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⁴ — Abstract

⁵ Quantum computation leverages the use of quantumly-controlled conditionals in order to achieve
⁶ computational advantage. However, since the different branches in the conditional may operate on
⁷ the same qubits, a typical approach to compilation involves performing the branches sequentially,
⁸ which can easily lead to an exponential blowup of the program complexity. We introduce and study a
⁹ compilation technique for avoiding branch sequentialization in a language that is sound and complete
¹⁰ for quantum polynomial time, improving on previously existing polynomial-size bounds and showing
¹¹ the existence of techniques that preserve the intuitive complexity of the program.
¹² 2012 ACM Subject Classification Theory of computation → Quantum complexity theory; Theory

13 of computation \rightarrow Quantum complexity theory

14 Keywords and phrases Formal methods, Quantum computation, Implicit Computational Complexity

1 Introduction

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Quantum computing is an emerging paradigm of computation where quantum physical 16 phenomena, such as entanglement and superposition, are used to obtain an advantage over 17 classical computation. A testament to the richness of the field is the variety of computational 18 models: quantum Turing machines [3], quantum circuits [18, 16], measurement-based quantum 19 computation [4, 6], linear optical circuits [13], among others. Some of these models have 20 been shown to be equivalent in terms of computational power and complexity. For instance, 21 Yao's equivalency result [18] shows that polynomial-time quantum Turing machine are 22 computationally equivalent to uniform and poly-size quantum circuit families. 23

A lot of effort has been put on developing high-level quantum programming languages to 24 allow programmers to abstract themselves from the technicalities of these low-level models. 25 Towards that end, several verification techniques such as type systems [9] or categorical 26 approaches for reasoning on programs semantics [2, 11] have been studied and developed to 27 ensure the physical reality of compiled programs, for example, by ensuring that it preserves 28 the main properties of quantum mechanics such as no-cloning theorem [1] or unitarity [8]. 29 An important line of research in this area involves checking polytime termination of quantum 30 programs [5, 17, 10]. 31

By Yao's Theorem, this property implies the feasibility of the corresponding quantum circuit by ensuring that its size is polynomially bounded in the program input size. However, there are still quite a few obstacles to the full use of these techniques. In particular, designing efficient compilation strategies is not trivial [10].

A prominent example is the time complexity of *quantum branching* in programs, i.e., when the flow in a loop or in a conditional is determined upon the state of a qubit. In the classical setting, the cost of branching is the maximum cost



Figure 1 Classical vs. quantum branching.

⁴² between the two branches (Figure 1). However, this is not necessarily the case in the ⁴³ quantum setting, as a consequence of no-cloning: in a quantum circuit, the two branches may

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contain operations on the same qubits, and thus require an implementation in series. This 44 results in a circuit whose total depth is the sum of the depths of the two branches as illustrated 45 by Figure 1. In [19], while trying to encode efficient operations over quantum data structures, 46 the authors encounter this problem which they have coined branch sequentialization. While 47 the authors provide a heuristic for avoiding branch sequentialization, it is only applicable 48 in a few precise examples. Given the importance of preserving the time complexity of a 49 program in its circuit implementation, there is an interest in discovering general techniques 50 that avoid the problem of branch sequentialization altogether. 51

Motivating Example. Consider the program PAIRS defined in Figure 2. The procedure 52 pairs takes as input a sorted set \bar{q} of qubits (i.e., a collection of pairwise distinct qubits) 53 on which it will perform operations. By language design, pairs immediately terminates 54 whenever \overline{q} is empty. First, pairs checks that the number of qubits in \overline{q} , given by its size $|\overline{q}|$, 55 is larger than 1 to enter the recursive case, otherwise it applies a NOT gate to the remaining 56 qubit (line 9). On line 3, the program will branch depending on the state $\bar{q}[1,2]$ of the first 57 two qubits in \bar{q} . Out of all four cases (lines 4-7), pairs only performs an operation when the 58 first two qubits are in state $|00\rangle$ or $|11\rangle$, in which case it performs a recursive call on $\bar{q} \ominus [1, 2]$, 59 the sorted set \bar{q} where the first and second qubits have been removed. 60

With $x \in \{0, 1\}^*$ and $y \in \{0, 1\}$, given the 61 input state $|xy\rangle$, pairs will apply a NOT 62 gate to y if and only if x is a string consisting 63 only of sequences of 00 and 11. Put another 64 way, pairs encodes a unitary transformation 65 that inverts the state of the last qubit of an 66 input when x belongs to the regular language 67 defined by $(00 | 11)^*$. 68

Since pairs performs at most one call
per branch, and consumes 2 qubits from its
input while doing so, we conclude that its
runtime complexity is bounded linearly.

⁷³ Let us now turn to finding a circuit im-

1	$\mathbf{decl} \; \mathtt{pairs}(ar{\mathrm{q}}) \{$
2	if $ \bar{\mathbf{q}} > 1$ then
3	qcase $\bar{q}[1,2]$ of $\{$
4	$00 \rightarrow call pairs(\bar{q} \ominus [1,2]);$
5	$01 \rightarrow \mathbf{skip};$
6	$10 \rightarrow \mathbf{skip};$
7	$11 \rightarrow \text{call pairs}(\bar{q} \ominus [1,2]);$
8	}
9	else $\bar{q}[1] *= NOT; \}$
10	$: call pairs(\bar{q});$

Figure 2 Branching program PAIRS.

plementation for the recursive case of **pairs**. Consider the two compilation strategies (a) 74 and (b) shown in Figure 3. While Strategy (a) could be considered the more direct approach 75 to building the circuit, at each recursive call the size of the circuit for pairs is the sum of 76 the sizes of each branch. On the other hand, while the strategy in (b) requires the creation 77 of an ancilla and the use of extra Toffoli gates, it only requires the implementation of one call 78 to pairs. As a consequence, the strategies (a) and (b) result in circuits of depth $\Theta(|\bar{q}|2^{|\bar{q}|})$ 79 and $\Theta(|\bar{q}|)$, respectively, showing how implementing the branches sequentially can result in 80 an exponential blowup in circuit size. It is simple enough to find a compilation strategy that 81 prevents the duplication of **pairs** in the recursive case. However, this becomes much less 82 trivial once we consider programs with more complex recursive calls. 83

Contribution. In this paper, we study the problem of branch sequentialization and solve it in
 the case of quantum polynomial time, in the following way:

We identify a programming language fragment BFOQ (for Basic FOQ) that is sound and complete for quantum polynomial time (Theorem 9). That is, any BFOQ program computes a function in FBQP, the class of functions computable in polynomial time by a quantum Turing machine with bounded error. Conversely, any function in FBQP can be computed by a BFOQ program. BFOQ is a strict but expressive subset of the PFOQ programming language of [10] whose expressive power is illustrated through many



Figure 3 Compilation strategies: branch sequentialization (a) vs optimized approach (b).

⁹² examples (see Table 1);

We introduce a compilation strategy compile⁺ from PFOQ to quantum circuits based on
 two subroutines compr⁺ (Algorithm 1) and optimize⁺ (Algorithm 2): while compr⁺
 just generates the compiled circuit by a simple structural induction on program statements,
 optimize⁺ perform some optimization by merging (recursive) procedure calls in different
 branches in the program.

We show that the **compile**⁺ is sound, i.e., the generated circuit fairly simulates the input program: this correctness result lies on the orthogonality of the control structures used in the **optimize**⁺ subroutine (Lemma 11).

On PFOQ programs, we exhibit a direct improvement on size complexity of the generated circuit with respect to the compilation algorithm studied in [10] (Theorem 12).

We show that, on BFOQ programs, **compile**⁺ produces circuits whose size is asymptotically bounded by their level (Theorem 13), i.e., by the maximal number of consecutive procedure calls in all branches (including quantum ones) of a program execution, thus avoiding branch sequentialization on a sound and complete language for quantum polynomial time.

Related work. Resource optimization in quantum computing is a well-studied subject for low
level computational models such as quantum circuits or ZX-diagrams: in this *constant-depth*scenario, (i.e., taking a specific and fixed circuit of constant size and, thus, constant depth),
is it possible to reduce its number of gates [15, 14] (or at least its number of non-Clifford
gates [12, 7]), with techniques such as gate substitution, graph-rewriting, among others.

