the Bell state is.

### 6.3.3 Extending the Type System to Support Circuits

Let us assume that the type system of the quantum lambda-calculus is extended with lists: \([A]\) stands for lists of elements of type \(A\) (see e.g. [146] to see how to do this). A function \([\text{qubit}] \to [\text{qubit}]\) inputs a list of qubits. It can apply unitary gates to these qubit arguments: It can in fact describe different circuits, depending on the size of the list. Such a function therefore describes a family of circuits. The quantum lambda-calculus is not expressive enough to extract one circuit out of this family of circuits and operate on it (e.g. by inversing or controlling it).

The ProtoQuipper language [139] and its successors [137, 65, 115] are formalized fragments of the programming language Quipper. They enforce structural properties of quantum programs using the linear type system of the quantum lambda-calculus, yet extending it to support circuit manipulation. The ProtoQuipper comes with a new type construct \(\text{Circ}(A, B)\): the type of circuits from \(A\) to \(B\), and two functions:

- box sends \(A \to B\) to \(\text{Circ}(A, B)\). It takes a function, partially evaluates it and store the emitted circuit.
- unbox sends \(\text{Circ}(A, B)\) to \(A \to B\). It takes a circuit from \(A\) to \(B\) and reads it as a function of input \(A\) and output \(B\).

One of the subtleties is the fact that box turns a function —possibly representing a family of many circuits— to one circuit. In the case of a function of type \([\text{qubit}] \to [\text{qubit}]\), this corresponds to choosing one size of list and building the circuit for this input size. Whenever the type system supports inductive types such as lists, the operator box then also take a shape as second argument, for deciding on the shape of circuit to build. In recent works [65], ProtoQuipper’s type system has been extended to very expressive dependent types, in order to characterize with a very fine-grain the shape structure of a family of circuits.

For instance, suppose that the program \(P\) sends \([\text{qubit}]\) to \([\text{qubit}]\). It corresponds to a family of circuits, but if we pick a choice of input size \(n\), the type gives no information on the output shape of the circuit —that is, the number of output wires—. Maybe \(P\) duplicates each input wires ? With dependent types, we can for instance index list-types with size, and type \(P\) with
\[
\forall n. [\text{qubit}]_n \to [\text{qubit}]_{2n}.
\]
This type tells us that \(P\) corresponds to a family of circuits of even output wires. This makes it possible to catch errors when using circuit combinators: for instance, the inverse operator can be typed with
\[
\forall n m. \text{Circ}([\text{qubit}]_m, [\text{qubit}]_n) \to \text{Circ}([\text{qubit}]_n, [\text{qubit}]_m)
\]
The inverse of \(P\) then becomes a function of type
\[
\forall n. [\text{qubit}]_{2n} \to [\text{qubit}]_n.
\]
In particular, this function can only be applied to lists of even sizes. This run-time error cannot be checked without shape information.

Although such a type system becomes very expressive, in general it fails to feature a type inference algorithm, as this would require to be able to solve arbitrary arithmetic equations.

6.3.4 Discussion

Type systems for quantum programming languages provide very efficient ways to encode and automatically verify some important properties of programs, and in particular to rule out at compile-time large classes of run-time errors specific to quantum computation. In particular, type systems have been used to characterize and enforce

- structure of parametric families of circuits
- linearity of non-duplicable elements
- only control and inversion of purely quantum circuits

However, to be able to go further and characterize functional correctness with respect to specification, or validate the number of gates of a circuit, or catch subtle bugs involving concatenation of inverted circuits, one needs to shift towards sophisticated dependent types. The gain in expressiveness is then at the expend of automation.

The quest for a finer trade-off, permitting automation while capturing some of what is currently only available with dependent type system is an active research area in the community.

7 High and Mid-Level Verification: Algorithms and Programs

Most quantum programming languages (Qiskit [132] Quipper [71], LiQUiD [165], Q# [155], ProjectQ [154], SILQ [20], etc) embed features for quantum circuit manipulations within a standard classical programming language. Such circuit-building quantum languages are the current consensus for high-level executable quantum programming languages. A current major challenge is to link this language design paradigm with formally verified programming. In the present section we introduce the main existing propositions in that direction.

7.1 Quantum Hoare Logic

Quantum Hoare logic (QHL) [28, 56, 92, 166, 158, 157, 15] is a general framework for reasoning about the high-level description of quantum algorithms. It is based on the intermediate assertion method [62, 81] — attach each program point with an assertion and whenever the data flow reaches a program point the attached assertion should be satisfied — which was originated with Alan Turing [8]. Hoare’s approach enables (interactive) theorem proving for high-level algorithmic description verification that proceeds at the same abstraction level as the language itself. This makes verification more human-friendly than lower-level (machine-friendly) verification.

7.1.1 Quantum Programming Language: Quantum WHILE-Programs

The guideline for the hybrid model introduced in Section 2.1.1 is summed up by the slogan “quantum data and classical control” [144]: quantum data can be superposed and entangled, they are manipulated by basic quantum operations — unitary evolution and measurement, but the high-level control is still classical (e.g. branch, loops, etc).
In light of this slogan, QHL introduces a minimal programming language for describing quantum algorithms [167]. Let $q$ (resp. $\bar{q}$) be a quantum variable (resp. a list of quantum variables); let $U$ be a unitary operator acting on the qubits $\bar{q}$ and let $M \triangleq \{M_m\}_m$ with $\sum_m M_m^\dagger M_m = I$ be a measurement on the qubits $\bar{q}$, each $M_m$ corresponding to a measurement result $m$. As a special case, let $M' \triangleq \{M_0, M_1\}$ with $M_0^\dagger M_0 + M_1^\dagger M_1 = I$. Then quantum WHILE-programs are generated by the following syntax.

$$\begin{align*}
S & \triangleq \text{skip} & \text{No operation} \\
& | q := |0\rangle & \text{Initialization} \\
& | \bar{q} *= U & \text{Unitary operation} \\
& | S_1; S_2 & \text{Sequential composition} \\
& | \text{if } \Box m \cdot M[\bar{q}] = m \rightarrow S_m \text{ fi} & \text{Probabilistic branching} \\
& | \text{while } M'[\bar{q}] = 1 \text{ do } S_0 \text{ od} & \text{Probabilistic while loop}
\end{align*}$$

The intended semantics of language constructs above is similar to that of their classical counterparts. To illustrate the quantum features contained in these constructs, we make the following comments:

(i) in the initialization, the choice of a fixed state $|0\rangle$ is due to the fact that any known quantum state can be prepared by applying a unitary operator to $|0\rangle$;

(ii) in the probabilistic branching (resp. while loop), different branches $\{S_m\}_m$ (resp. \{\text{skip}, S_0\}) are chosen according to (randomly distributed) outcomes of the measurement $M$ (resp. $M'$) on the qubits $\bar{q}$, potentially disturbing the current state.

We refer the reader to [166] for a detailed exposition of the syntax above.

**Example 7.1** (Preparation of the Bell state $|\beta_0\rangle$). Let $p$ and $q$ be quantum variables each denoting one qubit. Then the following program initiates them to $|0\rangle$ and implements the circuit from Figure 2, preparing state $|\beta_0\rangle$ from Example 2.1.:

$$
|\beta_0\rangle \triangleq p := |0\rangle; q := |0\rangle; p *\equiv H; (p, q) *\equiv \text{CNOT}
$$

Note that the quantum programming language defined above is in the spirit of the hybrid circuit model presented in Section 2. Indeed, the basic sequence of quantum operations (initialization, unitary operation, and measurement) are meant to be interpreted as a generalized quantum circuit to be executed on a quantum co-processor; and post-measurement branchings (in, e.g., probabilistic branching and while loop) are meant to be controlled by a classical computer.

### 7.1.2 Quantum States, Operations and Predicates

Measuring a quantum state transforms it, following the Born rule (see Section 2.1.2). The resulting probability distribution over quantum states is formalized as a *mixed state* (as opposed to *pure states* which are the usual quantum states, as introduced in Section 2.1.2 and used so far). For example, a measurement on any quantum pure state $|\psi\rangle \triangleq \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ or $|\psi\rangle \triangleq \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ will result in the mixed state $\mathcal{E} = \{(\frac{1}{2}, |0\rangle), (\frac{1}{2}, |1\rangle)\}$, with states $|0\rangle$ and $|1\rangle$ occurring with an equal probability of $\frac{1}{2}$ (notice that this observation makes both states $|+\rangle |-\rangle$ impossible to distinguish experimentally).

In this way, representation of the final state of applying a series of measurements to a quantum state could expand exponentially. To address this issue, a square-matrix representation of quantum states, i.e. partial density operator, is adopted instead. For example, pure quantum state $|+\rangle$ is represented as $|+\rangle \langle +|$, and mixed quantum state $\mathcal{E}$ as $\frac{1}{2} |0\rangle \langle 0| + \frac{1}{2} |1\rangle \langle 1|$. For more information on partial density operators, the reader is referred to [144, 167].
If we see the matrix representation of a quantum state (partial density operator) as a linear operator, then a quantum operation—initialization, unitary evolution and measurement—can be thought of as a super operator, i.e., a function from linear operators to linear operators. What’s interesting is that every quantum WHILE-program defined above can be interpreted as a quantum operation, and partial density operators are closed under quantum operations. This justifies the success of representing quantum states as partial density operators and defining the denotational semantics of quantum programs as quantum operations [144, 167].

Following [46], a quantum predicate on vector space $\mathcal{H}$ is defined as a Hermitian operator $M$ between the zero operator $0_\mathcal{H}$ (simulating the contradiction) and the identity operator $I_\mathcal{H}$ (simulating the tautology). Instead of the usual binary satisfaction judgment, QHL evaluates the satisfaction of a predicate by a state as a real value between 0 (false) and 1 (true). It is defined as the trace $tr(M\rho)$ $\dagger$ of the product $M\rho$. Intuitively, it represents the expectation for the truth value of $M$ in the mixed state $\rho$ (which is, again, a probability distribution over pure states).

Then, the intuition of implication between predicates is also probabilistic. It is filled by the *Löwner order* $M \sqsubseteq N$, relating operators $M$ and $N$, if and only if, for any state $\rho$, the expectation truth value of $N$ in $\rho$ it more or equal to that of $M$ in $\rho$. This condition is formalized as $tr(M\rho) \leq tr(N\rho)$ for all states $\rho$ (See, e.g., [166, Lemma 2.1]).

Adopting such quantum predicates as assertions, among many others (e.g., interpreted as physical observables), provides simple expression means for many properties of quantum effects. For example, quantum predicate $|+\rangle \langle +|$ expresses that a state $\rho$ is in the equal superposition $|+\rangle$ with probability $tr(|+\rangle \langle +| \rho)$; quantum predicate $|β_{00}\rangle \langle β_{00}|$ expresses that a state $\rho$ is in the maximal entanglement $|β_{00}\rangle$ with probability $tr(|β_{00}\rangle \langle β_{00}| \rho)$, etc.

### 7.1.3 Quantum Program Verification

For now, a quantum (partial) correctness formula can be the Hoare’s triple $\{P\} S \{Q\}$, where $S$ is a quantum WHILE-program, and $P, Q$ are quantum predicates. To define the partial-correctness semantics of quantum Hoare’s triples, in the sequel, let $[\lbrack S\rbrack]$ denote the semantic function of $S$ (Note that $[\lbrack S\rbrack]$ is a quantum operation defined by induction on $S$, cf. [167]), and $[\lbrack S\rbrack](\rho)$ the output of $S$ on the input $\rho$.