Resource optimization for high-level quantum programs is still a relatively undeveloped 112 research area as it involves the asymptotic consideration of families of circuits. Such 113 an issue has strong connections with programming language-based characterizations of 114 quantum polynomial time classes [17, 5, 10] as, by design, their set of programs is sound and 115 complete for uniform families of quantum circuits of polynomial size, as per Yao's equivalency 116 theorem. While [17, 5] provide non-constructive proofs of the existence of quantum circuits of 117 polynomial size, [10] introduces a programming language that avoids an exponential blowup 118 in the complexity of recursive (quantum) branching with a direct compilation strategy 119 for ensuring polysized circuit representations. However this strategy still performs branch 120 sequentialization and generates polynomial bounds whose degree is not accurate. 121

Figure 4 Syntax of FOQ programs.

¹²² **2** First-Order Quantum Programming Language

We consider the FOQ (First-Order Quantum) programming language with quantum control, introduced in [10] to characterize quantum polynomial time. A complete account of its syntax and its semantics is given in Appendix A.

126 2.1 Syntax

A FOQ program $P \triangleq D :: S$ is defined in Figure 4 by a list of procedure declarations D and 127 a program statement S. The language include 4 basic datatypes for expressions. Sorted 128 set expressions s are either variables \bar{q} , the empty sorted set nil, or $s \ominus [i]$, the sorted set s 129 where the i-th element has been removed. Intuitively, a sorted set is a list of unique (i.e., 130 non-duplicable) qubit pointers. Integer expressions, noted i, j, are either an integer variable x, 131 a constant n, an addition by a constant $i \pm n$ or the size of a sorted set |s|. Boolean expressions 132 b are defined in a standard way using boolean operators and arithmetic operators, e.g., 133 i > j. Finally, *qubit* expressions are of the shape s[i] which denotes the i-th qubit pointed 134 to in s. $s[i_1,\ldots,i_n]$ is a shorthand for $s[i_1],\ldots,s[i_n]$. Finally, we also allow for the syntactic 135 sugar on sorted state of pointing to the *n*-th last qubit in the set, by defining for any $n \ge 1$, 136 $\bar{\mathbf{q}}[-n] \triangleq \bar{\mathbf{q}}[|\bar{\mathbf{q}}| - n + 1].$ 137

A procedure of name proc is defined by a procedure declaration **decl** $\operatorname{proc}[x](\bar{q})\{S^{\operatorname{proc}}\}$ which takes a sorted set \bar{q} and an (optional) integer x as input parameters and executes the *procedure statement* S^{proc} . Let Procedures be an enumerable set of procedure names. We will write S instead of S^{proc} when the procedure is clear from context, and we denote by $\operatorname{proc} \in P$ the fact that proc appears in D. Given two statements S, S', S \in S' denotes the fact that S is a substatement of S'. Furthermore, we have that $\operatorname{proc} \in S$ holds if there are i and s such that **call** $\operatorname{proc}[i](s); \in S$.

Statements include the no-op instruction, unitary operations, sequences, classical and quantum conditionals, and procedures calls. Of these, we highlight the quantum conditional **qcase** $\bar{q}[i]$ of $\{0 \rightarrow S_0, 1 \rightarrow S_1\}$, which allows branching by executing statements S_0 and S_1 in superposition according to the state of qubit $\bar{q}[i]$, and also the procedure call rate call proc[i](s);, which runs procedure proc with *integer expression* i and *sorted set* expression s, a list of unique qubit pointers. The quantum conditional can be extended to *n* qubits **qcase** $\bar{q}[i_1, \ldots, i_n]$ of $\{0^n \rightarrow S_{0^n}, \ldots, 1^n \rightarrow S_{1^n}\}$ in a standard way as used in Figure 2.

In a statement $\bar{\mathbf{q}}[\mathbf{i}] *= \mathbf{U}^f(\mathbf{j});$, if the integer expression j evaluates to n, then the unitary operator $[\![\mathbf{U}^f]\!](n)$ corresponding to the unary construct $\mathbf{U}^f(\mathbf{j})$ is applied to qubit $\bar{\mathbf{q}}[\mathbf{i}]$. For expressivity purposes, these constructs are parameterized by some polynomial-time approximable total function $f \in \mathbb{Z} \to [0, 2\pi)$ and some integer expression j. For example, the gates of the quantum Fourier transform can be defined by $R_n \triangleq [\![\mathrm{Ph}^{\lambda x.\pi/2^{x-1}}]\!](n)$ with $[\![\mathrm{Ph}^f]\!](n) \triangleq (\begin{smallmatrix} 1 & 0 \\ 0 & e^{if(n)} \end{smallmatrix})$. Other basic unary gates are the *NOT* and the R_Y gate (see [10]). We also make use of some syntactic sugar to describe statements encoding constant-time

¹⁵⁹ quantum operations. For instance, the CNOT, SWAP, and Toffoli gates can be defined by:

 $\begin{array}{ccc} {}^{160}_{161} & & CNOT(\bar{q}[i], \bar{q}[j]) \ \triangleq \mathbf{qcase} \ \bar{q}[i] \ \mathbf{of} \ \left\{ 0 \rightarrow \ \mathbf{skip}; , 1 \rightarrow \bar{q}[j] \ \ast = \ NOT \right\} \end{array}$

 $_{162} \qquad \qquad SWAP(\bar{q}[i], \bar{q}[j]) \triangleq CNOT(\bar{q}[i], \bar{q}[j]) CNOT(\bar{q}[j], \bar{q}[i]) CNOT(\bar{q}[i], \bar{q}[j])$

 $\operatorname{TOF}(\bar{q}[i], \bar{q}[j], \bar{q}[k]) \triangleq \operatorname{\mathbf{qcase}} \bar{q}[i] \text{ of } \{0 \to \operatorname{\mathbf{skip}}; , 1 \to \operatorname{CNOT}(\bar{q}[i], \bar{q}[j])\}$

We define notions of rank that provide quantitative information on the recursion level of a given program or procedure.

Definition 1 (Rank). Given a FOQ program P, the rank of a procedure proc in P, denoted $rk_{\rm P}({\rm proc})$, is defined as follows:

$$rk_{\rm P}({\rm proc}) \triangleq \begin{cases} 0, & \text{if } \neg (\exists {\rm proc}', \ {\rm proc} \ge_{\rm P} \ {\rm proc}'), \\ \max_{\rm proc \ge_{\rm P} \ {\rm proc}'} \{rk_{\rm P}({\rm proc}')\}, & \text{if } \exists {\rm proc}', \ {\rm proc} \ge_{\rm P} \ {\rm proc}' \land \neg ({\rm proc} \sim_{\rm P} \ {\rm proc}), \\ 1 + \max_{\rm proc \ge_{\rm P} \ {\rm proc}'} \{rk_{\rm P}({\rm proc}')\}, & \text{if } \ {\rm proc} \sim_{\rm P} \ {\rm proc}, \end{cases}$$

where $\max(\emptyset) \triangleq 0$. The rank of a program is defined as the maximum rank among all procedures, i.e., for a program $P \triangleq D :: S$, we have that $rk(P) \triangleq \max_{\text{proc} \in D} rk_P(\text{proc})$.

Example 2. The program PAIRS given in Figure 2 has rank 1, since $rk(PAIRS) \triangleq \max_{\text{proc}\in PAIRS} rk_P(\text{proc}) = rk(\text{pairs}) = 1.$

174 2.2 Semantics

Let \mathcal{H}_{2^n} denote the Hilbert space of n qubits \mathbb{C}^{2^n} , $\mathcal{L}(\mathbb{N})$ denote the set of lists of natural numbers, and $\mathcal{P}(\mathbb{N})$ denote the powerset of natural numbers.

Expressions. For $\mathbb{K} \in \{\mathbb{N}, \mathbb{Z}, \mathbb{C}^{2\times 2}, \mathcal{L}(\mathbb{N})\}$, we write $(e, l) \Downarrow_{\mathbb{K}} v$ when the expression e evaluates to the value $v \in \mathbb{K}$ under the context $l \in \mathcal{L}(\mathbb{N})$. The context l is just the sorted set of qubit pointers into consideration when evaluating e. For example, we have that $(\bar{q}[2], [1, 4, 5]) \Downarrow_{\mathbb{N}}$ 4 (the second qubit is of index 4), $(\bar{q}[4], [1, 4, 5]) \Downarrow_{\mathbb{N}} 0$ (index 0 is used for error), and $(\bar{q} \in [3], [1, 4, 5]) \Downarrow_{\mathcal{L}(\mathbb{N})} [1, 4]$ (the third qubit has been removed).

Statements. Let $\operatorname{Conf}_n \triangleq (\operatorname{Statements} \cup \{\intercal, \bot\}) \times \mathcal{H}_{2^n} \times \mathcal{P}(\mathbb{N}) \times \mathcal{L}(\mathbb{N})$ be the set of configurations 182 of n qubits. In a configuration $c \triangleq (S, |\phi\rangle, S, l)$, S is the statement to be executed, $|\phi\rangle$ is the 183 quantum state, \mathcal{S} is a set of accessible (pointers to) qubits and l is the list of qubit pointers 184 under consideration. In case of error the program exits and the two special symbols \top and \perp 185 are markers for success (termination) and failure (error), respectively. The set \mathcal{S} of accessible 186 qubits is used to ensure that unitary operations on qubits can be physically implemented. For 187 example, statements S_0 and S_1 of a quantum branch **qcase** $\bar{q}[i]$ of $\{0 \rightarrow S_0, 1 \rightarrow S_1\}$ cannot 188 access $\bar{q}[i]$ to ensure that the operation can be physically implemented by a controlled-circuit. 189

The big-step semantics $\cdot \rightarrow \cdot$ is defined as a relation in $\bigcup_{n \in \mathbb{N}} \operatorname{Conf}_n \times \mathbb{N} \times \operatorname{Conf}_n$. When $c \xrightarrow{m} c'$ holds the *level* m is an integer corresponding to the maximum number of procedure calls performed over each (condition and quantum) branch during the evaluation of c. More formally, the level of a program P = D :: S on n qubits, denoted $\operatorname{level}_P(n)$, is defined by

$$\operatorname{level}_{\mathcal{P}}(n) \triangleq \max\{m \in \mathbb{N} \mid \exists |\phi\rangle, |\phi'\rangle \in \mathcal{H}_{2^{n}}, (S, |\phi\rangle, \mathcal{S}_{n}, l_{n}) \xrightarrow{m} (\mathsf{T}, |\phi'\rangle, \mathcal{S}_{n}, l_{n})\},\$$

with $\mathcal{S}_n \triangleq \{1, \ldots, n\}$ and $l_n \triangleq [1, \ldots, n]$.

Example 3. Consider the program PAIRS of Figure 2. We have that each procedure call removes two qubits until it reaches a case of input size $|\bar{q}|$ either 1 or 0 (depending on if *n* is odd or even) and for both sizes there are no more procedure calls. On an empty sorted set, the program exits after the first call. Then, $|\text{evel}_{\text{PAIRS}}(n) = \lfloor \frac{n}{2} \rfloor + 1 = O(n)$.

¹⁹⁵ 2.3 Polytime fragments of FOQ

In [10], the polynomial-time fragment of FOQ, denoted PFOQ, is defined by placing two restrictions on procedure calls: a well-foundedness criterion for termination and a restriction on the number of admissible recursive calls per (classical or quantum) branch to avoid exponentiation.

²⁰⁰ *PFOQ and Basic FOQ.* Given a program P \triangleq D :: S, the call relation →_P ⊆ Procedures × ²⁰¹ Procedures is defined for any two procedures proc₁, proc₂ ∈ S as proc₁ →_P proc₂ whenever ²⁰² proc₂ ∈ S^{proc₁}. The partial order ≥_P is then the transitive closure of →_P, and ~_P denotes the ²⁰³ equivalence relation where proc₁ ~_P proc₂ if proc₁ ≥_P proc₂ and proc₂ ≥_P proc₁ both hold. ²⁰⁴ **call** proc' ∈ S^{proc} is a *recursive* procedure call whenever proc ~_P proc'. The strict order >_P ²⁰⁵ is defined as proc₁ >_P proc₂ if proc₁ ≥_P proc₂ and proc₁ $\not/_P$ proc₂ both hold.

A program P is in WF if it satisfies the constraint that each recursive procedure call removes at least one qubit in its parameter. Programs in WF are terminating (well-founded) but still allow the programmer to write programs with exponential runtime. To avoid such programs, we use the notion of *width of a procedure* proc in a program P, noted width_P(proc), defined inductively on procedure declarations by counting the number of recursive calls in the procedure body, taking the maximum of each (classical or quantum) conditional.

▶ **Definition 4** (Width of a procedure). Given $P \in FOQ$ and $proc \in P$, the width of proc in P, noted width_P(proc), is defined as width_P(proc) $\triangleq w_P^{proc}(S^{proc})$, where $w_P^{proc}(S)$ is the width of the procedure proc in P relative to statement S, defined inductively as:

$$w_{\rm P}^{\rm proc}(\mathbf{skip};) = w_{\rm P}^{\rm proc}(\mathbf{q} *= \mathbf{U}^{f}(\mathbf{i});) \triangleq 0,$$

$$w_{\rm P}^{\rm proc}(\mathbf{S}_{1} \mathbf{S}_{2}) \triangleq w_{\rm P}^{\rm proc}(\mathbf{S}_{1}) + w_{\rm P}^{\rm proc}(\mathbf{S}_{2}),$$

$$w_{\rm P}^{\rm proc}(\mathbf{if} \mathbf{b} \mathbf{then} \mathbf{S}_{\mathbf{true}} \mathbf{else} \mathbf{S}_{\mathbf{false}}) \triangleq \max(w_{\rm P}^{\rm proc}(\mathbf{S}_{\mathbf{true}}), w_{\rm P}^{\rm proc}(\mathbf{S}_{\mathbf{false}})),$$

$$w_{\rm P}^{\rm proc}(\mathbf{qcase} \mathbf{q} \mathbf{of} \{0 \to \mathbf{S}_{0}, 1 \to \mathbf{S}_{1}\}) \triangleq \max(w_{\rm P}^{\rm proc}(\mathbf{S}_{0}), w_{\rm P}^{\rm proc}(\mathbf{S}_{1})),$$

$$w_{\rm P}^{\rm proc}(\mathbf{call} \operatorname{proc}'[\mathbf{i}](\mathbf{s});) \triangleq \begin{cases} 1 & \text{if proc } \sim_{\rm P} \operatorname{proc}', \\ 0 & \text{otherwise.} \end{cases}$$

Let $WIDTH_{\leq 1}$ be the set of programs with procedures of width at most 1. Finally, define PFOQ \triangleq FOQ \cap WF \cap WIDTH_{\leq 1}. We will show that PFOQ can be restricted to a fragment, denoted BFOQ (for Basic FOQ), that is still complete for polynomial time and where the compilation procedure conserves the intuitive complexity of the program. Let BASIC denote the set of programs where i) procedures do not use classical inputs ii) procedure call parameters are restricted to sorted set variables \bar{q} or to a fixed sorted set s (s is fixed for each BFOQ program). Then, we define BFOQ \triangleq BASIC \cap PFOQ. It trivially holds that BFOQ \subsetneq PFOQ \subsetneq FOQ.

▶ **Example 5** (Quantum Full Adder \in BFOQ). Let ADD encode the unitary transformation such that, for $a, b \in \{0, 1\}^n$ and $c_{\text{in}}, c_{\text{out}} \in \{0, 1\}$, ADD performs the following transformation, where η represents the *n* least significant bits of $(a + b + c_{\text{in}})$.

$$ADD |a_n b_n \dots a_1 b_1 0^n c_{\text{in}} \rangle \triangleq |a_n b_n \dots a_1 b_1 c_{\text{out}} \eta_1 \dots \eta_n \rangle$$

where $c_{\rm in}$ and $c_{\rm out}$ encode the *carry-in* and *carry-out* values, respectively. The operator

ADD corresponds to the circuit in Figure 6 and is described by the program FA below.

230	1	$\mathbf{decl} \; \mathtt{fullAdder}(ar{\mathrm{q}}) \{$
231	2	if $ \bar{\mathbf{q}} > 3$ then $/* \bar{\mathbf{q}}[1] = a, \bar{\mathbf{q}}[2] = b, \bar{\mathbf{q}}[-2] = 0\rangle$ and $\bar{\mathbf{q}}[-1] = c_{\text{in}} */$
232	3	$\mathrm{TOF}(ar{\mathrm{q}}[1],ar{\mathrm{q}}[2],ar{\mathrm{q}}[-2])$
233	4	$\operatorname{CNOT}(ar{\mathrm{q}}[1],ar{\mathrm{q}}[2])$
234	5	$\operatorname{TOF}(\bar{\mathbf{q}}[2], \bar{\mathbf{q}}[-1], \bar{\mathbf{q}}[-2]) /^{*} c_{\operatorname{out}} = (a \cdot b) \oplus (c_{\operatorname{in}} \cdot (a \oplus b)) * /$
235	6	$\operatorname{CNOT}(\bar{\mathbf{q}}[2], \bar{\mathbf{q}}[-1]) / * \eta = a \oplus b \oplus c_{\operatorname{in}} * /$
236	7	$\operatorname{CNOT}(ar{\mathrm{q}}[1],ar{\mathrm{q}}[2])$
237	8	$ extbf{call fullAdder}(ar{ extbf{q}} \ominus [1,2,-1]);$
238	9	else skip; $\}$,
238	10	" call fullAdder $(ar{ ext{q}});$

It holds that $FA \in FOQ \cap WF$ and that $width_{FA}(fullAdder) = 1$. Therefore, $FA \in PFOQ$. Also, FA is clearly in BFOQ as there is only one recursive call and no integer parameter.