**Definition 7.2** (Semantics of partial correctness, cf. [166]). Let $P, Q$ be quantum predicates and $S$ a quantum WHILE-program. We say that $S$ is (partially) correct w.r.t. precondition $P$ and postcondition $Q$, written $\models \{P\} S \{Q\}$, if

$$\forall \rho, \quad tr(P\rho) \leq tr(Q[\lbrack S\rbrack](\rho)) + [tr(\rho) − tr([\lbrack S\rbrack](\rho))] \). \quad (4)$$

Note that Inequality (4) can be seen as a probabilistic version of the following statement: if state $\rho$ satisfies predicate $P$, then, executing program $S$ on input $\rho$, either $S$ fails to terminate or the resulting state $[\lbrack S\rbrack](\rho)$ satisfies predicate $Q$.

The axiom system for proving partial correctness of quantum WHILE-programs is composed of axioms and inference rules manipulating quantum Hoare’s triples [166]. It is shown in Table 2 (where $\{|i\rangle_q\}$ is the computational basis for quantum variable $q$). Remark that each of these rules and axioms follows the intermediate assertion method. Here we only show how to derive the most complex rule (Par Loop Rule). The derivation of other proof rules can be done similarly.

$\dagger$ The trace of a square matrix $M$ with $n$ rows and columns is defined as the sum $\sum_{j \in [0,nq]} M(j,j)$ of its diagonal cells values.
Table 2: Proof system for partial correctness.

(Skip Axiom) \( \{ P \} \text{ skip } \{ P \} \)

(Init Axiom) \( \{ \sum_{l \in Q} \langle 0 | P \rangle | q \rangle | l \rangle = | 0 \rangle \} \{ P \} \)

(Unit Axiom) \( \{ U^+P_U \} \hat{q} = \{ P \} \)

(Comp Rule) \( \{ P \} S_1 \{ Q \} \{ Q \} S_2 \{ R \} \)

(If Rule) \( \{ P \} \sum_{m} \{ Q \} \) for all \( m \)

(Par Loop Rule) \( \{ P \} S_0 \{ M_0^{-1}Q M_0 + M_1^{-1}P M_1 \} \) while \( M_0^{-1}Q M_0 + M_1^{-1}P M_1 \) od \( \{ Q \} \)

(Order Rule) \( \frac{P \subseteq P'}{P \} S \{ Q' \} \quad Q' \subseteq Q \)

Intuition of (Par Loop Rule). To derive (Par Loop Rule), by intermediate assertion method, we attach each program point, say \( l_1, l_2, l_3 \), of a WHILE-statement with an assertion, say \( R, P, Q \), respectively:

\( \{ l_1 : R \} \quad \text{while } M'[\hat{q}] = 1 \quad \text{do } l_2 : P \quad \text{od } l_3 : Q \)

Fix the input \( \rho \) at the program point \( l_1 \) satisfying the assertion \( R \). By semantics of a WHILE loop, after the measurement \( M' \), one part \( M_1 \rho M_1^{-1} \) of the input will go to the loop body through the program point \( l_2 \) where the assertion \( P \) will be satisfied; the other part \( M_0 \rho M_0^{-1} \) will leave the while loop through the program point \( l_3 \) in which the assertion \( Q \) will be satisfied. Hence:

\[
tr(R\rho) \leq tr(Q(M_0 \rho M_0^{-1})) + tr(P(M_1 \rho M_1^{-1}))
\]

Due to the arbitrariness of \( \rho \), by properties of trace function and Löwner order, we have that \( R \subseteq M_0^{-1}Q M_0 + M_1^{-1}P M_1 \). Then, by weakening \( R \) to \( M_0^{-1}Q M_0 + M_1^{-1}P M_1 \) and lifting the above reasoning process into an inference rule, (Par Loop Rule) follows.

The following example illustrates how to derive a partially correct quantum Hoare triple using axioms and inference rules presented above.

Example 7.3 (Specification and correctness proof for the \( |\beta_{00}\rangle \) state construction program). Recall from Example 7.1 the definition of quantum program \( \beta_{00} \):

\[ \beta_{00} \triangleq p := |0\rangle; \; q := |0\rangle; \; p \equiv H; \; (p, q) \equiv \text{CNOT} \]

To show (partial) correctness of this program, it suffices to prove

\[ \{ I_p \otimes I_q \} \beta_{00} \{ |\beta_{00}\rangle \}_{p,q} \{ |\beta_{00}\rangle \} \]

This can be done as follows. By (Init Axiom), we have that

\[ \begin{align*}
\{ I_p \otimes I_q \} & \quad p := |0\rangle \quad \{ |0\rangle_p \otimes |0\rangle_q \\
\{ 0\rangle_p \otimes |0\rangle_q \} & \quad q := |0\rangle \quad \{ |0\rangle_p \otimes |0\rangle_q \} \langle 0 \mid q | 0 \rangle
\end{align*} \]
Applying (Comp Rule) to the last two triples, it follows that
\[
\{ I_p \otimes I_q \} \quad p := |0\rangle; \quad q := |0\rangle \quad \{ |0\rangle_p \otimes |0\rangle_q \langle 0| \}
\] (6)

By (Unit Axiom), we have that
\[
\{ |0\rangle_p \langle 0| \otimes |0\rangle_q \langle 0| \} \quad p \ast = H \quad \{ |+\rangle_p \langle +| \otimes |0\rangle_q \langle 0| \}
\]
\[
\{ |+\rangle_p \langle +| \otimes |0\rangle_q \langle 0| \} \quad (p.q) \ast = CNOT \quad \{ |\beta\rangle_p, q \langle \beta| \}
\] (7)

Finally, Hoare triple (5) follows by applying (Comp Rule) to (6) and (7).

### 7.1.4 Implementations and Extensions

Several works have taken advantage of extended Quantum Hoare Logic, e.g. algorithmic analysis of termination problem [112] or characterization and generation of loop invariants (i.e. \( M_0^t QM_0 + M_1^t PM_1 \) in (Par Loop Rule)) [169].

The practical illustration of QHL can be found in Liu et al. paper [117], containing an implementation in ISABELLE/HOL together with formalisation of Grover and QPE algorithms. Nevertheless in these examples, the central verification part is assumed through Python libraries uses.

More recent work [116] includes a full proof for a parametrized version of Grover algorithm. Although not holding the most general case for Grover algorithm, it constitutes an illustration of QHL use on a non trivial example.

### 7.1.5 Other Quantum Hoare Logics

Quantum relational Hoare logic [158, 15] allows to reason about how the outputs of two quantum programs relate to each other given a relation between their inputs, which can be used to analyze security of post-quantum cryptography and quantum protocols.

Quantum Hoare type theory [152] is inspired by classical Hoare type theory and extends the Quantum IO Monad [3] by indexing it with pre- and post-conditions that serve as program specifications, which has the potential to be a unified system for programming, specifying, and reasoning about quantum programs.

### 7.2 QBRICKS

QBRICKS [29] is a recently proposed circuit description language together with a deductive verification framework. It enables an automated proof support for program specifications, reducing the required human effort for the development of verified programs.

QBRICKS object language (QBRICKS-DSL) consists in a minimal functional language with features for the design of circuit families. Similarly to the formal contract style of algorithm descriptions (see Section 2.2.2), QBRICKS functions are written with explicit pre-and post conditions, specifying their complexity and the parametrized input-output quantum data registers function they implement. These specifications are written in a dedicated formal language, called QBRICKS-SPEC.

To support proofs, QBRICKS is given a Hoare style derivation rules system including derivation rules for each parametrized circuit constructor. These rules are enriched with equational theories enabling, in particular, reasoning about measurement and probabilities.
QBRICKS is a domain specific language, embedded in the Why3 [59] deductive verification framework: programs are written in ML language, and annotated with specifications in QBRICKS-DSL (pre and post conditions, loop invariants, calls for lemmas, etc). Compiling a QBRICKS program interprets these specifications as proof obligations. Then, a dedicated interface enables to directly access these proof obligations and either send them to a set of automatic SMT-solvers (CVC4, Alt-Ergo, Z3, etc.), or enter a number of interactive proof transformation commands (additional calls for lemmas or hypotheses, term substitutions, etc.) or even to proof assistants (COQ, ISABELLE/HOL).

7.2.1 Writing Quantum Circuits Functions in QBRICKS: QBRICKS-DSL

QBRICKS-DSL makes use of a regular inductive datatype for circuits, where the data constructors are elementary gates, sequential and parallel composition, and ancilla creation. In particular, unlike in e.g. QUIFPER or QWIRE, a quantum circuit in QBRICKS is not a function acting on qubits: it is a simple, static object. Nonetheless, for the sake of implementing quantum circuits from the literature, this does not restrict expressiveness as they are usually precisely represented as sequences of blocks.

The core of QBRICKS-DSL is presented in Figure 12. It is a small first-order functional, call-by-value language. To the elementary gates presented in Section 2.1.5, QBRICKS adds the qubit swapping gate SWAP and the identity ID. The constructors for high-level circuit operations are sequential composition SEQ, parallel composition PAR and ancilla creation/termination ANC.

```
Expression  e ::= x | c | f(e₁, ..., eₙ) | let (x₁, ..., xₙ) = e in e' |
                   if e₁ then e₂ else e₃ | iter f e₁ e₂

Data Constructor c ::= n | tt | ff | ⟨e₁, ..., eₙ⟩ | CNOT | SWAP | ID | H | Ph(e) | R₂(e) |
                     ANC(e) | SEQ(e₁, e₂) | PAR(e₁, e₂)

Function      f ::= f₁ | f₂

Declaration   d ::= let f₀(x₁, ..., xₙ) = e
```

Figure 12: Syntax for QBRICKS-DSL

The term constructs are limited to function calls, let-style composition, test with the ternary construct if-then-else and simple iteration: iter f n a stands for f(f(⋯f(a)⋯)), a succession of n calls to f.

Even if the language does not feature measurement, it is nonetheless possible to reason on probabilistic outputs of circuits, if we were to measure its output. This is expressed in a regular theory of real and complex numbers in the specification language (see Section 7.2.4 below for details).

7.2.2 Parametrized Path-Sums

To interpret circuit description functions, QBRICKS uses parametrized path-sums (pps), that are an extension of path-sums [5] (Section 5.2).