Example 6 (Quantum Fourier Transform \in BFOQ). The quantum Fourier transform can be described by the program QFT below

245	1	$\mathbf{decl} \ \mathtt{qft}(ar{\mathrm{q}})\{$	11	$\mathbf{decl} \ \mathtt{rot}(\bar{\mathrm{q}}) \{$
246	2	$\bar{\mathbf{q}}[1] \ast = \mathbf{H};$	12	if $ \bar{\mathbf{q}} > 1$ then
247	3	call $rot(\bar{q});$	13	qcase $\bar{q}[-1]$ of {
248	4	$\mathbf{call} \ \mathtt{shift}(\bar{\mathrm{q}});$	14	$0 \rightarrow \mathbf{skip};$
249	5	call qft($\bar{q} \ominus [-1]$);},	15	$1 \to \bar{q}[1] *= Ph^{\lambda x.\pi/2^{x-1}}(\bar{q}); \}$
250			16	call $rot(\bar{q} \ominus [-1]);$
251	6	$\mathbf{decl} \ \mathtt{shift}(\bar{\mathrm{q}}) \{$	17	$else skip; \}$
252	7	if $ \bar{\mathbf{q}} > 1$ then		
253	8	$\mathrm{SWAP}(ar{\mathrm{q}}[1],ar{\mathrm{q}}[-1])$	18	$:: \operatorname{call} qft(\bar{q});$
254	9	$\operatorname{\mathbf{call}}$ shift $(\bar{\mathrm{q}}\ominus [-1]);$		
355	10	else skip; $\}$,		

The program consists of three procedures, qft, shift, and rot, and is in PFOQ since it is in WF and width_{QFT}(qft) = width_{QFT}(shift) = width_{QFT}(rot) = 1. All procedure calls are performed on the set \bar{q} or $\bar{q} \ominus [-1]$, and therefore the program is also in BASIC. This program can be compiled to the circuit Figure 5 for input size 4, implementing the quantum Fourier transform. This circuit differs from (but is equivalent to) the standard implementation of the quantum Fourier transform. This is due to some of the restrictions put in BFOQ. The standard circuit can be obtained directly through compilation of a PFOQ program.

Properties of PFOQ and BFOQ programs. PFOQ programs have a consecutive number of procedure calls in the distinct branches of their execution (i.e., level) that is bounded polynomially in the input size (number of qubits). The degree of the polynomial can be obtained from the rank, which can be inferred syntactically.

▶ Lemma 7 (Polynomial level [10]). For any PFOQ program P, $evel_P(n) = O(n^{rk(P)})$.

The set PFOQ of programs was shown to be sound and complete for the class FBQP, of function computable in quantum polynomial time [10].

▶ **Theorem 8** (PFOQ-Soundness and Completeness [10]). For every function f in FBQP, there is a PFOQ program P that computes f with probability $\frac{2}{3}$ using at most a polynomial number of extra ancilla. Conversely, given a program P in PFOQ, if P computes $f: \{0,1\}^* \rightarrow \{0,1\}^*$, with probability $p \in (\frac{1}{2}, 1]$ then $f \in FBQP$.



Figure 5 Circuit for the QFT as defined by the program in Example 6.



Figure 6 Quantum Full Adder circuit (Example 5) for input size 10.

- Being a strict subset of PFOQ, BFOQ is trivially sound. Surprisingly, it is also complete. 275
- ▶ Theorem 9 (BFOQ-Soundness and Completeness). Theorem 8 holds for BFOQ. 276

Proof. Soundness is trivial since BFOQ is contained in PFOQ, and completeness is given 277 analogously to the proof of [10, Theorem 5], by noticing that all programs constructed in the 278 proof are also contained in BFOQ. 279

3 **Circuit compilation** 280

In this section, we introduce a compilation strategy for PFOQ programs that strictly improves 281 on the compilation algorithm of [10]. We also show that, in the BFOQ fragment, circuit 282 complexity scales in such a way that the cost of branching is the maximum cost of each 283 branch, thereby avoiding branch sequentialization. 284

3.1 A new compilation algorithm 285

The compilation algorithm $compile^+$ takes as input a program P and a natural number n (the number of input qubits) and returns a circuit implementation of P for an input size of nqubits. $compile^+$ is defined by its subroutine $compr^+$ (Algorithm 1) in the following way:

$$\operatorname{compile}^+(\mathbf{P}, n) \triangleq \operatorname{compr}^+(\mathbf{P}, [1, \dots, n], \cdot, \{\}),$$

where P is the program to be compiled, $[1, \ldots, n]$ is list of qubit pointers (initially all qubits), 286 · is an empty control structure, and {} an empty dictionary. A control structure is a partial 287 function in $\mathbb{N} \to \{0,1\}$ mapping qubit pointers to their control values in a quantum case. For 288 $n \in \mathbb{N}$ and $k \in \{0, 1\}, cs[n \coloneqq k]$ is the control structure obtained from cs by setting $cs(n) \triangleq k$. 289 We denote by dom(cs) the domain of the control structure. For a given $x \in \{0,1\}^*$, we say 290 that state $|x\rangle$ satisfies cs if, $\forall n \in dom(cs), cs(n) = k$ implies that $x_n = k$. The purpose of 291 control structures in the algorithm is to preserve the information of each quantum branch 292 and to allow for merging using ancillas. 293

Algorithm 1 (**compr** $^+)$ **Input:** (D :: S, l, cs, Anc) \in Programs $\times \mathcal{L}(\mathbb{N}) \times (\mathbb{N} \to \{0, 1\}) \times \mathcal{D}$ 1: if S = skip; then $C \leftarrow 1$ 2: \triangleright Identity circuit 3: 4: else if S = s[i] *= U^f(j); and (s[i], l) $\Downarrow_{\mathbb{N}} n$ and $(U^{f}(j), l) \Downarrow_{\mathbb{C}^{2\times 2}} M$ then $C \leftarrow M(cs, [n])$ \triangleright Controlled gate 5:6: 7: else if $S = S_1 S_2$ then 8: $C \leftarrow \mathbf{compr}^+(D :: S_1, l, cs, Anc) \circ \mathbf{compr}^+(D :: S_2, l, cs, Anc)$ \triangleright Composition 9: else if S = if b then S_{true} else S_{false} and $(b, l) \downarrow_{\mathbb{B}} b$ then 10:▷ Conditional 11: $C \leftarrow \mathbf{compr}^+(\mathbf{D} :: \mathbf{S}_b, l, cs, \mathbf{Anc})$ 12:else if S = qcase s[i] of $\{0 \rightarrow S_0, 1 \rightarrow S_1\}$ and $(s[i], l) \downarrow_{\mathbb{N}} n$ then 13: \triangleright Quantum case $C \leftarrow \mathbf{compr}^+(D :: S_0, l, cs[n := 0], Anc) \circ \mathbf{compr}^+(D :: S_1, l, cs[n := 1], Anc)$ 14: 15:16: else if S = call proc[i](s); and (s, l) $\downarrow_{\mathcal{L}(\mathbb{N})}$ [] then $C \leftarrow 1$ \triangleright Nil call 17:18:19: else if S = call proc[i](s); and $(s,l) \downarrow_{\mathcal{L}(\mathbb{N})} l' \neq []$ and $(i,l) \downarrow_{\mathbb{Z}} n$ then \triangleright Procedure call 20: $a \leftarrow \mathbf{new} \ ancilla()$ Anc[proc', $n, |l'|] \leftarrow (a, l');$ 21: $C \leftarrow \mathbf{optimize}^+(\mathbf{D}, [(\cdot [a=1], \mathbf{S}^{\mathrm{proc}}\{n/\mathbf{x}\})], \mathrm{proc}, l', \mathrm{Anc})$ 22: 23: end if 24: return C

The aim of subroutine \mathbf{compr}^+ is just to generate the quantum circuit corresponding 294 to P on n qubits inductively on the statement of P. When the analyzed statement is a 295 (possibly recursive) procedure call, **compr**⁺ calls the **optimize**⁺ subroutine (Algorithm 2) to 296 perform an optimization of the generated quantum circuit. $\mathbf{optimize}^+$ has the same inputs 297 as $compr^+$ with the addition of a list of *controlled statements* l_{Cst} and the name proc of 298 the procedure under analysis. A controlled statement is defined as a pair (cs, S) where cs299 is a control structure and S is a FOQ statement. This will allow us to generate the circuit 300 implementation of S (which may contain multiple gates) while keeping track of the branch 301 on which it is implemented. 302

The compilation algorithm **compile**⁺ is based on the process of merging procedure calls by reasoning about the orthogonality relations within the circuit. It is similar to the compilation algorithm **compile** of [10] based on the subroutines **compr** and **optimize**, with the differences highlighted in the code of Algorithms 1 and 2: **optimize**⁺ strictly improves on **optimize** (Theorem 12) by extending this analysis to procedures of different ranks.