In QBRICKS setting, a path-sum $P$ is an object from an opaque type with four parameters, presented in Table 3 with their types and identifier shortcuts: two integer constants $\text{pps.width}(P)$ (the width of the target circuit) and $\text{pps.range}(P)$ (the range, meaning that the output sum of kets has a term for each bit vector $\vec{y}$ of length $\text{pps.range}(P)$ — written $\vec{y} \in \text{BV}_{\text{pps.range}(P)}$—) and two functions $\text{pps.angle}(P)$ and $\text{pps.ket}(P)$: for any input bit vector $\vec{x}$ of length $\text{pps.width}(p)$ (standing for a basis ket input to the target circuit) and for any index bit vector $\vec{y}$ of length $\text{pps.range}(p)$, func-
tions \texttt{pps_angle}(P) and \texttt{pps_ket}(P) respectively define a real scalar and a bit vector of length \texttt{pps_width}(p) (standing for a basis ket output to the target circuit)\textsuperscript{6}.

| Identifier     | Type                   | Id-abbreviation |
|----------------|------------------------|-----------------|
| \texttt{pps_width} | int                    | \texttt{p_w}   |
| \texttt{pps_range}  | int                    | \texttt{p_r}   |
| \texttt{pps_angle}  | \texttt{bit_vector} → \texttt{bit_vector} → real | \texttt{p_a}   |
| \texttt{pps_ket}    | \texttt{bit_vector} → \texttt{bit_vector} → \texttt{bit_vector} | \texttt{p_k}   |

Table 3: Pps accessors and types

Then for any bit vector \(\vec{x}\) of size \(\texttt{p_w}(P)\), the expression

\[
Ps(h, |\vec{x}\rangle) = \frac{1}{\sqrt{2^{\text{p_r}(P)}}} \sum_{\vec{y} \in \text{BV}_{\text{p_r}(P)}} e^{2\pi i \cdot \text{p_a}(P)(\vec{x}, \vec{y})} |\text{p_k}(P)(\vec{x}, \vec{y})\rangle_{\text{p_w}(P)}
\]

combines these different element together to define a linear application for quantum state vectors. Function \(Ps\) is extended by linearity to any ket \(|u\rangle\) of length \(\texttt{p_w}(P)\)\textsuperscript{7}.

A path-sum \(P\) is said to \textit{correctly interpret a given circuit} \(C\) (written \((C \triangleright p)\)) if and only if \(C\) has width \(n = \texttt{pps_width}(P)\) and for any bit vector \(\vec{x}\) of length \(n\), \(\text{Mat}(C) \cdot |\vec{x}\rangle = Ps(P, |\vec{x}\rangle)\). The relation \((\triangleright, \_\_)\) enjoys nice composition properties along \texttt{QBRICKS-DSL} circuit constructors (see [29]).

\texttt{QBRICKS-SPEC} generalizes path-sums by introducing Parametrized path-sums (\texttt{pps}). Basically, a \texttt{pps} is a function which inputs a set of parameters and outputs a path-sum. Then, it can be seen as a family of path-sums (one for each possible value of its parameters) describing the effects of the different circuit members in a family of quantum circuits. Hence, it is well-fitted for the specification of parametrized algorithm such as Shor order finding (Shor-OF see Figure 4).

The main strength of \texttt{pps} semantics, with regards to formal verification, is that each of the path-sum parameterized accessors (see Table 3) combines compositionally along circuit constructors.

Hence, it enables reasoning about parametrized quantum circuits and their semantics without manipulating sum terms or other higher-order objects. Thanks to this tool, the automatic generation of proof obligations for \texttt{QBRICKS} specifications results in only first-order formulas, enabling an high level of automation when sent to SMT-solvers.

7.2.3 From Quantum Circuits to Path-Sums

The specification language for \texttt{QBRICKS} is a first-order predicate language, equipped with various equational theories. For any quantum circuit family \(C\), \texttt{QBRICKS-DSL} enables to identify a \texttt{pps} \texttt{circ_to_pps}(C). Each of its parameterized accessors is defined inductively upon the structure of \(C\) and it is proved that \((C \triangleright \texttt{circ_to_pps}(C))\), for any instance of circuit. These accessors are listed and given abbreviations in Table 4.

\textsuperscript{6}In the rest of this section, type \texttt{bit_vector} corresponds to bit vectors \(\vec{x}\), encoded by an integer \texttt{length}(\vec{x}) (the length of the vector) and a function \texttt{get_bv}(\vec{x}) : \texttt{int} → \texttt{int}. For any integer \(i\), we commonly abbreviate \texttt{get_bv}(\vec{x})\(i\) as \(\vec{x}_i\); if \(i \in [0, \text{length}(\vec{x})]\) then it is such that \(0 \leq \vec{x}_i < 2^n\).

\textsuperscript{7}That is, to any linear combination of basis kets \(|\vec{x}\rangle\) of length \(\texttt{p_w}(P)\).
Table 4: Function \texttt{circ.to.pps} and accessors

| Accessor                        | Abbreviation |
|---------------------------------|--------------|
| \texttt{pps.width(circ.to.pps(C))} | \texttt{Cw(C)} |
| \texttt{pps.range(circ.to.pps(C))} | \texttt{Cr(C)} |
| \texttt{pps.angle(circ.to.pps(C))} | \texttt{Ca(C,\text{-,\text{-})}} |
| \texttt{pps.ket(circ.to.pps(C))}   | \texttt{Ck(C,\text{-,\text{-})}} |

7.2.4 Probabilistic Reasoning

QBRICKS-DSL does not contain any constructor for measurement of quantum registers. Nevertheless, QBRICKS-SPEC provides reasoning tools about it. In particular, function

\[
\text{proba.measure}: \text{circ} \times \text{ket} \times \text{int} \rightarrow \text{real}
\]

inputs a circuit \(C\), a quantum data register \(|v\rangle^n\) and an index \(j \in \llbracket 0, 2^n \rrbracket\). It outputs the probability, for one measuring the quantum register resulting from applying circuit \(C\) to \(|v\rangle\), to get \(j\) as a result. Function \text{proba.measure} is defined, for any input ket \(|u\rangle\) of length \texttt{pps.width(C)}, by application of the Born rule (see Section 2.1.2), as

\[
\text{proba.measure}(C, |i\rangle^m, j) = |(Ps(circ.to.pps, |i\rangle)^m(j))|^2.
\]

7.2.5 Verified Properties

The QBRICKS framework aims at providing tools for writing and verifying the standard format of quantum algorithm specifications as they appear in algorithm (see, e.g., Figure 4): to perform a given computation task with a given amount of resources. Hence, as illustrated above, QBRICKS-SPEC is designed for the formalization of both:

- parameterized input/output relations for families of circuits. For a family of circuit, they typically consist in characterizing their parametrized output ket vector. Thanks to function \text{proba.measure}, QBRICKS enables to identify probability to get a given result after measurement and derivated probability reasoning (such as bounding the parametrized probability of success of a computation, \textit{wrt} a pre-defined success condition). Proof support for these specifications is processed through the \texttt{pps} formalism,

- complexity requirements: QBRICKS enables to specify the parametrized width, number of required ancilla qubits and number of elementary gates of a circuit family.

Example 7.4 (Pps specifications for the Bell generating circuit). For example, a specification for the Bell generating circuit can be written using accessors of \texttt{pps circ.to.pps} (\textit{Bell-circuit}), as below

\[
\begin{align*}
\Gamma, \vec{x}, \vec{y}: \text{bit vector}, j: \text{int} & \vdash \\
\{ \text{bv.length}(\vec{x}) = 2 \land \text{bv.length}(\vec{y}) = 1 \land j \in \llbracket 0, 2 \rrbracket \} & \\
\text{Bell-circuit} & \\
\begin{cases}
\text{Cw(result)} = 2 \land \text{Ck(result, } \vec{x}, \vec{y}) = x(0) \cdot (1 - x(1)) \\ 
\text{Cr(result)} = 1 \land \text{Ca(result, } \vec{x}, \vec{y}) = x(0) \ast y(0) \\ 
\text{width(result)} = 2 \land \text{size(result)} = 2 \land \text{ancillas(result)} = 0
\end{cases}
\end{align*}
\]

This Hoare style writing, \{\text{Pre}\}p\{\text{Post}\} states that whenever \text{Pre} is satisfied, then running \(p\) ensures that \text{Post} is satisfied. Formula \text{Post} uses \text{result} as a variable standing for program \(p\). The
specification uses free bit vectors variables $\vec{x}$ and $\vec{y}$ and integer variable $j$. It requires $\vec{x}$ and $\vec{y}$ to have respective lengths 2 and 1 and $j$ to be in $\{0, 2\}$. Given these preconditions, the specifications ensures that the angle $C_a$ outputs $\vec{x}_0 \ast \vec{y}_0$ for inputs $\vec{x}$ and $\vec{y}$ and the ket function $C_k$ outputs $\vec{x}_0 \cdot (1 - \vec{x}_1)$ for inputs $\vec{x}, \vec{y}$ and $j$. Then, one easily verifies that, applying equation 8 on each bit-vector $a \cdot b$ of length 2 results in the corresponding output $\ket{\beta_{ab}}$, formally:

$$Ps\left(\text{circ_to_pps}(\text{Bell-circuit}), \ket{ab}\right) = \text{Mat}(\text{Bell-circuit}) \cdot \ket{ab}$$

So the postcondition, by use of $C_w, C_r, C_a$ and $C_k$, enables a complete characterization of the input/output function performed by the Bell circuit. In addition, the specification brings some complexity related post-condition: the circuit has width 2 and size 2 (ie, length of the required quantum register and number of performed elementary operations), and does not use any additional ancilla qubit.

### 7.2.6 Deduction and Proof Support

Proof support in QBRICKS strongly lies on the compositional structure of quantum circuits, enabling compositional reasoning on both pps and complexity features. As an example, in Figure 13 we give some of the rules used for the characterization of circuits size. Gates $\text{ID}$ and $\text{SWAP}$ are considered as free, so they count for null. The other elementary gates have size 1, both sequence and parallel compositions sum the size of their components and ancilla creation/termination does not affect circuit size.

Similar deduction rules are defined for circuit width, number of ancilla qubits and pps accessors. We do not introduce them here for sake of concision but we again refer the desirous reader to [29].

$$
\frac{C \in \{\text{ID, SWAP}\}}{\text{width}(C) = 0} \quad \frac{C \in \{\text{H, Ph(n), R_z(n)}\}}{\text{size}(C) = 1}
$$

$$
\frac{\Gamma \vdash \text{size}(C_1) = n_1 \quad \Gamma \vdash \text{size}(C_2) = n_2 \quad \Gamma \vdash \text{width}(C_1) = \text{width}(C_2)}{\Gamma \vdash \text{size}(\text{SEQ}(C_1, C_2)) = n_1 + n_2} \quad (\text{seq-size})
$$

$$
\frac{\Gamma \vdash \text{size}(C_1) = n_1 \quad \Gamma \vdash \text{size}(C_2) = n_2}{\Gamma \vdash \text{size}(\text{PAR}(C_1, C_2)) = n_1 + n_2} \quad (\text{par-size})
$$

$$
\frac{\Gamma \vdash \text{size}(C) = n}{\Gamma \vdash \text{size}(\text{ANC}(C)) = n} \quad (\text{anc-size})
$$

Figure 13: Deduction rules for QBRICKS: size (number of gates)

### 7.2.7 Implementation and Case Studies

QBRICKS enabled to implement, specify and formalize parametrized versions for some of the most emblematic quantum algorithms from the literature (Quantum Fourier Transform, Grover search algorithm, QPE, Shor order finding, etc). The main specificity of these QBRICKS implementations is to hold an high-level of proof support automation. This is largely due to the reduction of proof obligations to first-order logic predicates by use of pps characterizations.
7.3 SQIR

The SQIR language [78, 77] is the representation language used by the VOQC optimizer (see Section 5.3). On its own, it also constitutes a solution for formally proved correct quantum programs. It is developed concurrently with QBRICKS and holds similar concerns: basically, to reduce the expressivity of programming languages such as QUIPPER and QWIRE so as to (1) still enable the whole implementation of emblematic algorithms (2) enable formal proof of specifications.