308 3.2 Soundness and optimization

The correctness of **optimize**⁺ is a consequence of an orthogonality property between elements of the circuit being compiled that remains invariant throughout the compilation. In Algorithm 2, a recursive procedure proc is compiled by generating three separate circuits $C_{\rm L}$, $C_{\rm M}$, and $C_{\rm R}$. The compilation process makes use of a list $l_{\rm Cst}$ of controlled statements which Algorithm 2 (optimize⁺) Build circuit for recursive procedure proc Inputs: $(D, l_{Cst}, proc, l, Anc) \in Decl \times \mathcal{L}(Cst) \times Procedures \times \mathcal{L}(\mathbb{N}) \times \mathcal{D}$

```
1: C_{\rm L} \leftarrow 1; C_{\rm R} \leftarrow 1; C_{\rm M} \leftarrow 1; P \leftarrow D :: skip;
  2: while l_{\text{Cst}} \neq [] do
             (cs, S) \leftarrow hd(l_{Cst}); \ l_{Cst} \leftarrow tl(l_{Cst})
  3:
  4:
             if S = S_1 S_2 then
  5:
                    Anc' \leftarrow Anc.copy() /* create copy of ancilla dictionary */
  6:
                    if w_{\mathrm{P}}^{\mathrm{proc}}(\mathrm{S}_1) = 1 then
  7:
                          l_{\text{Cst}} \leftarrow l_{\text{Cst}} @[(cs, S_1)]; C_{\text{M}} \leftarrow \text{compr}^+(\text{D} :: S_2, l, cs, \text{Anc'}) \circ C_{\text{M}}
  8:
  9:
                    else
                          l_{\text{Cst}} \leftarrow l_{\text{Cst}} @[(cs, S_2)]; C_{\text{M}} \leftarrow \text{compr}^+(\text{D} :: S_1, l, cs, \text{Anc}') \circ C_{\text{M}}
10:
                    end if
11:
             end if
12:
13:
             if S = if b then S<sub>true</sub> else S<sub>false</sub> and (b, l) \Downarrow_{\mathbb{B}} b then
14:
                    if w_{\rm P}^{\rm proc}(S_b) = 1 then
15:
                          l_{\text{Cst}} \leftarrow l_{\text{Cst}} @[(cs, S_b)]
16:
17:
                    else
                          C_{\mathrm{M}} \leftarrow \mathbf{compr}^{+}(\mathrm{D} :: \mathrm{S}_{b}, l, cs, \mathrm{Anc}) \circ C_{\mathrm{M}}
18:
                    end if
19:
20:
             end if
21:
22:
             if S = \mathbf{qcase} \ s[i] of \{0 \rightarrow S_0, 1 \rightarrow S_1\} and (s[i], l) \Downarrow_{\mathbb{N}} n then
                    if w_{\rm P}^{\rm proc}(S_0) = 1 and w_{\rm P}^{\rm proc}(S_1) = 1 then
23:
24:
                          l_{\text{Cst}} \leftarrow l_{\text{Cst}} @[(cs[n \coloneqq 0], S_0), (cs[n \coloneqq 1], S_1)]
                    else if w_{\rm P}^{\rm proc}({\rm S}_1) = 0 then
25:
                          l_{\text{Cst}} \leftarrow l_{\text{Cst}} \otimes [(cs[n \coloneqq 0], S_0)];
26:
                          C_{\mathrm{M}} \leftarrow \mathbf{compr}^{+}(\mathrm{D} :: \mathrm{S}_{1}, l, cs[n := 1], \mathrm{Anc}) \circ C_{\mathrm{M}}
27:
                    else if w_{\rm P}^{\rm proc}(S_0) = 0 then
28:
                          l_{\text{Cst}} \leftarrow l_{\text{Cst}} @[(cs[n \coloneqq 1], S_1)];
29:
                          C_{\mathrm{M}} \leftarrow \mathbf{compr}^{+}(\mathrm{D} :: \mathrm{S}_{0}, l, cs[n := 0], \mathrm{Anc}) \circ C_{\mathrm{M}}
30:
                    end if
31:
             end if
32:
33:
             if S = call proc'[i](s) and (s, l) \downarrow_{\mathcal{L}(\mathbb{N})} l' \neq [] and (i, l) \downarrow_{\mathbb{Z}} n then
34:
35:
                    if (\text{proc}', n, |l'|) \in \text{Anc then}
                          Let (a, l'') = \operatorname{Anc}[\operatorname{proc}', n, |l'|] in
36:
                          e \leftarrow \text{new ancilla()}; /* \text{ compatible procedure already exists: merging case }*/
37:
                          C_{\rm L} \leftarrow C_{\rm L} \circ NOT(cs, e) \circ NOT(\cdot [e=1], a) \circ SWAP(\cdot [e=1], l', l'');
38:
                          C_{\mathrm{R}} \leftarrow SWAP(\cdot[e=1], l'', l') \circ NOT(\cdot[e=1], a) \circ NOT(cs, e) \circ C_{\mathrm{R}}
39:
40:
                    else
                          a \leftarrow \text{new ancilla()} /* no compatible procedure: create new ancilla */
41:
42:
                          Anc[proc', n, |l'|] \leftarrow (a, l');
                          C_{\rm L} \leftarrow C_{\rm L} \circ NOT(cs, a); \ C_{\rm R} \leftarrow NOT(cs, a) \circ C_{\rm R};
43:
                          l_{\text{Cst}} \leftarrow l_{\text{Cst}} @[(\cdot[a=1], \text{S}^{\text{proc}'}\{n/\mathbf{x}\})]
44:
                    end if
45:
             end if
46:
47: end while
48: return C_{\rm L} \circ C_{\rm M} \circ C_{\rm R}
```

have not yet been compiled. Given a program P and an input procedure proc, the list $l_{\rm Cst}$ contains controlled statements (cs, S) such that $w_{\rm P}^{\rm proc}(S) = 1$, whereas $C_{\rm M}$ contains circuits for statements such that $w_{\rm P}^{\rm proc}(S) = 0$ but that are nonetheless orthogonal to those in $l_{\rm Cst}$, for which merging will be possible. Circuits $C_{\rm L}$ and $C_{\rm R}$ contain circuits for statements for which $w_{\rm P}^{\rm proc}(S) = 0$ and that are not orthogonal to the elements of $l_{\rm Cst}$. The circuit below pictures how the output circuit is generated from the circuits $C_{\rm L}$, $C_{\rm M}$, and $C_{\rm R}$ and the list $l_{\rm Cst}$.



34



The steps of **optimize**⁺ are depicted in Figure 7, where in each case we treat a controlled statement $(cs, S) \in l_{Cst}$. A gate placed inside the violet box \square denotes the new controlled statement that replaces (cs, S) in l_{Cst} . A gate placed inside a grey box \square indicates a circuit that is compiled and added to C_{M} . The notation is agnostic to the precise placement of these objects within l_{Cst} and C_{M} , making use of the orthogonality relation described in Lemma 11 which renders the choice inconsequential. Figures 7a, 7b, and 7c contain two circuits consisting of the different possible cases of compilation:

In Figure 7a, we consider a sequence S_1 S_2 . This includes the case where S_2 is recursive (left) and the one where S_1 is recursive (right). Given the WIDTH_{≥ 1} condition, there are no more cases.

In Figure 7b, the case of classical control, we have the step where S_b contains a recursive call (above) and where it does not (below).

For the case of quantum branching (Figure 7c), it is possible that only one of the two statements, say S_0 , contains a recursive call (left) and the case where both do (right).