The development of SQIR followed that of QWIRE (see Section 6.1.3), when the authors observed the difficulty to hold formal verification, mainly linked to the management of memory wires. Hence SQIR and QWIRE share common authors and developers, they are both deeply embedded in the COQ proof assistant and they share the same mathematical libraries for, e.g., matrices and complex numbers. Schematically, compared to QWIRE, SQIR has a reduced expressivity (disabling, e.g., the identification of qubit wires), making tractable the formal verification of functional program properties.

7.3.1 Programming Language

Just as QBRICKS, the programming part of SQIR is reduced to the minimum enabling implementation of main quantum programming features. It is two-layered: the unitary part corresponds to the design of what we called circuits so far and a generalized circuit layer adds branching measurement and kets initialization.

In SQIR, quantum circuits have type \( \mathbb{N} \rightarrow \text{Set} \), with a positive integer parameter corresponding to their width. Quantum memory wires are identified by integer indexes, bounded by a global register size parameter \( d \). Then, the type for unitary operators in SQIR (ucom) features the application of a circuit to a quantum register with \( d \) wires. It is defined inductively as follows.

\[
\text{Inductive } \text{ucom} \ (U: \mathbb{N} \rightarrow \text{Set}) \ (d: \mathbb{N}) : \text{Set} := \\
\ | \text{useq} : \text{ucom } U \ d \rightarrow \text{ucom } U \ d \rightarrow \text{ucom } U \ d \\
\ | \text{uapp1} : U \ 1 \rightarrow \mathbb{N} \rightarrow \text{ucom } U \ d \\
\ | \text{uapp2} : U \ 2 \rightarrow \mathbb{N} \rightarrow \mathbb{N} \rightarrow \text{ucom } U \ d \\
\ | \text{uapp3} : U \ 3 \rightarrow \mathbb{N} \rightarrow \mathbb{N} \rightarrow \mathbb{N} \rightarrow \text{ucom } U \ d 
\]

This definition holds two kinds of operations:

- the sequential composition, useq, which inputs two circuits and outputs their composition,
- the application of an elementary gates to (a) given wire(s), depending on the width of this gate. There are three different versions of this operations, for gates of width 1, 2 or 3, named respectively uapp1, uapp2 and uapp3. As an example, uapp1 inputs a gate \( U \) of width 1 and a parameter \( i \). It outputs the result of applying \( U \) on wire \( i \) in a register of size \( d \).

Then, SQIR provides a generalized circuit building layer, enabling the sequential composition of unitary commands, their initialization and branching measurement. Again, a circuit is an object com of type \( \mathbb{N} \rightarrow \text{Set} \) applied on a register of specified size \( d \). It is defined, inductively, as follows.

\[
\text{Inductive } \text{com} \ (U: \mathbb{N} \rightarrow \text{Set}) \ (d: \mathbb{N}) : \text{Set} := \\
\ | \text{uc} : \text{ucom } U \ d \rightarrow \text{com } U \ d \rightarrow \text{ucom } U \ d \\
\ | \text{skip} : \text{com } U \ d \\
\ | \text{meas} : \mathbb{N} \rightarrow \text{com } U \ d \rightarrow \text{com } U \ d \rightarrow \text{com } U \ d \\
\ | \text{seq} : \text{com } U \ d \rightarrow \text{com } U \ d \rightarrow \text{com } U \ d 
\]

Note that, for this construction to make sense, the parameter \( i \) should not be greater than \( d \). This condition is encoded by the semantics of SQIR.
A generalized circuit is built as either the lifting of a circuit into a generalized circuit, the empty skip operation, the branching measurement with inputs a wire identifier for a qubit to measure and two generalized circuits to execute depending on the measurement result) and the sequence of two different generalized circuits.

7.3.2 Matrix Semantics and Specifications

The semantics for SQIR programs is based on the standard matrix apparatus. For the unitary fragment it uses the matrix semantics presented in Section 2.1.5. It is extended for generalized circuits by density operators semantics, similarly as in Section 7.1.

In its present state of development, SQIR enables to specify functional properties, describing the input-output relation, similarly as the one for QBRICKS introduced in Section 7.2.5.

7.3.3 Implementation and Case Studies

SQIR is implemented as an embedded DSL into the COQ proof assistant. It was illustrated with specified and proved parametrized implementations of some emblematic quantum algorithm (Simon algorithm, QPE, Grover algorithm).

7.3.4 Comparison Between QBRICKS and SQIR

QBRICKS and SQIR are being developed concurrently, with very similar objectives. In particular they both trade off between offering user friendly programming features and reducing the language expressivity to the minimal, so as to enable functional formal verification. The solutions they provide share many common points. We discuss their main design differences.

- SQIR elementary operations consist in applying quantum gates on given wires of a quantum register, whereas QBRICKS proceeds by assembling quantum gates together into a quantum circuit, just as brick of a wall. Both views are actually inter-simulable: QBRICKS provides a macro with integer parameters specifying the wire identifier a given sub-circuit should be applied to and the size of the overall circuit (corresponding to the size of the available quantum register). This macro is built by parallel combination of its sub-circuit arguments with the appropriate number of occurrences of ID gate. It is of similar use as SQIR function uapp. On the other hand, QBRICKS gates assemblage is trivially simulable through SQIR uapp;

- Regarding the available operations over quantum circuits, SQIR lacks parallel composition and ancilla creation/annihilation. The lack of native parallelism is not a problem as it can be simulated through the successive applications of subcircuits on different parts of a quantum register. However, ancilla qubits are an hardly avoidable feature of quantum programming. They are commonly used in the algorithm literature and enable both to optimize the implementation of quantum circuits and to lower the size of required quantum registers for these implementations;

- On the other hand, SQIR provides a generalized circuit building layer, including measurement and classical control. Nevertheless, this upper layer is formalized through density operators, which are cumbersome objects for formal reasoning. So far, this part of the language only received illustrations with toy examples, such as superdense coding or quantum teleportation. In more involved implementations (such as QPE or Grover), SQIR authors followed a specification and proof strategy similar to that of QBRICKS: by reasoning on the quantum data
outputs of circuits, specifying over the probability distribution of result if a measurement were performed. Hence, designing a generalized circuit building language with probed semantics is still an open challenge;

- As introduced in Section 4.2.2, complexity properties of circuits constitute a fundamental aspect of quantum certification, decisive with regards to both the physical reliability of a computation and the quantum advantage it may provide. In the present state of development, SQIR does not offer a solution for this type of specifications. Still, this could be merely implemented in SQIR as an additional functionality.

7.4 Conclusion about Formal Verification of Quantum Programs

In Table 5 we sum up the main concrete case study realizations of formally verified quantum algorithms: instances of Grover algorithm from QBRICKS, SQIR and QHL, Deutsch-Jozsa and QPE instances from QBRICKS and SQIR, and Shor-OF implementation from QBRICKS. For each of these implementations, we give the length of the code (column LoC) and a measure of the human proof effort required for the specification proofs. It was obtained by adding the length of the program specifications (Spec stands for the number of lines of specifications and intermediary lemmas) and the number of proof commands that was required to prove these specifications (column Cmd).

Table 5: Compared implementations of formally verified quantum algorithms

|                     | QBRICKS [29] | SQIR [77, 78] | QHL [116] |
|---------------------|-------------|---------------|-----------|
|                     | LoC Spec+Cmd| LoC Spec+Cmd  | LoC Spec+Cmd |
| DJ                  | 11 85       | 10 261        |           |
| Grover              | 39 279      | 15 926        | 90 2975   |
| QPE                 | 23 246      | 40 812        |           |
| Shor-OF             | 132 1212    |               |           |

To the best of our knowledge Table 5 is comprehensive regarding parametrized formally proved quantum algorithm ⁹. Let us stress out how this field is young (in complement to the reduced number of concrete realizations, note that none of them is dated earlier than 2019). Nevertheless, it has already given promising results.

One of the main challenges for formal verification is to reduce the human proof effort that is required for the certification of programs. As Table 5 shows, comparing this effort to the length of effective programs, QBRICKS offers a quite stable ratio ≃ 10. In a quite regular way, SQIR adds a ≃ 3.5 factor to this ratio and QHL, for the case of Grover algorithm, requires ≃ 10 times more human effort ¹⁰.

⁹ An additional formalization of Deutsch Jozsa algorithm is presented by Bordg et al. [23]. We do not include it in Table 5 since it is not generated by a programming language but directly led as an algebraic proof. The total length of the proof is over 1 700 lines.

¹⁰ Note that the QHL implementation of Grover algorithm concerns a restricted case, with regards to the two others figuring in Table 5. Furthermore, it does contain the gate-to-gate circuit building but uses large circuit portions as primitives instead. Therefore, factor ≃ 10 is actually an underestimation.
8 Discussion and Bibliographical Notes

We end up this chapter by providing some additional references for usage of formal methods in quantum information and quantum computing.

8.1 Deductive Verification

Deductive verification appears to be the most promising direction for the development of formal methods in quantum computing. In particular, it is particularly adequate for the formal verification of functional specifications, which is crucial for quantum programming and prone to play, there, a role similar to that of testing and debugging in classical computing (see Section 4.1). Indeed, so far, occurrences from the literature of actual specified and verified quantum algorithms [116] or quantum algorithm implementations [29, 78], are all based either on deductive verification or interactive proofs.

8.2 Model-Checking

Attempts for functional verification of quantum algorithms with model-checking techniques were also led prior to these developments [66, 168]. They enabled to verify toy examples of quantum processes in a completely automated way. Nevertheless, this direction is limited by its high scale-sensitivity, which is specifically problematic for quantum programs, since they are designed to tackle large problems instances.

8.3 Type Checking

Apart from functional specification, specialized type systems for quantum programming languages also facilitate programming and debugging. In Section 4.1 we introduced the verification of structural constraints and the non duplicability of quantum information. Type checking may also have further use in quantum computing.

Recently, the SiLQ language was proposed. It is based on a linear type system which, upon other features, enables to verify, for any quantum circuit, whether it can be uncomputed, a computation feature required at many stages of quantum implementations. Based on this type system, SiLQ enables to automatically generate the uncomputation steps of circuits. This partial automation of the development lower the expertise requirements for developers and the length of programs with regards to language such as Q# or Quipper.

8.4 Assertion Checking

First, recall from Section 1 that proving quantum programs is mainly meant to replace the standard classical debugging method of testing and assertion checking. Apart from the development of formal proofs as an alternative, efforts are led to adapt this classical strategy to the quantum case. There, we still decorate programs with formal specifications (called assertions in this context) describing the evolution of the system state through an execution. But instead of mathematical proofs, these assertions are probed by statistical testing over program fragments. The challenges faced by such methods are mainly twofold:

**Destructive measurement**: memory reading destructs the superposition of quantum state, therefore one cannot continue the execution after checking. Hence, assertion checking can be applied only to fragments of an execution.
Non determinism: what we aim to check is a superposition of states, which induces a probability distribution of outcomes when measurement is performed. Then, checking an assertion requires a number of testing runs large enough to build a representative statistical distribution.

To overcome these difficulties, a first strategy is to reduce the specifications so as to express only properties that may be handled by assertion checking. Huand and Martonosi propose a “runtime-monitoring like” verification method for quantum circuits [83]. The annotation language is reduced so as to specify, for a quantum register, to be either in a classical state, in a superposition or entangled, without any concern about further description of the state.