Finally, we consider the case of a procedure call. Either there is already a compatible procedure and merging is performed (Figure 7d) or a new ancilla is used to anchor the procedure (Figure 7e).

³³⁷ We formalize orthogonality between controlled statements as follows.

³³⁸ ► **Definition 10** (Orthogonality between control structures). We say that two control structures ³³⁹ are orthogonal, also denoted $cs \perp cs'$, if $\exists i \in \mathbb{N}$ such that $i \in dom(cs) \cap dom(cs')$ and where ³⁴⁰ cs(i) + cs'(i) = 1.

Hence, two control structures are orthogonal if there is no base state that satisfies them both.
We now show that the steps of **optimize**⁺ respect an orthogonality invariant.

▶ Lemma 11 (Orthogonality invariant). At each step of the subroutine optimize⁺, the list l_{Cst} and the circuit C_M satisfy the following properties:

 $_{345}$ 1. All controlled statements in l_{Cst} are mutually orthogonal:

 $\forall (cs, S), (cs', S') \in l_{Cst} \text{ such that } (cs, S) \neq (cs', S'), \text{ we have that } cs \perp cs'.$

 $_{347}$ 2. Any controlled statement in l_{Cst} commutes with any element of C_{M} :

$$\forall (cs, S) \in l_{Cst}, \forall M(cs', [n]) \in C_M \text{ we have that } cs \perp cs'.$$

³⁴⁹ **Proof.** We start **optimize**⁺ with a single procedure statement and an empty control structure, ³⁵⁰ i.e. $C_{\rm M}$ is empty and $l_{\rm Cst} = \{(\cdot, S^{\rm proc})\}$, in which case the lemma is clearly true.

We now prove by induction that it is an invariant. Let $(cs, S) \in l_{Cst}$ be the controlled statement being treated. If $S = S_1 S_2$, let $w_P^{\text{proc}}(S_1) = 1$ and $w_P^{\text{proc}}(S_2) = 0$. Then, (cs, S)



(d) S = call proc'[i](s); (merging).

(e)

363



(e) S = call proc'[i](s); and (i, l) $\Downarrow_{\mathbb{Z}} n$ (anchoring).

cs

Figure 7 A step of the **optimize**⁺ subroutine.

is replaced with (cs, S_1) in l_{Cst} and C_M is unchanged – therefore, the invariant property 353 remains true. The case where $w_{\rm P}^{\rm proc}({\rm S}_1) = 0$ and $w_{\rm P}^{\rm proc}({\rm S}_2) = 1$ is analogous. 354

If S = if b then S₀ else S₁, then consider the case (b, l) $\Downarrow_{\mathbb{B}} 0$, where if $w_{\mathbb{P}}^{\text{proc}}(S_0) = 1$ we 355 have that (cs, S) is replaced with (cs, S_0) in l_{Cst} and C_M remains the same, and therefore 356 the property remains true. If $w_{\rm P}^{\rm proc}(S_0) = 0$ we have that (cs, S) is removed from $l_{\rm Cst}$ and 357 $C_{\mathrm{M}} \leftarrow [(cs, \mathrm{S})] \circ C_{\mathrm{M}}$. By the induction hypothesis all other cs_i in l_{Cst} are orthogonal to cs358 and therefore the property is conserved. The same can be shown for the case of $(b, l) \downarrow_{\mathbb{B}} 1$. 359

If S = qcase s[i] of $\{0 \to S_0, 1 \to S_1\}$ with $(s[i], l) \downarrow_{\mathbb{N}} n$, notice first that $cs_i \perp cs_{i'}$ implies 360 both $cs_i \perp cs_{i'}[n=0]$ and $cs_i \perp cs_{i'}[n=1]$, and that clearly $cs_{i'}[n=0] \perp cs_{i'}[n=1]$. Then, 361 all cases preserve the condition. 362

If S = call proc'[i](s) with $(s, l) \downarrow_{\mathcal{L}(\mathbb{N})} l' \neq []$ and $(i, l) \downarrow_{\mathbb{Z}} n$, we consider two cases:

(i) A corresponding ancilla *a* already exists (merging), which by the constraints of PFOQ 364 implies that $\cdot [a = 1] \perp cs_i$ for all cs_i in l_{Cst} . Therefore, by the induction hypothesis, 365 adding cs to a preserves the orthogonality conditions. 366

(ii) No corresponding ancilla exists (anchoring), in which case the creation of the ancilla 367 does not change the orthogonality between statements, as intended. 368

We now show that algorithm **compile**⁺ strictly improves on the asymptotic size of circuit, 369 compared to the **compile** algorithm of [10]. 370

Theorem 12. For any PFOQ program P, #compile⁺(P, n) = O(#compile(P, n)). Furthermore, there exist programs for which #compile⁺(P, n) = o(#compile(P, n)).

³⁷³ **Proof.** The circuit size in both cases is asymptotically bounded by the number of ancillas
³⁷⁴ created. Since we do more merging than before the result follows. Table 1 provides some
³⁷⁵ examples to show the second claim.

Theorem 13 (No branch sequentialization). For $P \in BFOQ$ and $n \in \mathbb{N}$, $\#compile^+(P, n) = O(level_P(n))$.

Proof. The theorem can be shown by structural induction on the program body, by checking that it is the case in each scenario that the circuit size scales with the level of the program. All cases are straightforward except the one of the quantum control case, which is proven at the end. The BASIC restrictions give us the following two properties during the compilation: (a) merging can be done in constant time, since there is no need for controlled-swap gates, and (b) a call to a recursive function only result in at most O(n) calls to procedures of the same rank with unique ancillas.

We proceed by structural induction on the program body, considering that the statement is part of a procedure call for procedure proc.

 $(S = skip; or S = \bar{q}[i] *= U;)$ in this case we have that, $level_P(n) = 0$ and the the circuit is of constant size.

 $(S = S_1 S_2)$ In this case, S_1 and S_2 are compiled in series (Figure 7a). The size of the circuit for S is then given by the sum of the sizes of the circuits of S_1 and S_2 , and by definition the level of S is the sum of the levels.

 $(S = if b then S_0 else S_1)$ Depending on the value of b the circuit for S either it corresponds to the circuit for S₀ or S₁. Therefore the size of the circuit is bounded by the maximum of between the two statements, as in the definition of level.

(S = call proc[i](s);) This case also follows the definition of level since the circuit size is the one given inductively by the non-procedure-call operations (constant size) plus the circuit given by the procedure calls.

Notice that, for all statements besides the **qcase**, the size of the circuit follows the definition of level. We check that the number of ancillas created for S is bounded by the maximum number of ancillas for S_0 and S_1 separately. To show this, we proceed by induction on the rank r of the procedure.

The base case is given by (b), therefore we may consider r > 1. For the inductive case, we consider three possible scenarios:

 $w_{\text{proc}}^{P}(S_{0}) = w_{\text{proc}}^{P}(S_{1}) = 0$. Therefore, S_{0} and S_{1} contain only calls to procedures of rank strictly lower than r. This may only occur a constant number of times in the depth of a program, therefore we may simply consider the sum of the number of ancillas as a sufficient upper bound on the asymptotic number of ancillas for S.

 $w_{\text{proc}}^{P}(S_0) = w_{\text{proc}}^{P}(S_1) = 1$. In this case, S_0 and S_1 are of the same rank, r, and all their procedure calls may be merged. Therefore, the asymptotic number of such calls is bounded between the maximum between S_0 and S_1 (consider that, if there is no overlap between the ancillas needed, their number is still bounded linearly). Applying the IH on the procedures of rank r - 1 we obtain the desired result.

 $w_{\text{proc}}^{\text{P}}(S_0) = 0 \text{ and } w_{\text{proc}}^{\text{P}}(S_1) = 1.$ Therefore, S_0 contains calls to procedures of rank r' < rwhereas S_1 contains calls to procedures of rank r. The number of procedures of rank r'is bounded asymptotically by the maximum between those in S_0 and S_1 , therefore we obtain our result.

		Circuit complexity	
Problem	Example	[10]	$\mathbf{compile}^{\scriptscriptstyle +}$
Full Adder	Example 5	$\Theta(n)$	$\Theta(n)$
Quantum Fourier Transform	Example 6	$\Theta(n^2)$	$\Theta(n^2)$
Palindromes	Example 14	$\Theta(n)$	$\Theta(n)$
Chained Substring	Example 15	$\Theta(n^3)$	$\Theta(n)$
$\operatorname{Sum}(r), r \ge 1$	Example 18	$\Theta(n^r)$	$\Theta(n)$

Table 1 Circuit size complexity bounds given by the compilation strategy in [10] and **compile**⁺ described in this work. For all of these problems, we give the corresponding programs in BFOQ.