More recently, Li et al. [111] developed an assertion-checking based method for the verification of fine quantum registers states properties, including functional descriptions of circuit behaviors. This methods is based on:

- an assertion language, based on QHL predicates (see Section 7.1), enabling functional specifications about computations at state;
- the use and formalization of gentle measurements: quantum registers are not measured in the usual computation basis, but in a basis containing an output that is very close to the expected state;
- an appropriate formalization of the notion of distance between quantum states, enabling verification in terms of confidence interval between the current state of the system and its expected value.

Hence, gentle measurement enables to test executions over full functional state specifications. In addition to bring expressivity to the specifications, it lowers the undesired effects of destructive measurement: since a gentle measurement operator contains an eigenstate that is an approximation of the expected quantum state, in most cases the measurement effect on the system state can be considered negligible and the execution can be pursued. Furthermore, the test result probability distribution is centered on a specific value. Therefore, a much reduced set of runs bring valuable statistical conclusions.

However, verification following this strategy only holds for a particular instance of a circuit, instead of a family of quantum circuits with unassigned inputs as in propositions from Section 7. Furthermore, in the general case gentle measurements are implemented by applying (1) a unitary $U$ uncomputing the system state into a ket of the computational basis (2) a measurement in the computational basis (3) unitary $U^\dagger$, so as to recover the initial state. Then, assertion checking inputs unitaries $U$ and $U^\dagger$ that are themselves prone to error. More precisely, to test against the exact expected value of the state, operator $U^\dagger$ should be equivalent to the computation under test. Practically, gentle measurements approximates the state under test. This enables a simplification of the measurement operator, at cost the robustness of the procedure.

8.5 Verification of Quantum Communication Protocols

Another challenge for formal methods in the verification of quantum information processes concerns quantum protocols.

Quantum key distribution protocols [141, 18, 113, 119] enable secured information exchanges between two parties. These protocols basically exploits the fact that, due to the destructive measurement, physics laws prevent any possibility for a potential eavesdropping in the exchange of quantum information. In particular, several formally verified implementations of the BB84 quantum
key distribution protocol [18] have been proposed in the literature, based either on process calculus [122, 103], formalization in Coq [21] or model-checking [53, 57].

Bordg et al. [23] propose a formalization of quantum information in the ISABELLE/HOL proof assistant. They illustrate their methods through the cases of quantum teleportation and the quantum prisoner dilemma. This work also contains a formally verified implementation of the Deutsch-Jozsa algorithm in ISABELLE/HOL.

In a more fundamental prospect, Echenim et al. [51] provide an ISABELLE/HOL proof for the CHSH inequalities [35]. These are probability distributions about crossed measurement results of quantum observables. They provide a proof for the Bell theorem [17], inducing that no classical theory could account for the entanglement phenomenon (hence that quantum physics cannot be reduced to local classical theories).

9 Conclusion

9.1 Summary

Throughout this chapter, we introduced the context, the main challenges and the most promising results in formally verified quantum programmatic. The current state of affairs in this emerging domain can be summed up as follows:

- Quantum computing is an emerging field, with huge potential application fields and promises. Progresses in the development of concrete machines are reaching the practical relevance landmark: prototypes are getting powerful enough to overpass classical computers. Consequently, quantum software development is becoming a crucial industrial short-term need;

- Quantum software deals with an entirely new programming paradigm. Upon its main particularities are the dual nature of information (either classical or quantum), the destructive measurement and irreducibly probabilistic computations;

- These specificities make programming particularly non-intuitive and prone to error. Furthermore, they make it very hard to directly import usual debugging methods from the classical practice (based on test and assertion checking). The technique presented in Section 8.4 might bring some hope, but this is still so far at a very preliminary stage.

- Formal methods appear as the privileged alternative for debugging strategies. Apart from providing solutions to the destructive measurement challenge, they have additional decisive advantages: mainly, they provide absolute guarantee of the correction of programs, and they hold for any instance of programs they verify;

- During the last ten years (the genesis of formal quantum programming), this new field as shown promising results in the different stages of software development: high-level program designs, circuit building languages, verification, compilation, optimization, etc.

9.2 Main Current Challenges

Although encouraging, these early successes draw the road map for rising the field from academic proof of concepts to practical usable programming solutions. We present the main coming challenges for this development in three categories: providing relevant integrated development solutions for the NISQ era, offering practical wide spreadable user experience and developing a full-fledged formally verified quantum compilation toolchain.
Provide relevant integrated development solutions for the NISQ era. So far, quantum formal verification mainly proved its relevance by offering solutions for the unitary core of quantum computations. As a matter of fact, illustrations and concrete implementations using these techniques primarily treated historical emblematic algorithms such as Shor, Phase Estimation or Grover search. The classical treatment in these algorithms can be completely decoupled from their quantum core.

However, the first generation of quantum computing machine (so called NISQ era) hints towards a radically distinct mode of operation. NISQ machine will have limited, noisy resources. A major consequence is that these quantum processors are too small to support the error correction mechanisms required for Shor and Grover’s algorithms. Such NISQ processors aim instead at different kinds of quantum algorithms: hybrid algorithms such as variational algorithms [120]. An hybrid algorithms tightly mix quantum and classical data treatments: one cannot decouple the quantum part of the algorithm from its classical part.

Adapting the quantum formal methods to the NISQ setting in order to support hybrid quantum/classical computation is a challenge and an active current research avenue.

Offer practical wide spreadable user experience: formalism, language design automation. In the present state of development, programming languages enabling formal verification usually sacrifice their expressivity to formal reasoning. In particular, all the solutions that have been probed against actual parametric quantum algorithms fail to satisfy essential elements of the requirements listed in Section 6.1.2 for scalable quantum programming languages: in addition to classical processing mentioned above, they lack the possibility to manipulate quantum registers and wire references. Verified programming should address these limitations.

Another issue, while concerning any method of quantum programming, is specially critical in the case of formally verified programming. It concerns the level of qualifications required from developers. The interpretation of quantum computations indeed requires unusual and non-intuitive mathematical formalism (including Kronecker products, complex phase amplitudes, probabilistic reasoning, etc). While the need for qualified programmers is prone to grow rapidly in the coming years, integrating formal verification should come with the development of user-friendly specification languages and highly automated mathematical reasoning engines.

Formally verified quantum compilation toolchain. In addition to the preceding considerations, in its early academic ages, quantum formal verification focused on idealized representations of quantum circuits, directly extracted from algorithm descriptions. As introduced in Section 2.3.2, these logical qubits are merely abstract model for actual computations to be ran. A major addition that is left for future works in quantum formal verification is error correction, with formal verification that the state of the system preserves the functional correctness of computations (assuming a given error model, and possibly with probabilistic requirements). Presented in Section 5.3, VOQC is a first step towards this goal.

Another future direction concerns the integration in widespread classical development environment. Recall from Section 6.1.3 that many widespread quantum programming languages benefit from embeddings in usual programming languages — such as python. Today most formal verification solutions are embedded in more academic functional development environment (such as Haskell, Ocaml, proof assistants or deductive verification environments). Interfaces should be developed so as to integrate formally verified quantum computations into comprehensive projects.

At the other extremity of the development stack, formal verification should accompany the implementation of compiled programs on concrete machines. This induces verified solutions for qubit mapping problem and gate simulation (see Section 2.3.3), depending on constraints that depend on the particular target material.
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References

[1] Scott Aaronson and Alex Arkhipov. The computational complexity of linear optics. In Proceedings of the forty-third annual ACM symposium on Theory of computing, pages 333–342, 2011.

[2] Samson Abramsky and Bob Coecke. Categorical quantum mechanics. In Handbook of Quantum Logic and Quantum Structures, pages 261–323. Elsevier, 2009.

[3] Thorsten Altenkirch and Alexander S Green. The quantum IO monad. Semantic Techniques in Quantum Computation, pages 173–205, 2010.

[4] Matthew Amy. Formal Methods in Quantum Circuit Design. PhD thesis, University of Waterloo, Ontario, Canada, 2019.

[5] Matthew Amy. Towards large-scale functional verification of universal quantum circuits. In Peter Selinger and Giulio Chiribella, editors, Proceedings 15th International Conference on Quantum Physics and Logic, QPL 2018, volume 287 of Electronic Proceedings in Theoretical Computer Science, pages 1–21, Halifax, Canada, 2019. EPTCS.

[6] Matthew Amy, Jianxin Chen, and Neil J. Ross. A finite presentation of CNOT-dihedral operators. In Bob Coecke and Aleks Kissinger, editors, Proceedings 14th International Conference on Quantum Physics and Logic, Nijmegen, The Netherlands, 3-7 July 2017, volume 266 of Electronic Proceedings in Theoretical Computer Science, pages 84–97, 2018.

[7] Matthew Amy, Dmitri Maslov, and Michele Mosca. Polynomial-time T-depth optimization of Clifford+T circuits via matroid partitioning. IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems, 33(10):1476–1489, 2014.

[8] Krzysztof R. Apt and Ernst-Rüdiger Olderog. Fifty years of Hoare’s logic. Formal Aspects Comput., 31(6):751–807, 2019.

[9] Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C. Bardin, Rami Barends, Rupak Biswas, Sergio Boixo, Fernando G. S. L. Brandao, David A. Buell, et al. Quantum supremacy using a programmable superconducting processor. Nature, 574(7779):505–510, 2019.

[10] Miriam Backens. The ZX-calculus is complete for stabilizer quantum mechanics. In New Journal of Physics, volume 16, page 093021. IOP Publishing, Sep 2014.

[11] Miriam Backens, Hector Miller-Bakewell, Giovanni de Felice, Leo Lobski, and John van de Wetering. There and back again: A circuit extraction tale. Quantum, 5:421, 2021.
[12] Thomas Ball, Byron Cook, Vladimir Levin, and Sriram K. Rajamani. Slam and static driver verifier: Technology transfer of formal methods inside microsoft. In Integrated Formal Methods, 4th International Conference, IFM 2004. Springer, 2004.

[13] Henk P. Barendregt. The Lambda-Calculus, its Syntax and Semantics, volume 103 of Studies in Logic and the Foundation of Mathematics. North Holland, second edition, 1984.

[14] Mike Barnett, Manuel Fähndrich, K. Rustan M. Leino, Peter Mülle, Wolfram Schulte, and Herman Venter. Specification and verification: the SPEC# experience. Commun. ACM, 54(6):81–91, 2011.

[15] Gilles Barthe, Justin Hsu, Mingsheng Ying, Nengkun Yu, and Li Zhou. Relational proofs for quantum programs. PACMPL, 4:21:1–21:29, 2020.

[16] Patrick Behm, Paul Benoit, Alain Faivre, and Jean-Marc Meynadier. Météor: A successful application of B in a large project. In In Proceedings of the World Congress on Formal Methods in the Development of Computing Systems (FM’99). Springer, 1999.

[17] John S Bell. On the Einstein Podolsky Rosen paradox. Physics Physique Fizika, 1(3):195–200, 1964.

[18] C. H. Bennett and G. Brassard. Quantum cryptography: Public key distribution and coin tossing. In Proceedings of IEEE International Conference on Computers, Systems and Signal Processing, pages 175–179, Bengalore, India, 1984.

[19] Jacob Biamonte, Peter Wittek, Nicola Pancotti, Patrick Rebentrost, Nathan Wiebe, and Seth Lloyd. Quantum machine learning. Nature, 549(7671):195, 2017.

[20] Benjamin Bichsel, Maximilian Baader, Timon Gehr, and Martin T. Vechev. Silq: a high-level quantum language with safe uncomputation and intuitive semantics. In Alastair F. Donaldson and Emina Torlak, editors, Proceedings of the 41st ACM SIGPLAN International Conference on Programming Language Design and Implementation, PLDI 2020, London, UK, June 15-20, 2020, pages 286–300. ACM, 2020.

[21] Jaap Boender, Florian Kammlüller, and Rajagopal Nagarajan. Formalization of quantum protocols using Coq. In Chris Heunen, Peter Selinger, and Jamie Vicary, editors, Proceedings of the 12th International Workshop on Quantum Physics and Logic (QPL 2015), volume 195 of Electronic Proceedings in Theoretical Computer Science, pages 71–83, Oxford, UK, 2015. EPTCS.

[22] Adam D Bookatz. QMA-complete problems. Quantum Information & Computation, 14(5&6):361–383, 2014.

[23] Anthony Bordg, Hanna Lachnitt, and Yijun He. Certified quantum computation in Isabelle/HOL. Journal of Automated Reasoning, 65(5):691–709, 2021.

[24] E. Bounimova, P. Godefroid, and D. Molnar. Billions and billions of constraints: Whitebox fuzz testing in production. In 35th International Conference on Software Engineering (ICSE), pages 122–131. IEEE/ACM, 2013.

[25] Daniel E Browne, Elham Kashefi, Mehdi Mhalla, and Simon Perdrix. Generalized flow and determinism in measurement-based quantum computation. New Journal of Physics, 9(8):250–250, aug 2007.
Formal methods for quantum algorithms

[26] Cristian Cadar and Koushik Sen. Symbolic execution for software testing: three decades later. *Commun. ACM*, 56(2):82–90, 2013.

[27] Titouan Carette, Emmanuel Jeandel, Simon Perdrix, and Renaud Vilmart. Completeness of Graphical Languages for Mixed States Quantum Mechanics. In Christel Baier, Ioannis Chatzigiannakis, Paola Flocchini, and Stefano Leonardi, editors, *46th International Colloquium on Automata, Languages, and Programming (ICALP 2019)*, volume 132 of *Leibniz International Proceedings in Informatics (LIPIcs)*, pages 108:1–108:15, Dagstuhl, Germany, 2019. Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik.

[28] Rohit Chadha, Paulo Mateus, and Amilcar Sernadas. Reasoning about imperative quantum programs. *Electronic Notes in Theoretical Computer Science*, 158:19–39, 2006.

[29] Christophe Charette, Sébastien Bardin, François Bobot, Valentin Perrelle, and Benoît Valiron. An automated deductive verification framework for circuit-building quantum programs. In Nobuko Yoshida, editor, *Programming Languages and Systems - 30th European Symposium on Programming, ESOP 2021, Luxembourg City, Luxembourg, March 27 - April 1, 2021, Proceedings*, volume 12648 of *Lecture Notes in Computer Science*, pages 148–177. Springer, 2021.

[30] Lily Chen, Lily Chen, Stephen Jordan, Yi-Kai Liu, Dustin Moody, Rene Peralta, Ray Perlner, and Daniel Smith-Tone. Report on post-quantum cryptography, volume 12. US Department of Commerce, National Institute of Standards and Technology, 2016.

[31] John Chiaverini, Dietrich Leibfried, Tobias Schaetz, Murray D Barrett, RB Blakestad, J Britton, Wayne M Itano, Juergen D Jost, Emanuel Knill, Christopher Langer, et al. Realization of quantum error correction. *Nature*, 432(7017):602–605, 2004.

[32] Edmund M. Clarke and E. Allen Emerson. Design and synthesis of synchronization skeletons using branching-time temporal logic. In *Logics of Programs, Workshop, LNCS 131*, pages 52–71. Springer, 1981.

[33] Edmund M. Clarke, Thomas A. Henzinger, Helmut Veith, and Roderick Bloem. *Handbook of Model Checking*. Springer, 2018.

[34] Edmund M. Clarke and Jeannette M. Wing. Formal methods: State of the art and future directions. *ACM Computing Surveys (CSUR)*, 28(4):626–643, 1996.

[35] John F Clauser, Michael A Horne, Abner Shimony, and Richard A Holt. Proposed experiment to test local hidden-variable theories. *Physical review letters*, 23(15):880, 1969.

[36] Bob Coecke and Ross Duncan. Interacting quantum observables: Categorical algebra and diagrammatics. *New Journal of Physics*, 13(4):043016, Apr 2011.

[37] Bob Coecke and Aleks Kissinger. *Picturing quantum processes*. Cambridge University Press, Cambridge, United Kingdom, 2017.

[38] Bob Coecke and Simon Perdrix. Environment and classical channels in categorical quantum mechanics. *Log. Methods Comput. Sci.*, 8(4), 2010.

[39] Patrick Cousot and Radhia Cousot. Abstract interpretation : A unified lattice model for static analysis of programs by construction or approximation of fixpoints. In *Proceedings of the Fourth ACM Symposium on Principles of Programming Languages (POPL)*, pages 238–252. ACM, 1977.
[40] Patrick Cousot, Radhia Cousot, Jerôme Feret, Laurent Mauborgne, Antoine Miné, David Monniaux, and Xavier Rival. The ASTRÉE analyzer. In European Symposium on Programming Languages and Systems, ESOP 2005. Springer, 2005.

[41] Andrew W. Cross, Lev S. Bishop, John A. Smolin, and Jay M. Gambetta. Open quantum assembly language, 2017.

[42] Vincent Danos and Elham Kashefi. Determinism in the one-way model. Phys. Rev. A, 74:052310, Nov 2006.

[43] Niel de Beaudrap, Xiaoning Bian, and Quanlong Wang. Fast and effective techniques for T-count reduction via spider nest identities. In Steven T. Flammia, editor, 15th Conference on the Theory of Quantum Computation, Communication and Cryptography, TQC 2020, June 9-12, 2020, Riga, Latvia, volume 158 of LIPIcs, pages 11:1–11:23. Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 2020.

[44] Niel de Beaudrap, Ross Duncan, Dominic Horsman, and Simon Perdrix. Pauli fusion: a computational model to realise quantum transformations from ZX terms. In QPL’19: International Conference on Quantum Physics and Logic, Los Angeles, United States, June 2019.

[45] Niel de Beaudrap and Dominic Horsman. The ZX calculus is a language for surface code lattice surgery. Quantum, 4:218, January 2020.

[46] Ellie D’Hondt and Prakash Panangaden. Quantum weakest preconditions. Mathematical Structures in Computer Science, 16(3):429–451, 2006.

[47] Alejandro Díaz-Caro. A lambda calculus for density matrices with classical and probabilistic controls. In Bor-Yuh Evan Chang, editor, Proceedings of the 15th Asian Symposium on Programming Languages and Systems (APLAS’17), volume 10695 of Lecture Notes in Computer Science, pages 448–467, Suzhou, China, 2017. Springer.

[48] Alejandro Díaz-Caro and Octavio Malherbe. A concrete categorical semantics of lambda-S. In Beniamino Accattoli and Carlos Olarte, editors, Proceedings of the 13th Workshop on Logical and Semantic Frameworks with Applications, LSFA 2018, Fortaleza, Brazil, September 26-28, 2018, volume 344 of Electronic Notes in Theoretical Computer Science, pages 83–100. Elsevier, 2019.

[49] Edsger W. Dijkstra. A Discipline of Programming. Prentice-Hall, 1976.

[50] Ross Duncan, Aleks Kissinger, Simon Perdrix, and John van de Wetering. Graph-theoretic simplification of quantum circuits with the ZX-calculus. Quantum, 4:279, 2020.

[51] Mnacho Echenim, Mehdi Mhalla. Quantum projective measurements and the CHSH inequality. Arch. Formal Proofs, 2021, 2021.

[52] Albert Einstein, Boris Podolsky, and Nathan Rosen. Can quantum-mechanical description of physical reality be considered complete? Physical review, 47(10):777, 1935.

[53] Mohamed Elboukhari, Mostafa Azizi, and Abdelmalek Azizi. Verification of quantum cryptography protocols by model checking. Int. J. Network Security & Appl, 2(4):43–53, 2010.
[54] Edward Farhi, Jeffrey Goldstone, and Sam Gutmann. A quantum approximate optimization algorithm. Technical Report MIT-CTP/4610, MIT, 2014.

[55] Edward Farhi, Jeffrey Goldstone, Sam Gutmann, Joshua Lapan, Andrew Lundgren, and Daniel Preda. A quantum adiabatic evolution algorithm applied to random instances of an np-complete problem. Science, 292(5516):472–475, 2001.

[56] Yuan Feng, Runyao Duan, Zhengfeng Ji, and Mingsheng Ying. Proof rules for the correctness of quantum programs. Theoretical Computer Science, 386(1-2):151–166, 2007.

[57] Verónica Fernández, María-José García-Martínez, Luis Hernández-Encinas, and Agustín Martín. Formal verification of the security of a free-space quantum key distribution system. In Proc. World Congr. Comput. Sci. Comput. Eng. Appl. Comput.(WORLDCOMP) Int. Conf. Security Manag.(SAM), 2011.

[58] Richard P. Feynman. Simulating physics with computers. International Journal of Theoretical Physics, 21(6–7):467–488, 1982.

[59] Jean-Christophe Filliâtre and Andrei Paskevich. Why3 - where programs meet provers. In Matthias Felleisen and Philippa Gardner, editors, Proceedings of the 22nd European Symposium on Programming Languages and Systems (ESOP 2013), Held as Part of the European Joint Conferences on Theory and Practice of Software (ETAPS 2013), volume 7792 of Lecture Notes in Computer Science, pages 125–128, Rome, Italy, 2013. Springer.

[60] Jean-Christophe Filliâtre. Deductive software verification. STTT, 13(5):397–403, 2011.

[61] R. W. Floyd. Assigning meanings to programs. In Mathematical Aspects of Computer Science, Proceedings of Symposia in Applied Mathematics, pages 19–32. American Mathematical Society, 1967.

[62] Robert W Floyd. Assigning meanings to programs. Mathematical aspects of computer science, 19(19-32):1, 1967.

[63] Austin G. Fowler, Matteo Mariantoni, John M. Martinis, and Andrew N. Cleland. Surface codes: Towards practical large-scale quantum computation. Phys. Rev. A, 86:032324, Sep 2012.

[64] Michael Freedman, Alexei Kitaev, Michael Larsen, and Zhenghan Wang. Topological quantum computation. Bulletin of the American Mathematical Society, 40(1):31–38, 2003.

[65] Peng Fu, Kohei Kishida, and Peter Selinger. Linear dependent type theory for quantum programming languages. In Proceedings of the 35th Annual ACM/IEEE Symposium on Logic in Computer Science, pages 440–453, 2020.

[66] Simon J. Gay, Rajagopal Nagarajan, and Nikolaos Papanikolaou. QMC: a model checker for quantum systems. In Aarti Gupta and Sharad Malik, editors, Proceeding of the 20th International Conference on Computer Aided Verification (CAV 2008), volume 5123 of Lecture Notes in Computer Science, pages 543–547, Princeton, NJ, USA, 2008. Springer.

[67] Jean-Yves Girard. Linear logic. Theoretical Computer Science, 50(1):1–101, 1987.