417 **4** Examples

In this section, we provide several examples illustrating our results, including general examples
on regular expressions. We show that any regular language can be decided by a BFOQ program
whose compiled quantum circuit of linear size (Theorem 17). A benchmark, illustrating the
difference between our compilation algorithm and the one in [10], is provided in Table 1.

▶ **Example 14** (Palindromes). Consider the following BFOQ program PALINDROME.

1 decl palindrome (\bar{q}) { if $|\bar{q}| > 2$ then 2 3 qcase $\bar{q}[1, |\bar{q}| - 1]$ of { $00 \rightarrow call palindrome(\bar{q} \ominus [1, -2]);$ 4 $01 \rightarrow \mathbf{skip};$ 5 423 $10 \rightarrow \mathbf{skip};$ 6 $11 \rightarrow call palindrome(\bar{q} \ominus [1, -2]);$ 7 } 8 else $\bar{q}[-1] \ast = NOT; \}$ 9

10 :: call palindrome (\bar{q}) ;

PALINDROME \in WF since all recursive procedure calls decrease the input sorted set. Furthermore, at most one recursive call is done per branch, and therefore PALINDROME \in WIDTH_{≤ 1} and so the program is also in PFOQ. Further checking that all procedure calls in the program are either of the form \bar{q} or $\bar{q} \in [1, |\bar{q}| - 1]$, we conclude that it is also in BFOQ. We are therefore in a position to apply Theorem 13.

Since $rk(PALINDROME) = rk_{PALINDROME}(palindrome) = 1$, by Lemma 7, we obtain the conclusion that $\#optimize^+(P, n) = O(n)$, i.e., the compilation procedure generates a circuit of size linear on the input. Indeed, for PALINDROME, **compile**⁺ generates the following circuit in the case where n is even:





⁴³⁰ The circuit makes use of n/2 ancillas that are reset to zero, only applying a *NOT* gate to ⁴³¹ $\bar{q}[n]$ if $\bar{q}[1, ..., n-1]$ forms a palindrome.

⁴³² ► Example 15 (Chained substring). Let $s_0 = 001$ and $s_1 = 11$. Let \mathcal{L} be the regular language ⁴³³ defined by identifying strings containing an instance of s_0 followed eventually by an instance ⁴³⁴ of s_1 in a word, i.e., the language defined by the regular expression $*s_0 * s_1 *$. We can define ⁴³⁵ a BFOQ program (Appendix C) that detects inputs in \mathcal{L} using the following call graph:



436

The program has as body a procedure call **call** $\mathbf{f}_0(\bar{\mathbf{q}})$; and consists of 5 procedures \mathbf{f}_i and a terminating procedure \oplus . An arrow $s \rightarrow^b t$ with $b \in \{0, 1\}$ indicates a procedure call of the form **call** $t(\bar{\mathbf{q}} \ominus [1])$; appears in the body of procedure s done in a branch with $\bar{\mathbf{q}}[1]$ in state b. The maximum rank of a procedure is 3 (for \mathbf{f}_0 and \mathbf{f}_1) and the circuit obtained by the technique in [10] gives a circuit of size $\Theta(n^3)$. On the other hand, the size of the circuit produced by **compile**⁺ grows linearly on the input size.

In the previous example, the bound obtained by **compile**⁺ was linear, which is the expected complexity in the case of detecting a regular language. It is straightforward to show that this is the case for any regular language, using the bound on the size of BFOQ circuits given in Theorem 13.

▶ Definition 16. Let $A: \{0,1\}^* \to \{0,1\}$ be a decision problem. Given a FOQ program P, we say that P decides A if, for $\bar{x} \in \{0,1\}^*$ and $y \in \{0,1\}$, we have that $[P](|\bar{x}y\rangle) = |\bar{x}(y \oplus A(\bar{x}))\rangle$.

▶ **Theorem 17** (Regular languages). For any regular language \mathcal{L} , there exists a BFOQ program P that decides if $\bar{x} \in \mathcal{L}$, for any $\bar{x} \in \{0,1\}^*$, such that #**compile**⁺(P,n) $\in O(n)$.

Proof sketch. Since \mathcal{L} is regular, there exists a deterministic finite automaton \mathcal{D} that decides it. It is relatively simple to construct from \mathcal{D} an BFOQ program that decides the language in the sense given in Definition 16. Since \mathcal{D} is deterministic, the level of the corresponding program is bounded linearly. Using Theorem 13 we obtain the desired result.

Example 18. Let SUM_r be the decision problem of checking if an input bitstring contains precisely r 1s. This corresponds to identifying bitstrings in the regular expression $(0^*1)^r 0^*$ and therefore, by Theorem 17, there exists a BFOQ program deciding SUM_r such that **compile**⁺ outputs a family of circuits of linear size.

5 Conclusions and Future Work

In this paper, we have delineated an expressive fragment, named BFOQ, of the first-order 460 quantum programming language with quantum control of [10]. We have shown that BFOQ 461 is sound and complete for polynomial time computation (Theorem 9) and that the branch 462 sequentialization problem introduced by [19] is solved for BFOQ programs: the compiled 463 circuit has size upper-bounded by the maximal complexity of program branches (Theorem 13). 464 As a consequence, the compilation procedure generates circuits with a better size complexity 465 than the compilation algorithm of [10] (Theorem 12). This result and the expressivity of 466 BFOQ are illustrated by the Examples of Table 1. A future and challenging research direction 467 includes the extension of this work to higher-order. 468

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517 **A**

Semantics of FOQ programs

In Section 2, we have defined $\mathcal{L}(\mathbb{N})$ as the set of lists of natural numbers $[n_1, \ldots, n_k]$ (the empty list being denoted by []), which are used to represent list of (unique) qubit pointers in the semantics.

⁵²¹ Basic data types τ are interpreted as follows:

522	$\llbracket Integers \rrbracket \triangleq \mathbb{Z}$	$\llbracket \text{Booleans} \rrbracket \triangleq \mathbb{B}$	$\llbracket \text{SortedSets} \rrbracket \triangleq \mathcal{L}(\mathbb{N})$
523 524	$\llbracket \text{Qubits} \rrbracket \triangleq \mathbb{N}$	$[\![Operators]\!] \triangleq \tilde{\mathbb{C}}^{2 \times 2}$	

Each basic operation op $\in \{+, -, >, \geq, =, \land, \lor, \neg\}$ of arity n, with $1 \leq n \leq 2$, has a type signature $\tau_1 \times \ldots \times \tau_n \to \tau$ fixed by the program syntax. For example, the operation + has signature Integers × Integers \to Integers. A total function $[\![op]\!] \in [\![\tau_1]\!] \times \ldots \times [\![\tau_n]\!] \to [\![\tau]\!]$ is associated to each basic operation op.

529 A function $\llbracket U^f \rrbracket \in \mathbb{Z} \to \tilde{\mathbb{C}}^{2 \times 2}$ is associated to each U^f as follows:

$$\llbracket \operatorname{NOT} \rrbracket(n) \triangleq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \llbracket \operatorname{R}^{f}_{Y} \rrbracket(n) \triangleq \begin{pmatrix} \cos(f(n)) & -\sin(f(n)) \\ \sin(f(n)) & \cos(f(n)) \end{pmatrix}, \quad \llbracket \operatorname{Ph}^{f} \rrbracket(n) \triangleq \begin{pmatrix} 1 & 0 \\ 0 & e^{if(n)} \end{pmatrix},$$

where \mathbb{C} is the set of polynomial time computable complex numbers, i.e., complex numbers whose both real and imaginary part are in \mathbb{R} . Each of the above matrices is unitary, *i.e.*, the matrix M satisfies $M^* \circ M = M \circ M^* = I$, with M^* being the conjugate transpose of M and *I* being the identity matrix.