[68] Georges Gonthier. Formal proof – the four-color theorem. Notices of the AMS, 55(11):1382–1393, 2008.
[69] Daniel Gottesman. *Stabilizer codes and quantum error correction*. PhD thesis, Caltech, 1997.

[70] Alexander S. Green, Peter LeFanu Lumsdaine, Neil J. Ross, Peter Selinger, and Benoît Valiron. An introduction to quantum programming in Quipper. In Gerhard W. Dueck and D. Michael Miller, editors, *Proceedings of the 5th International Conference on Reversible Computation (RC’13)*, volume 7948 of *Lecture Notes in Computer Science*, pages 110–124, Victoria, BC, Canada, 2013. Springer.

[71] Alexander S. Green, Peter LeFanu Lumsdaine, Neil J. Ross, Peter Selinger, and Benoît Valiron. Quipper: A scalable quantum programming language. In Hans-Juergen Boehm and Cormac Flanagan, editors, *Proceedings of the ACM SIGPLAN Conference on Programming Language Design and Implementation, (PLDI’13)*, pages 333–342, Seattle, WA, USA, 2013. ACM.

[72] Lov K. Grover. A fast quantum mechanical algorithm for database search. In Gary L. Miller, editor, *Proceedings of the Twenty-Eighth Annual ACM Symposium on the Theory of Computing (STOC)*, pages 212–219, Philadelphia, Pennsylvania, USA, 1996. ACM.

[73] Amar Hadzihasanovic, Kang Feng Ng, and Quanlong Wang. Two complete axiomatisations of pure-state qubit quantum computing. In *Proceedings of the 33rd Annual ACM/IEEE Symposium on Logic in Computer Science*, LICS ’18, pages 502–511, New York, NY, USA, 2018. ACM.

[74] Aram W. Harrow, Avinatan Hassidim, and Seth Lloyd. Quantum algorithm for linear systems of equations. *Physical Review Letters*, 103:150502, Oct 2009.

[75] Ichiro Hasuo and Naohiko Hoshino. Semantics of higher-order quantum computation via geometry of interaction. *Annals of Pure and Applied Logic*, 168(2):404 – 469, 2017.

[76] Thomas A. Henzinger, Ranjit Jhala, Rupak Majumdar, and Grégoire Sutre. Software verification with Blast. In *Proceedings of the 10th International Conference on Model Checking Software, SPIN’03*. Springer, 2003.

[77] Kesha Hietala, Robert Rand, Shih-Han Hung, Liyi Li, and Michael Hicks. Proving quantum programs correct. In Liron Cohen and Cezary Kaliszyk, editors, *12th International Conference on Interactive Theorem Proving, ITP 2021, June 29 to July 1, 2021, Rome, Italy (Virtual Conference)*, volume 193 of *LIPIcs*, pages 21:1–21:19, 2021.

[78] Kesha Hietala, Robert Rand, Shih-Han Hung, Xiaodi Wu, and Michael Hicks. A verified optimizer for quantum circuits. *Proc. ACM Program. Lang.*, 5(POPL):1–29, 2021.

[79] Anne Hillebrand. Quantum protocols involving multiparticle entanglement and their representations. Master’s thesis, University of Oxford, 2011.

[80] R. Hindley. The principal type-scheme of an object in combinatory logic. *Transactions of the American Mathematical Society*, 146:29–60, 1969.

[81] C. A. R. Hoare. An axiomatic basis for computer programming. *Commun. ACM*, 12(10):576–580, 1969.

[82] Clare Horsman, Austin G. Fowler, Simon Devitt, and Rodney Van Meter. Surface code quantum computing by lattice surgery. *New Journal of Physics*, 14(12):123011, December 2012.
[83] Yipeng Huang and Margaret Martonosi. Statistical assertions for validating patterns and finding bugs in quantum programs. In Srilatha Bobbie Manne, Hillery C. Hunter, and Erik R. Altman, editors, Proceedings of the 46th International Symposium on Computer Architecture (ISCA 2019), pages 541–553, Phoenix, AZ, USA, 2019. ACM.

[84] Shih-Han Hung, Kesha Hietala, Shaopeng Zhu, Mingsheng Ying, Michael Hicks, and Xiaodi Wu. Quantitative robustness analysis of quantum programs. Proceedings of the ACM on Programming Languages, 3(POPL):1–29, 2019.

[85] Dominik Janzing, Pawel Wocjan, and Thomas Beth. “non-identity-check” is QMA-complete. International Journal of Quantum Information, 03(03):463–473, 2005.

[86] Ali JavadiAbhari, Shruti Patil, Daniel Kudrow, Jeff Heckey, Alexey Lvov, Frederic T. Chong, and Margaret Martonosi. ScaffCC: Scalable compilation and analysis of quantum programs. Parallel Computing, 45:2–17, 2015.

[87] Emmanuel Jeandel. The rational fragment of the ZX-calculus, 2018.

[88] Emmanuel Jeandel, Simon Perdrix, and Renaud Vilmart. A complete axiomatisation of the ZX-calculus for Clifford+T quantum mechanics. In Proceedings of the 33rd Annual ACM/IEEE Symposium on Logic in Computer Science, LICS ’18, pages 559–568, New York, NY, USA, 2018. ACM.

[89] Emmanuel Jeandel, Simon Perdrix, and Renaud Vilmart. Diagrammatic reasoning beyond Clifford+T quantum mechanics. In Proceedings of the 33rd Annual ACM/IEEE Symposium on Logic in Computer Science, LICS ’18, pages 569–578, New York, NY, USA, 2018. ACM.

[90] Emmanuel Jeandel, Simon Perdrix, and Renaud Vilmart. A generic normal form for ZX-diagrams and application to the rational angle completeness. In 2019 34th Annual ACM/IEEE Symposium on Logic in Computer Science (LICS), pages 1–10, 2019.

[91] Emmanuel Jeandel, Simon Perdrix, and Renaud Vilmart. Completeness of the ZX-calculus. Logical Methods in Computer Science, 16(2), 2020.

[92] Yoshihiko Kakutani. A logic for formal verification of quantum programs. In Annual Asian Computing Science Conference, pages 79–93. Springer, 2009.

[93] Nathan Killoran, Josh Izaac, Nicolás Quesada, Ville Bergholm, Matthew Amy, and Christian Weedbrook. Strawberry Fields: A software platform for photonic quantum computing. Quantum, 3:129, 2019.

[94] Florent Kirchner, Nikolai Kosmatov, Virgile Prevosto, Julien Signoles, and Boris Yakobowski. Frama-C : A software analysis perspective. Formal Asp. Comput., 27(3):573–609, 2015.

[95] Aleks Kissinger, Lucas Dixon, Ross Duncan, Benjamin Frot, Alex Merry, David Quick, Matvey Soloviev, and Vladimir Zamdzhiev. Quantomatic, 2011.

[96] Aleks Kissinger and John van de Wetering. PyZX, 2018.

[97] Aleks Kissinger and John van de Wetering. PyZX: Large scale automated diagrammatic reasoning. Electronic Proceedings in Theoretical Computer Science, 318:229–241, May 2020.

[98] Aleks Kissinger and John van de Wetering. Reducing the number of non-clifford gates in quantum circuits. Phys. Rev. A, 102:022406, Aug 2020.
[99] Aleks Kissinger and Vladimir Zamdzhiev. Quantomatic: A proof assistant for diagrammatic reasoning. In Amy P. Felty and Aart Middeldorp, editors, Proceedings for the 25th International Conference on Automated Deduction (CADE-25), volume 9195 of Lecture Notes in Computer Science, pages 326–336, Berlin, Germany, 2015. Springer.

[100] Erwin Klein, June Andronick, Kevin Elphinstone, Gernot Heiser, David Cock, Philip Derrin, Dhammika Elkaduwe, Kai Engelhardt, Rafal Kolanski, Michael Norrish, Thomas Sewell, Harvey Tuch, and Simon Winwood. sel4: formal verification of an operating-system kernel. Commun. ACM, 53(6):107–115, 2010.

[101] Emmanuel Knill. Conventions for quantum pseudocode. Technical report, Los Alamos National Lab., NM (United States), 1996.

[102] Daniel Kroening and Michael Tautschnig. Cbmc - c bounded model checker. In Tools and Algorithms for the Construction and Analysis of Systems - 20th International Conference, TACAS 2014, pages 389–391. Springer, 2014.

[103] Takahiro Kubota, Yoshihiko Kakutani, Go Kato, Yasuhiro Kawano, and Hideki Sakurada. Semi-automated verification of security proofs of quantum cryptographic protocols. Journal of Symbolic Computation, 73:192–220, 2016.

[104] Hidenori Kuwakado and Masakatu Morii. Quantum distinguisher between the 3-round Feistel cipher and the random permutation. In 2010 IEEE International Symposium on Information Theory, pages 2682–2685. IEEE, 2010.

[105] Hidenori Kuwakado and Masakatu Morii. Security on the quantum-type Even-Mansour cipher. In 2012 International Symposium on Information Theory and its Applications, pages 312–316. IEEE, 2012.

[106] Ugo Dal Lago, Claudia Faggian, Benoît Valiron, and Akira Yoshimizu. The geometry of parallelism: classical, probabilistic, and quantum effects. In Giuseppe Castagna and Andrew D. Gordon, editors, Proceedings of the 44th ACM SIGPLAN Symposium on Principles of Programming Languages (POPL'17), pages 833–845, Paris, France, 2017. ACM.

[107] R LaRose. Review of the CirQ quantum software framework, 2019. Available online.

[108] Louis Lemonnier, John van de Wetering, and Aleks Kissinger. Hypergraph simplification: Linking the path-sum approach to the ZH-calculus, 2020. To appear in the Proceedings of QPL 2020.

[109] Xavier Leroy. Formal verification of a realistic compiler. Commun. ACM, 52(7):107–115, 2009.

[110] Jerzy Lewandowski. Volume and quantizations. Classical and Quantum Gravity, 14(1):71, 1997.

[111] Gushu Li, Li Zhou, Nengkun Yu, Yufei Ding, Mingsheng Ying, and Yuan Xie. Projection-based runtime assertions for testing and debugging quantum programs. Proceedings of the ACM on Programming Languages, 4(OOPSLA):1–29, 2020.

[112] Yangjia Li and Mingsheng Ying. Algorithmic analysis of termination problems for quantum programs. In ACM SIGPLAN Notices, volume 53, pages 35:1–29. ACM, 2018.

11https://quantumcomputingreport.com/review-of-the-cirq-quantum-software-framework/
[113] Sheng-Kai Liao, Wen-Qi Cai, Wei-Yue Liu, Liang Zhang, Yang Li, Ji-Gang Ren, Juan Yin, Qi Shen, Yuan Cao, Zheng-Ping Li, et al. Satellite-to-ground quantum key distribution. Nature, 549(7670):43–47, 2017.

[114] Daniel A Lidar and Todd A Brun. Quantum Error Correction. Cambridge University Press, 2013.

[115] Bert Lindenhovius, Michael Mislove, and Vladimir Zamdzhiev. Enriching a linear/non-linear lambda calculus: A programming language for string diagrams. In Proceedings of the 33rd Annual ACM/IEEE Symposium on Logic in Computer Science, pages 659–668, 2018.