For each basic type τ , the reduction $\bigcup_{[\tau]}$ is a map in $\tau \times \mathcal{L}(\mathbb{N}) \to [[\tau]]$. Intuitively, it maps an expression of type τ to its value in $[[\tau]]$ for a given list l of pointers in memory. These reductions are defined in Figure 8, where e and d denote either an integer expression i or a Boolean expression b.

$$\frac{(\mathbf{e},l) \Downarrow_{\llbracket\tau1} m \quad (\mathbf{d},l) \Downarrow_{\llbracket\tau2} n}{(\mathbf{e} \text{ op } \mathbf{d},l) \Downarrow_{\llbracket\sigmap}(\llbracket\tau1],\llbracket\tau2]} [\![\mathbf{op}]\!](m,n)} (\mathbf{Op}) \qquad \frac{(\mathbf{i},l) \Downarrow_{\mathbb{Z}} n}{(\mathbf{U}^{f}(\mathbf{i}),l) \Downarrow_{\mathbb{C}^{2\times2}} [\![\mathbf{U}^{f}]\!](n)} (\text{Unit})$$

$$\frac{\overline{(n,l)} \Downarrow_{\mathbb{Z}} n}{(n,l) \Downarrow_{\mathbb{Z}} n} (\mathbf{Cst}) \qquad \frac{(\mathbf{s},l) \Downarrow_{\mathcal{L}(\mathbb{N})} [x_{1},\ldots,x_{m}] \quad (\mathbf{i},l) \Downarrow_{\mathbb{Z}} k \in [1,m]}{(\mathbf{s} \in [\mathbf{i}],l) \Downarrow_{\mathcal{L}(\mathbb{N})} [x_{1},\ldots,x_{m}] \quad (\mathbf{i},l) \Downarrow_{\mathbb{Z}} k \notin [1,m]} (\mathbf{Rm}_{\epsilon})$$

$$\frac{(\mathbf{s},l) \Downarrow_{\mathcal{L}(\mathbb{N})} [x_{1},\ldots,x_{n}]}{(|\mathbf{s}|,l) \Downarrow_{\mathbb{Z}} n} (\mathbf{Size}) \qquad \frac{(\mathbf{s},l) \Downarrow_{\mathcal{L}(\mathbb{N})} [x_{1},\ldots,x_{m}] \quad (\mathbf{i},l) \Downarrow_{\mathbb{Z}} k \notin [1,m]}{(\mathbf{s} \in [\mathbf{i}],l) \Downarrow_{\mathcal{L}(\mathbb{N})} [1} (\mathbf{Rm}_{\epsilon})$$

$$\frac{\overline{(nil,l)} \Downarrow_{\mathcal{L}(\mathbb{N})} [1]}{(\mathbf{nil},l) \Downarrow_{\mathcal{L}(\mathbb{N})} [1]} (\mathbf{Nil}) \qquad \frac{(\mathbf{s},l) \Downarrow_{\mathcal{L}(\mathbb{N})} [x_{1},\ldots,x_{m}] \quad (\mathbf{i},l) \Downarrow_{\mathbb{Z}} k \notin [1,m]}{(\mathbf{s}[\mathbf{i}],l) \Downarrow_{\mathbb{N}} x_{k}} (\mathbf{Qu}_{\epsilon})$$

$$\frac{\overline{(q,l)} \Downarrow_{\mathcal{L}(\mathbb{N})} l}{(\mathbf{s}[\mathbf{i}],l) \Downarrow_{\mathbb{N}} 0} (\mathbf{Var}) \qquad \frac{(\mathbf{s},l) \Downarrow_{\mathcal{L}(\mathbb{N})} [x_{1},\ldots,x_{m}] \quad (\mathbf{i},l) \Downarrow_{\mathbb{Z}} k \notin [1,m]}{(\mathbf{s}[\mathbf{i}],l) \Downarrow_{\mathbb{N}} 0} (\mathbf{Qu}_{\epsilon})$$

Figure 8 Semantics of expressions

Recall from Section 2 that the set of *configurations* over n qubits, denoted $Conf_n$, is defined by

 $\operatorname{Conf}_n \triangleq (\operatorname{Statements} \cup \{\mathsf{T}, \bot\}) \times \mathcal{H}_{2^n} \times \mathcal{P}(\mathbb{N}) \times \mathcal{L}(\mathbb{N}),$

where $\mathcal{P}(\mathbb{N})$ being the powerset over \mathbb{N} and where \top and \bot are two special symbols for termination and error, respectively. Let \diamond stand for a symbol in $\{\top, \bot\}$.

A configuration $c = (S, |\psi\rangle, S, l) \in \text{Conf}_n$ contains a statement S to be executed (provided that $S \notin \{T, \bot\}$), a quantum state $|\psi\rangle$ of length n, a set S containing the qubit pointers that are allowed to be accessed by statement S, and a list l of qubit pointers.

The program big-step semantics $\cdot \xrightarrow{\cdot} \cdot$, described in Figure 9, is defined as a relation in $\bigcup_{n \in \mathbb{N}} \operatorname{Conf}_n \times \mathbb{N} \times \operatorname{Conf}_n$.

Figure 9 Semantics of statements

545 **B Proofs**

In this section, we provide the full proof of Theorem 17. Towards that end, we first define a
 notion of call-graph.

Definition 19 (Call graph). A call graph \mathcal{G} is a triple (proc, V, E) where

549 proc $\in V$ is the entry node;

550 \bigvee V \subseteq Procedures is a set of nodes containing a special procedure \oplus ;

 $E \subseteq V \times L \times V$ is a set of labeled directed edges, where labels correspond to combinations of quantum and classical conditionals.

Procedure \oplus only applies a NOT gate to the last qubit in the input and terminates. Labels L are defined as follows: values $\{0,1\}$ denote a quantum if statement on the first qubit, and $|\bar{\mathbf{q}}| = n \text{ or } |\bar{\mathbf{q}}| > n$ denotes a boolean condition on the size of the input.

▶ Theorem 17 (Regular languages). For any regular language \mathcal{L} , there exists a BFOQ program P that decides if $\bar{x} \in \mathcal{L}$, for any $\bar{x} \in \{0,1\}^*$, such that $\#\text{compile}^+(\mathbf{P},n) \in O(n)$.

Proof. Let \mathcal{D} be a deterministic finite automaton deciding \mathcal{L} . We will construct the PFOQ program P by using \mathcal{D} to define the call graph for P. The subtlety in the transformation is in the difference between the acceptance condition in \mathcal{D} (i.e., termination in an accept state) and the *acceptance nodes* of the call graph, referring here to the \oplus nodes. For a base state $|\bar{x}y\rangle$, the program P outputs $|\bar{x}(\neg y)\rangle$ iff it *ever* reaches a \oplus node, at which point P terminates.

The call graph is then defined as follows. The call graph contains a node for each state of \mathcal{C} , with the same transitions, except for those that constitute incoming our outgoing edges of an accept state, i.e., edges x_i, y_i, z_i in the following diagram:



567

⁵⁶⁸ These edges are encoded in the call graph as follows:



569

with an extra procedure d for each accept state and using edges with classical conditions to handle the acceptance condition of the program. P is then defined as the program given by the call graph where the procedures consist only of the procedure calls defined in the graph. For a set of conditions c_i , with i = 1...m, we denote by $\{c_i\}_{i=1...m}$ a set of m edges each labelled with a conditions c_i .

Since each procedure performs at most one procedure call per branch (recursive or otherwise) its level will be linear on the input size.

C Regular languages (Example 15)

⁵⁷⁸ The following is the program defined by the call graph given in Example 15.

```
decl f_0(\bar{q}){
                 1
579
                            qcase \bar{q}[1] of \{0 \rightarrow \text{call } f_1(\bar{q} \ominus [1]), 1 \rightarrow \text{call } f_0(\bar{q} \ominus [1])\},\
                 2
580
581
                       decl f_1(\bar{q}){
582
                 3
                           qcase \bar{q}[1] of \{0 \rightarrow \text{call } f_2(\bar{q} \ominus [1]), 1 \rightarrow \text{call } f_0(\bar{q} \ominus [1])\},\
                 4
583
584
                       decl f_2(\bar{q}){
585
                 5
                            qcase \bar{q}[1] of \{0 \rightarrow \text{call } f_2(\bar{q} \ominus [1]), 1 \rightarrow \text{call } f_3(\bar{q} \ominus [1])\},\
                 6
586
587
                       decl f_3(\bar{q}){
                 7
588
                            qcase \bar{q}[1] of \{0 \rightarrow \text{call } f_3(\bar{q} \ominus [1]), 1 \rightarrow \text{call } f_4(\bar{q} \ominus [1])\},\
589
                 8
590
                       decl f_4(\bar{q}){
                 9
591
                            qcase \bar{q}[1] of \{0 \rightarrow \text{call } f_3(\bar{q} \ominus [1]), 1 \rightarrow \text{call } \oplus (\bar{q} \ominus [1])\},\
592
593
                       decl \oplus (\bar{q}){
               11
594
                           \bar{q}[-1] *= NOT; }
595
               12
596
                        :: call f_0(\bar{q});
               13
<u>59</u>7
```

It is straightforward to verify that all conditions of BFOQ are met and that the level of the program is linearly bounded.