[116] Junyi Liu, Bohua Zhan, Shuling Wang, Shenggang Ying, Tao Liu, Yangjia Li, Mingsheng Ying, and Naijun Zhan. Formal verification of quantum algorithms using quantum Hoare logic. In Isil Dillig and Serdar Tasiran, editors, Computer Aided Verification, pages 187–207, Cham, 2019. Springer International Publishing.

[117] Tao Liu, Yangjia Li, Shuling Wang, Mingsheng Ying, and Naijun Zhan. A theorem prover for quantum Hoare logic and its applications. Available as arXiv:1601.03835, 2016.

[118] Seth Lloyd, Masoud Mohseni, and Patrick Rebentrost. Quantum algorithms for supervised and unsupervised machine learning. arXiv preprint arXiv:1307.0411, 2013.

[119] Hoi-Kwong Lo, Xiongfeng Ma, and Kai Chen. Decoy state quantum key distribution. Physical review letters, 94(23):230504, 2005.

[120] Jarrod R McClean, Jonathan Romero, Ryan Babbush, and Alán Aspuru-Guzik. The theory of variational hybrid quantum-classical algorithms. New Journal of Physics, 18(2):023023, 2016.

[121] Robin Milner. A theory of type polymorphism in programming. Journal of Computer and System Sciences, 17(3):348–375, 1978.

[122] Rajagopal Nagarajan and Simon Gay. Formal verification of quantum protocols. Available online as arXiv:quant-ph/0203086, 2002.

[123] Yunseong Nam, Neil J Ross, Yuan Su, Andrew M Childs, and Dmitri Maslov. Automated optimization of large quantum circuits with continuous parameters. npj Quantum Information, 4(1):1–12, 2018.

[124] Michael A. Nielsen and Isaac Chuang. Quantum computation and quantum information. Cambridge University Press, Cambridge, United Kingdom, 2002.

[125] Tobias Nipkow, Lawrence C. Paulson, and Markus Wenzel. Isabelle/HOL: a proof assistant for higher-order logic. Springer, 2002.

[126] Berhnard Ömer. Structured Quantum Programming. PhD thesis, TU Wien, 2003.

[127] Michele Pagani, Peter Selinger, and Benoît Valiron. Applying quantitative semantics to higher-order quantum computing. In Proceedings of the 41st ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL ’14, page 647–658, New York, NY, USA, 2014. Association for Computing Machinery.
[128] Luca Paolini and Margherita Zorzi. qPCF: A language for quantum circuit computations. In T. V. Gopal, Gerhard Jäger, and Silvia Steila, editors, \textit{Proceedings of the 14th Annual Conference on Theory and Applications of Models of Computation (TAMC’17)}, volume 10185 of \textit{Lecture Notes in Computer Science}, pages 455–469, Bern, Switzerland, 2017.

[129] Christine Paulin-Mohring. Introduction to the calculus of inductive constructions, 2015.

[130] Jennifer Paykin, Robert Rand, and Steve Zdancewic. QWIRE: a core language for quantum circuits. In Giuseppe Castagna and Andrew D. Gordon, editors, \textit{Proceedings of the 44th ACM SIGPLAN Symposium on Principles of Programming Languages (POPL’17)}, pages 846–858, Paris, France, 2017. ACM.

[131] Benjamin C. Pierce. \textit{Types and Programming Languages}. MIT Press, 2002.

[132] Qiskit Development Team. Qiskit documentation. Available online\footnote{https://qiskit.org/documentation/}.

[133] Quantum Computing Report. List of tools. Available online\footnote{https://quantumcomputingreport.com/resources/tools/}, 2019.

[134] Robert Rand, Kesha Hietala, and Michael Hicks. Formal verification vs. quantum uncertainty. In \textit{3rd Summit on Advances in Programming Languages (SNAPL 2019)}. Schloss Dagstuhl-Leibniz-Zentrum fuer Informatik, 2019.

[135] Robert Rand, Jennifer Paykin, and Steve Zdancewic. QWIRE practice: Formal verification of quantum circuits in Coq. In Bob Coecke and Aleks Kissinger, editors, \textit{Proceedings 14th International Conference on Quantum Physics and Logic (QPL 2017)}, volume 266 of \textit{Electronic Proceedings in Theoretical Computer Science}, pages 119–132, Nijmegen, The Netherlands, 2017. EPTCS.

[136] Robert Raussendorf, Daniel E Browne, and Hans J Briegel. Measurement-based quantum computation on cluster states. \textit{Physical review A}, 68(2):022312, 2003.

[137] Francisco Rios and Peter Selinger. A categorical model for a quantum circuit description language. In Bob Coecke and Aleks Kissinger, editors, \textit{Proceedings 14th International Conference on Quantum Physics and Logic (QPL 2017)}, volume 266 of \textit{Electronic Proceedings in Theoretical Computer Science}, pages 164–178, Nijmegen, The Netherlands, 2018.

[138] Xavier Rival and Kwangkeun Yi. \textit{Introduction to Static Analysis: An Abstract Interpretation Perspective}. The MIT Press, 2020.

[139] Neil J. Ross. \textit{Algebraic and Logical Methods in Quantum Computation}. PhD thesis, Dalhousie University, 2015. Available as \texttt{arxiv:1510.02198}.

[140] Thomas Santoli and Christian Schaffner. Using Simon’s algorithm to attack symmetric-key cryptographic primitives. \textit{Quantum Inf. Comput.}, 17(1&2):65–78, 2017.

[141] Valerio Scarani, Helle Bechmann-Pasquinucci, Nicolas J Cerf, Miloslav Dušek, Norbert Lütkenhaus, and Mømchil Peev. The security of practical quantum key distribution. \textit{Reviews of modern physics}, 81(3):1301, 2009.
[142] Artur Scherer, Benoît Valiron, Siun-Chuon Mau, Scott Alexander, Eric Van den Berg, and Thomas E Chapuran. Concrete resource analysis of the quantum linear-system algorithm used to compute the electromagnetic scattering cross section of a 2d target. *Quantum Information Processing*, 16(3):60, 2017.

[143] Maria Schuld. *Supervised Learning with Quantum Computers*. Springer, 2018.

[144] Peter Selinger. Towards a quantum programming language. *Mathematical Structures in Computer Science*, 14(4):527–586, 2004.

[145] Peter Selinger. Generators and relations for n-qubit Clifford operators. *Logical Methods in Computer Science*, 11(2), Jun 2015.

[146] Peter Selinger and Benoît Valiron. A lambda calculus for quantum computation with classical control. In Paweł Urzyczyn, editor, * Typed Lambda Calculi and Applications*, pages 354–368, Berlin, Heidelberg, 2005. Springer Berlin Heidelberg.

[147] Peter Selinger and Benoît Valiron. A lambda calculus for quantum computation with classical control. *Mathematical Structures in Computer Science*, 16:527–552, 2006.

[148] Peter Selinger and Benoît Valiron. A linear-non-linear model for a computational call-by-value lambda calculus (extended abstract). In Roberto M. Amadio, editor, *Proceedings of the 11th International Conference on Foundations of Software Science and Computational Structures (FOSSACS’08)*, volume 4962 of *Lecture Notes in Computer Science*, pages 81–96, Budapest, Hungary, 2008. Springer.

[149] Peter W. Shor. Algorithms for quantum computation: Discrete log and factoring. In *Proceedings of the 35th Annual Symposium on Foundations of Computer Science (FOCS’94)*, pages 124–134, Santa Fe, New Mexico, US., 1994. IEEE, IEEE Computer Society Press.

[150] Peter W Shor. Scheme for reducing decoherence in quantum computer memory. *Physical review A*, 52(4):R2493, 1995.

[151] Daniel R Simon. On the power of quantum computation. *SIAM journal on computing*, 26(5):1474–1483, 1997.

[152] Kartik Singhal and John Reppy. Quantum Hoare type theory. In *17th International Conference on Quantum Physics and Logic 2020*, QPL ’20, may 2020. To appear.

[153] Seyon Sivarajah, Silas Dilkes, Alexander Cowtan, Will Simmons, Alec Edgington, and Ross Duncan. tket: a retargetable compiler for NISQ devices. *Quantum Science and Technology*, 6(1):014003, 2020.

[154] Damian S Steiger, Thomas Häner, and Matthias Troyer. ProjectQ: an open source software framework for quantum computing. *Quantum*, 2(49):10–22331, 2018.

[155] Krysta M Svore, Alan Geller, Matthias Troyer, John Azariah, Christopher Granade, Bettina Heim, Vadym Kluchnikov, Maria Mykhailova, Andres Paz, and Martin Roetteler. Q#: Enabling scalable quantum computing and development with a high-level domain-specific language. Available online as arXiv:1803.00652, 2018.

[156] Quingo Development Team. Quingo: A programming framework for heterogeneous quantum-classical computing with NISQ features. Draft available as arXiv:2009.01686., 2020.
[157] Dominique Unruh. Quantum Hoare logic with ghost variables. In 2019 34th Annual ACM/IEEE Symposium on Logic in Computer Science (LICS), pages 1–13. IEEE, 2019.

[158] Dominique Unruh. Quantum relational Hoare logic. Proceedings of the ACM on Programming Languages, 3(POPL):1–31, 2019.

[159] Wim Van Dam, Sean Hallgren, and Lawrence Ip. Quantum algorithms for some hidden shift problems. SIAM Journal on Computing, 36(3):763–778, 2006.

[160] André van Tonder. A lambda calculus for quantum computation. SIAM Journal on Computing, 33(5):1109–1135, 2004.

[161] Renaud Vilmart. A near-minimal axiomatisation of ZX-calculus for pure qubit quantum mechanics. In 2019 34th Annual ACM/IEEE Symposium on Logic in Computer Science (LICS), pages 1–10, June 2019.

[162] Renaud Vilmart. The structure of sum-over-paths, its consequences, and completeness for Clifford, 2020. Available online as arXiv:2003.05678.

[163] Willem Visser, Corina S. Pasareanu, and Sarfraz Khurshid. Test input generation with Java Pathfinder. In 2004 ACM SIGSOFT International Symposium on Software Testing and Analysis, ISSTA ’04. ACM, 2004.

[164] Chuan Wang, Fu-Guo Deng, Yan-Song Li, Xiao-Shu Liu, and Gui Lu Long. Quantum secure direct communication with high-dimension quantum superdense coding. Phys. Rev. A, 71:044305, Apr 2005.

[165] Dave Wecker and Krysta M Svore. LIQUi⟩: A software design architecture and domain-specific language for quantum computing. Available online as arXiv:1402.4467, 2014.

[166] Mingsheng Ying. Floyd-Hoare logic for quantum programs. ACM Transactions on Programming Languages and Systems (TOPLAS), 33(6):19:1–19:49, 2011.

[167] Mingsheng Ying. Foundations of Quantum Programming. Morgan Kaufmann, 2016.

[168] Mingsheng Ying, Yangjia Li, Nengkun Yu, and Yuan Feng. Model-checking linear-time properties of quantum systems. ACM Transactions on Computational Logic, 15(3):22:1–22:31, 2014.

[169] Mingsheng Ying, Shenggang Ying, and Xiaodi Wu. Invariants of quantum programs: characterisations and generation. In ACM SIGPLAN Notices, volume 52, pages 818–832. ACM, 2017.

[170] Shengyu Zhang. BQP-complete problems. In Grzegorz Rozenberg, Thomas Bäck, and Joost N. Kok, editors, Handbook of Natural Computing, pages 1545–1571. Springer, 2012.